Passivity-based nonlinear control of CSTR via asymptotic observers ☆

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ABSTRACT

This work makes use of a passivity-based approach (PBA) and tools from Lyapunov theory to design a nonlinear controller for the asymptotic stabilization of a class of nonisothermal Continuous Stirred Tank Reactors (CSTR) around any desired stationary point. The convergence and stability proofs are derived in the port Hamiltonian framework. Asymptotic observers that do not require knowledge of reaction kinetics are also proposed for a system with incomplete state measurement. Numerical simulations are given to illustrate the application of the theoretical results to a CSTR with multiple steady states.

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1. Introduction

Lyapunov theory (Khalil, 2002), or more generally the Passivity Based Approach (PBA) (Brogliato, Lozano, Maschke, & Egeland, 2007; van der Schaft, 2000a; Willems, 1972) combined with generalized energetic arguments as expressed through a Hamiltonian function, is one of the most efficient ways to investigate stability and design controllers for nonlinear dynamical systems (Jeltsema, Ortega, & Scherpen, 2004; Ortega, van der schaft, Mareels, & Maschke, 2001; Ortega, Jeltsema, & Scherpen, 2003). The key idea of the PBA in the Port Hamiltonian framework (Ortega, van der Schaft, Maschke, & Escobar, 2002) is to define transformations (by means of control input or shaped dynamics) to obtain a certain structured representation of the original system by rendering it passive with respect to a given storage function. The PBA was first proposed and successfully applied for stability analysis and control design for the electro-mechanical systems (Maschke, Ortega, & van der Schaft, 2000; van der Schaft, 2000b). In these systems the connections between the energy and the dynamical behavior of the system are well established by the fact that the system reaches its stable state if and only if the total energy is at its minimum. As a consequence, a Lyapunov function candidate can be assigned to the total energy and passivity can then be related to energy dissipation due to friction or resistance. Unfortunately, the link

between Lyapunov stability theory and the energy of chemical reactive systems is far from being understood at present (Alvarez, Alvarez-Ramírez, Espinosa-Perez, & Schaum, 2011; Favache & Dochain, 2010). This topic has therefore been an active research area (Hangos, Bokor, & Szederkényi, 2001; Hoang, Couenne, Jallut, & Le Gorrec, 2012; Hudon & Bao, 2012; Ramírez, Sbarbaro, & Ortega, 2009).

The Continuous Stirred Tank Reactors (CSTRs) (Luyben, 1990) provide a benchmark both in chemical engineering and in dynamical systems theory due to their highly nonlinear dynamics. CSTRs may exhibit nonminimum phase behavior (Niemiec & Kravaris, 2003), instability and multiple steady states (Favache & Dochain, 2010; Viel, Jadot, & Bastin, 1997). Studies on CSTRs have investigated control synthesis for stabilization (Alvarez et al., 2011; Favache, Dochain, & Winkin, 2011; Georgakis, 1986; Hoang, Couenne, Jallut, & Le Gorrec, 2011; Hoang et al., 2012) and state observer design (Alvarez-Ramírez, 1995; Dochain, Couenne, & Jallut, 2009; Gibon-Fargeot, Hammouri, & Celle, 1994; Soroush, 1997). The combination of these is an important field of research.

The underlying motivation for nonlinear control of the CSTRs is that industrial chemical reactors may have to be operated at unstable operating conditions (Bruns & Bailey, 1975). Numerous control strategies have been developed to achieve this objective. Input/output feedback linearization (Viel et al., 1997) for control under constraints, nonlinear PI control (Alvarez-Ramírez & Morales, 2000), direct Lyapunov based control (Antonelli & Astolfi, 2003), (pseudo) Hamiltonian framework (Dörfler, Johnsen, & Allgöwer, 2009; Hangos et al., 2001; Hoang et al., 2011; Ramírez et al., 2009), power/energy-shaping control (Alvarez et al., 2011; Favache & Dochain, 2010), inventory control (Farschman, Viswanath, & Ydstie, 1998) and dissipativity based decentralized control of interconnected chemical reactors (Hudon, Höffner, & Guay, 2008; Hudon &

Bao, 2012) provide some examples. Thermodynamics/physics based control has also been proposed to the stabilization of chemical reactors in Georgakis (1986), Ydstie and Alonso (1997) and more recently in Hoang et al. (2012) using the availability function as its point of departure.

State estimation for CSTRs has attracted the attention of researchers for a long time. Papers (Dochain, 2003; Kravaris, Hahn, & Chu, 2012) and references therein provide good overviews of recent developments. Strategies have been developed for industrial applications since on-line measurements of all reactant concentrations are difficult and/or quite expensive to implement and the reactor temperature is in some cases the only measurement available online (Alvarez-Ramírez, 1995; Gibon-Fargeot et al., 1994). The missing state variables can be estimated by different tools (Alvarez-Ramírez, 1995; Dochain, Perrier, & Ydstie, 1992; Dochain et al., 2009; Gibon-Fargeot et al., 1994; Soroush, 1997). The results given in the papers referred above relate to systems where feedback is not imposed. Closed loop stability can therefore not be guaranteed in general.

In this work we focus on the combined control and state estimation problems. First, we propose a passive nonlinear controller for the stabilization of the fully actuated CSTR with chemical reactions around a steady state which may be unstable. This approach is based on the passive Hamiltonian concepts defined in Brogliato et al. (2007), van der Schaft (2000a), Maschke et al. (2000). The shaped Hamiltonian storage function is chosen by using the techniques in Viel et al. (1997), Farschman et al. (1998), Hoang et al. (2012) such that the resulting state feedback is admissible (Hoang et al., 2012). Second, we assume that only the reactor temperature and a subset of concentrations are available online. Following the same concepts used for the passivity-based control, we propose a state estimation strategy based on chemical reaction invariants via the so-called *asymptotic observers* (Dochain et al., 1992; Dochain et al., 2009). We show, analytically and/or with simulations, that exponential convergence of the estimated state variables and closed loop stability of the CSTR are guaranteed.

This paper is organized as follows. The passivity based approach is introduced and the state feedback control law is derived in Section 2. The dynamical model of the CSTR case study is presented and preliminary results are presented in Section 3. Section 4 is devoted to the design of a passive nonlinear controller within the port Hamiltonian framework. It is shown that the resulting control is asymptotically stable and admissible in terms of the amplitude and variation rate as long as the chosen closed loop Hamiltonian function is appropriate. The results generalize previous ones (Viel et al., 1997) without constraint on control input. Furthermore, they allow to rewrite the closed loop system dynamics into a port Hamiltonian representation. A state reconstruction method is then proposed via the so-called asymptotic observers (Dochain et al., 1992; Dochain et al., 2009). The theoretical developments are then illustrated by simulation studies reported in Section 5. Conclusions and future perspectives of the work are given in Section 6.

2. The Passivity Based Approach (PBA)

Let us consider nonlinear systems that are affine in the control input u and whose dynamics is given by the following set of ordinary differential equations (ODEs) (Khalil, 2002):

$$\frac{dx}{dt} = f(x) + g(x)u \tag{1}$$

where $x = x(t) \in \mathbb{R}^n$ is the state vector, the nonlinear function $f(x) \in \mathbb{R}^n$ and the input-state map $g(x) \in \mathbb{R}^{n \times m}$ are smooth and $u \in \mathbb{R}^m$ is the control input.

The purpose of the PBA is to find a static state-feedback control $u = \beta(x)$ such that the closed loop dynamics becomes a dissipative Port Controlled Hamiltonian (PCH) system (Maschke et al., 2000; Ortega et al., 2002). The dynamics can then be written:

$$\frac{dx}{dt} = Q_d(x)\frac{\partial \mathcal{H}_d(x)}{\partial x} \tag{2}$$

where the controlled Hamiltonian storage function $\mathcal{H}_d(x)$ has a strict local minimum at the desired equilibrium x_d; and $Q_d(x) = [J_d(x) - R_d(x)]$ is the difference of a skew-symmetric matrix $J_d(x)$ and a symmetric one $R_d(x)$ so that:

$$J_d(x) = \frac{Q_d(x) - Q_d(x)^T}{2}, \quad R_d(x) = -\frac{Q_d(x) + Q_d(x)^T}{2} \tag{3}$$

Furthermore, the damping matrix $R_d(x)$ in Eq. (3) fulfills:

$$R_d(x) = R_d(x)^T \geqslant 0 \tag{4}$$

The system (2) is then dissipative in the sense that the time derivative

$$\frac{d\mathcal{H}_d(x)}{dt} = -\left[\frac{\partial \mathcal{H}_d(x)}{\partial x}\right]^T R_d(x)\left[\frac{\partial \mathcal{H}_d(x)}{\partial x}\right] \tag{5}$$

is always negative and the Hamiltonian $\mathcal{H}_d(x)$ is bounded from below (Brogliato et al., 2007; van der Schaft, 2000a). Consequently, it plays role of Lyapunov function for stabilization at the desired equilibrium x_d. The following matching equation[1] that follows from Eqs. (1) and (2) has to be solved to find $u = \beta(x)$:

$$f(x) + g(x)\beta(x) = Q_d(x)\frac{\partial \mathcal{H}_d(x)}{\partial x} \tag{6}$$

We assume that there exists a full rank left annihilator of $g(x)$ denoted $g(x)^\perp$ such that $g(x)^\perp g(x) = 0$. If $J_d(x)$, $R_d(x)$ and $\mathcal{H}_d(x)$ are chosen such that:

$$g(x)^\perp f(x) = g(x)^\perp Q_d(x)\frac{\partial \mathcal{H}_d(x)}{\partial x} \tag{7}$$

then the control variable is deduced from the state feedback $\beta(x)$ given by Ortega et al. (2002):

$$\beta(x) = g(x)^T (g(x)g(x)^T)^{-1}\left(Q_d(x)\frac{\partial \mathcal{H}_d(x)}{\partial x} - f(x)\right) \tag{8}$$

Thus, a general methodology for the PBA in the port Hamiltonian framework is derived from Eqs. (3), (4), (6), (7) and (8). Three different guidelines can be considered:

(i) We first choose an appropriate Hamiltonian storage function $\mathcal{H}_d(x)$. The matrix $Q_d(x)$ fulfilling (3) and (4) has to be found by considering (7). The feedback u is then synthesized using (8) (Hoang, Couenne, Le Gorrec, Chen, & Ydstie, 2012; Ramírez et al., 2009).

(ii) We choose an appropriate matrix $Q_d(x)$ fulfilling (3) and (4). The Hamiltonian storage function $\mathcal{H}_d(x)$ remains to be found by considering (7). From this the feedback u is obtained using (8) (Hoang et al., 2011).

(iii) The matrix $Q_d(x)$ fulfilling (3) and (4) and the Hamiltonian storage function $\mathcal{H}_d(x)$ are simultaneously solved by considering (7). The feedback u is then given by (8) (Dörfler et al., 2009). This guideline becomes quite difficult to implement as degrees of freedom increase (Ortega et al., 2002).

In what follows, we shall show that the PBA is useful, not only for controller synthesis but also asymptotic observers design of a

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[1] A partial differential equation (PDE) (Ortega et al., 2002).

class of the nonisothermal CSTR with chemical reactions. The use of the PBA with the guideline (i) is applied.

3. The CSTR case study with chemical transformation

3.1. The CSTR modeling

Consider a CSTR with n_r chemical reactions[2] with n_c active components $\mathcal{C}_i$ of molar mass M_i ($i = 1, 2, \ldots, n_c$). Such a reaction network is characterized by the following reaction invariant:

$$\sum_{i=1}^{n_c} v_{ij} M_i = 0, \quad j = 1, 2, \ldots, n_r \tag{9}$$

where v_{ij} is the signed stoichiometric coefficient of species i as it enters in reaction j (Hoang et al., 2011; Srinivasan, Amrhein, & Bonvin, 1998). For modeling purposes, we make the following hypotheses:

(**H1**) The fluid mixture is isobaric, ideal and incompressible.
(**H2**) The heat flow from the jacket to the reactor is given by:

$$\dot{Q}_J = \lambda(T_J - T) \tag{10}$$

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

(**H3**) The reactor is fed by the species k ($k = 1, 2, \ldots$) at a fixed temperature T_I and dilution rate d. The specific heat capacities c_{pk} ($k = 1, 2, \ldots$) are assumed to be constant.

Remark 1. Any reversible reaction l ($l \in \{1, \ldots, n_r\}$) of the network (9) can be considered to be irreversible (Couenne, Jallut, Maschke, Breedveld, & Tayakout, 2006) when we define the reduced reaction rate:

$$r_l = (r_l)^{(f)} - (r_l)^{(r)} \tag{11}$$

where $(r_l)^{(f)}$ and $(r_l)^{(r)}$ are the forward and reserve reaction rates respectively.

Under (**H1**), the energy balance is written using the enthalpy H. Hence the material and energy balances are finally given as follows (Favache et al., 2011; Favache & Dochain, 2010; Hoang et al., 2012; Luyben, 1990):

$$\begin{cases} \frac{dN_1}{dt} = d(N_{1I} - N_1) + \sum_{j=1}^{n_r} v_{1j} r_j \\[2mm] \frac{dN_2}{dt} = d(N_{2I} - N_2) + \sum_{j=1}^{n_r} v_{2j} r_j \\[2mm] \vdots \\[2mm] \frac{dN_n}{dt} = d(N_{n_c I} - N_{n_c}) + \sum_{j=1}^{n_r} v_{nj} r_j \\[2mm] \frac{dH}{dt} = d(H_I - H) + \dot{Q}_J \end{cases} \tag{12}$$

where:

- N_i is mole number of species i ($i = 1, \ldots, n_c$);
- H and r_j represent the total enthalpy and the reaction rate of the reaction j ($j = 1, \ldots, n_r$);
- d stands for the dilution rate which is assumed to be constant. The subscript I written in Eq. (12) denotes "Inlet".

Remark 2. Species N_{ot} that are *Inert* and/or *Catalyst* can be added to the dynamics by setting:

[2] Without loss of generality, we assume that all considered reactions are irreversible.

$$\frac{d\mathbf{N}_{ot}}{dt} = d(\mathbf{N}_{otI} - \mathbf{N}_{ot}) \tag{13}$$

where $\mathbf{N}_{ot}$ is a vector containing all these species. But we can easily check that the differential Eq. (13) is stable and the state converges to $\mathbf{N}_{otI}$. We shall therefore only consider the dynamics of n_c active species (12) from the point of view of chemical reaction. However, the presence of *Inert* and/or *Catalyst* should be considered in the energy balance since the total enthalpy H in definition (14), the total heat capacity C_p in definition (17) and the total mass m_t depend not only on ($N_1, \ldots, N_{n_c}$) but also $\mathbf{N}_{ot}$.

Remark 3. The total enthalpy H of the reaction system is given by:

$$H = \sum_i h_i(T) N_i \tag{14}$$

with $h_i(T) = c_{pi}(T - T_{ref}) + h_{iref}$ where T_{ref} and h_{iref} are the reference values. By using the local equilibrium hypothesis, the energy balance $\frac{dH}{dt}$ in (12) can be rewritten in terms of temperature (Hoang et al., 2012) so that:

$$\frac{dT}{dt} = \frac{\sum_{j=1}^{r} (-\Delta H_{Rj}) r_j}{C_p} + d(T_I - T) \frac{C_{pI}}{C_p} + \frac{1}{C_p} \dot{Q}_J \tag{15}$$

where

$$\Delta H_{Rj} = \sum_{i=1}^{n_c} v_{ij} h_i(T) \tag{16}$$
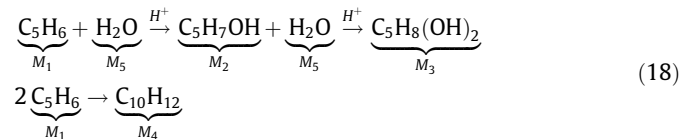
represents the enthalpy of the chemical reaction j ($j = 1, \ldots, n_r$) and,

$$C_p = \sum_i c_{pi} N_i \tag{17}$$

is the total heat capacity.

The system dynamics with state variables ($H, N_1, \ldots, N_{n_c}$) given by Eq. (12) or ($T, N_1, \ldots, N_{n_c}$) defined by Eqs. (15) and (12) are mathematically equivalent due to definition (14). The dynamical representation corresponding to the state vector ($T, N_1, \ldots, N_{n_c}$) given by ODEs (12) and (15) will be used for controller synthesis. Asymptotic observer design will be solved with the dynamics corresponding to the state vector ($H, N_1, \ldots, N_{n_c}$) in Eq. (12). The transient behavior of the differential Eq. (13) is considered for the energy balance in both cases.

Example 1. We consider the production of cyclopentenol C_5H_7OH from cyclopentadiene C_5H_6 by sulfuric acid-catalyzed addition of water in a dilute solution (Niemiec & Kravaris, 2003). The total mass of the liquid phase mixture m_t is assumed to be constant. The process is described by the Van de Vusse reaction system (van de Vusse, 1964). The stoichiometry is written as in (9) with $n_r = 3$ and $n_c = 5$:

$$\underset{M_1}{\underbrace{C_5H_6}} + \underset{M_5}{\underbrace{H_2O}} \xrightarrow{H^+} \underset{M_2}{\underbrace{C_5H_7OH}} + \underset{M_5}{\underbrace{H_2O}} \xrightarrow{H^+} \underset{M_3}{\underbrace{C_5H_8(OH)_2}}$$
$$2\underset{M_1}{\underbrace{C_5H_6}} \rightarrow \underset{M_4}{\underbrace{C_{10}H_{12}}} \tag{18}$$

The system dynamics (12) with 5 active species is given by:

$$\begin{cases} \frac{dN_1}{dt} = d(N_{1I} - N_1) - r_1 - 2r_3 \\[2mm] \frac{dN_2}{dt} = d(N_{2I} - N_2) + r_1 - r_2 \\[2mm] \frac{dN_3}{dt} = d(N_{3I} - N_3) + r_2 \\[2mm] \frac{dN_4}{dt} = d(N_{4I} - N_4) + r_3 \\[2mm] \frac{dN_5}{dt} = d(N_{5I} - N_5) - r_1 - r_2 \\[2mm] \frac{dH}{dt} = d(H_I - H) + \dot{Q}_J \end{cases} \tag{19}$$

Note that sulfuric acid is present as a catalyst. From Remark 2, we therefore have:

$$\frac{dN_{ot}}{dt} = d(N_{otl} - N_{ot}) \tag{20}$$

In differential Eqs. (19) and (20), we have $d = \frac{q_m}{m_t}$ and $N_{il} = x_{il} \frac{m_t}{M_i}$ where $\sum_i x_{il} = 1$ and q_m is the mass flow rate. Finally, the energy balance $\frac{dH}{dt}$ in Eq. (19) is written in terms of the temperature T (see Remark 3) so that:

$$\frac{dT}{dt} = \frac{\sum_{j=1}^{3}(-\Delta H_{Rj})r_j}{C_p} + d(T_I - T)\frac{C_{pl}}{C_p} + \frac{1}{C_p}\dot{Q}_J \tag{21}$$

where:

$$\begin{cases} \Delta H_{R1} = -h_1 - h_5 + h_2 > 0 \\ \Delta H_{R2} = -h_2 - h_5 + h_3 < 0 \\ \Delta H_{R3} = -2h_1 + h_4 < 0 \end{cases} \tag{22}$$

and,

$$C_p = c_{p1}N_1 + c_{p2}N_2 + c_{p3}N_3 + c_{p4}N_4 + c_{p5}N_5 + c_{pot}N_{ot} \tag{23}$$

3.2. Preliminaries

The following assumptions are now made to characterize the dynamical behavior of the system (12):

(**A1**) The reaction rates r_j ($j = 1, \ldots, n_r$) are described by the mass action laws,

$$r_j = k_j(T)F_j(N_1^{|\nu_{1j}|}, N_2^{|\nu_{2j}|}, \ldots), \quad j = 1, \ldots, n_r \tag{24}$$

where F_j ($j = 1, \ldots, n_r$) are nonlinear functions with respect to their arguments and $k_j(T)$ ($j = 1, \ldots, n_r$) are reaction rate constants fulfilling the condition that $k_j(T)$ is monotone, nonnegative and bounded in accordance to thermodynamic principles (Favache & Dochain, 2010; Hoang et al., 2012; Luyben, 1990) so that:

$$\lim_{T \to 0} k_j(T) = 0 \quad \text{and} \quad \lim_{T \to +\infty} k_j(T) = k_{j\max} \tag{25}$$

The Arrhenius law

$$k_j(T) = k_{0j} \exp\left(\frac{-k_{1j}}{T}\right) \tag{26}$$

where k_{0j} is the kinetic constant and k_{1j} is the activation temperature, is compatible with the limits in Eq. (25).

(**A2**) The temperature and mole numbers are nonnegative.

Assumption (**A2**) describes measurable physical quantities (Antonelli & Astolfi, 2003) and implies that the CSTR is a positive system. In what follows, we first present the following results which are instrumental in proving the main results of this work.

3.2.1. Boundedness of material dynamics
Lemma 1 generalizes the results of Theorem 2.1 (i) presented in Viel et al. (1997) by considering multi-component homogeneous mixtures.

Lemma 1. *The domain* $\Omega = \{N_1, \ldots, N_{n_c} | 0 \leqslant \sum_{i=1}^{n_c} M_i N_i \leqslant \sum_{i=1}^{n_c} M_i N_{il}\}$ *is positively invariant.*

Proof. Define $\eta = \sum_{i=1}^{n_c} M_i N_i$. By using the mass conservation property given by Eq. (9), we obtain from Eq. (12):

$$\frac{d\eta}{dt} = d\left(\sum_{i=1}^{n_c} M_i N_{il} - \eta\right)$$

$\eta(t) \leqslant \sum_{i=1}^{n_c} M_i N_{il}$ for all $\eta(t = 0) \leqslant \sum_{i=1}^{n_c} M_i N_{il}$ since $d > 0$. Using (**A2**), one gets $\eta(t) \geqslant 0$. The latter completes the proof. □

3.2.2. Stability of the isothermal dynamics
Let $(N_{1d}, N_{2d}, \ldots, N_{Nd}, T_d)$ be the steady state of the reaction system defined by Eqs. (12) and (15). Let us note that possible steady states are calculated by considering that all time derivatives vanish and that there may be more than one stationary solution to the problem (Favache & Dochain, 2010). An additional assumption (used in Viel et al. (1997), Alvarez-Ramírez & Morales (2000), Antonelli & Astolfi (2003) or recently Favache & Dochain, 2010) is considered:

(**A3**) For the isothermal conditions ($T = T_d$), the system dynamics (12) admits a single equilibrium point ($N_{1d}, \ldots, N_{nd}$) which is globally asymptotically stable.

From a control point of view, we can show by means of Lyapunov converse theorems (Khalil, 2002) together with the above assumption, that there exists a positive function $\mathcal{V}(N_1, \ldots, N_{n_c})$ with $\frac{d\mathcal{V}}{dt} < 0$ along the isothermal dynamics. Several industrial chemical reaction processes verify this assumption. Let us illustrate with the Van de Vusse reaction system in Example 1.

Example 2. We rewrite the isothermal dynamics derived from Eq. (19) into the explicit form using (**A1**) so that:

$$\begin{cases} \frac{dN_1}{dt} = d(N_{1I} - N_1) - k_1(T_d)N_1 - 2k_3(T_d)N_1^2 \\ \frac{dN_2}{dt} = d(N_{2I} - N_2) + k_1(T_d)N_1 - k_2(T_d)N_2 \\ \frac{dN_3}{dt} = d(N_{3I} - N_3) + k_2(T_d)N_2 \\ \frac{dN_4}{dt} = d(N_{4I} - N_4) + k_3(T_d)N_1^2 \\ \frac{dN_5}{dt} = d(N_{5I} - N_5) - k_1(T_d)N_1 - k_2(T_d)N_2 \end{cases} \tag{27}$$

The existence of the positive-definite function $\mathcal{V}(N_1, \ldots, N_{n_c})$ is derived by considering the separable dynamics of (27). Indeed the dynamics on N_1 (27) can be rewritten as follows:

$$\frac{dN_1}{dt} = -2k_3(T_d)(N_1 - N_{1d})(N_1 - \overline{N}_{1d}) \tag{28}$$

where $N_{1d} > 0$ and $\overline{N}_{1d} < 0$ are roots of the second-order polynomial equation that follow by setting $\frac{dN_1}{dt} = 0$ in Eq. (27):

$$\begin{cases} N_{1d} = \frac{(d + k_1(T_d)) - \sqrt{(d + k_1(T_d))^2 + 8dk_3(T_d)N_{1I}}}{-4k_3(T_d)} \\ \overline{N}_{1d} = \frac{(d + k_1(T_d)) + \sqrt{(d + k_1(T_d))^2 + 8dk_3(T_d)N_{1I}}}{-4k_3(T_d)} \end{cases} \tag{29}$$

Lemma 1 shows that there exits a positive constant $\varrho > 0$ so that (28) can be rewritten as follows:

$$\frac{dN_1}{dt} \leqslant -2\varrho k_3(T_d)(N_1 - N_{1d}) \tag{30}$$

It is now clear that the positive-definite function $\mathcal{V}_1(N_1) = \frac{1}{2}(N_1 - N_{1d})^2$ is a Lyapunov function candidate for the stabilization of (30) at N_{1d}. The same argument sequentially applies to N_2, N_3, N_4 and N_5. Finally, the (global) Lyapunov function of the isothermal dynamics (27) is defined so that:

$$\mathcal{V}(N_1, \ldots, N_{n_c}) = \sum_{k=1}^{5} \mathcal{V}_k(N_k) \tag{31}$$

In the following we focus our attention on nonlinear control and state estimation problems of nonisothermal CSTR (27). These two problems will be effectively solved in the framework of the passivity theory.

4. Main results

4.1. Controller design

For controller synthesis, it is convenient to let the state vector $x = (N_1, \ldots, N_{n_c}, T)$ represent the reaction system dynamics (15) and (12). The dynamics (1) is then obtained with:

$$
f(x) = \begin{pmatrix} d(N_{1I} - N_1) + \sum_{j=1}^{n_r} v_{1j} r_j \\ d(N_{2I} - N_2) + \sum_{j=1}^{n_r} v_{2j} r_j \\ \vdots \\ d(N_{n_cI} - N_{n_c}) + \sum_{j=1}^{n_r} v_{nj} r_j V \\ \dfrac{\sum_{j=1}^{n_r} (-\Delta H_{Rj}) r_j - \lambda T}{C_p} + d(T_I - T)\dfrac{C_{pl}}{C_p} \end{pmatrix}, \quad g(x) = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \dfrac{\lambda}{C_p} \end{pmatrix} \quad \text{and } u = T_J
$$

(32)

The PBA with the guideline (i) (in Section 2) will be used to design a passive nonlinear controller for the stabilization of the reaction system (1) with (32) at a given desired state x_d. The problem first consists of choosing an appropriate closed loop Hamiltonian storage function $\mathcal{H}_d(x)$. Let us note that in previous works (Alvarez-Ramírez & Morales, 2000; Viel et al., 1997), a Lyapunov function candidate based on thermal deviation $\frac{1}{2}(T - T_d)^2$ is considered for the temperature stabilization problem. Farschman and coworkers in Farschman et al. (1998) have proposed an inventory-based quadratic storage function $\frac{1}{2}(x - x_d)^2$ for control of chemical process systems. In Hoang et al. (2011), Hoang et al. (2012), the thermodynamic availability and its individual contributions have been used as the desired closed loop storage functions. We now show that the matrix $Q_d(x)$ can be found using the PBA with the Hamiltonian function:

$$
\mathcal{H}_d(x) = \mathcal{H}_d(T, N_1, \ldots, N_{n_c})
$$

$$
= \frac{(T - T_d)^2}{2}\left(1 + \sum_{i=1}^{n_c} K_i (N_i - N_{id})^2\right)
$$

(33)

where $K_i \geqslant 0$. One consequence of definition (33) is that sufficient damping is introduced to allow the stabilization problem to be accomplished with a smooth control law in terms of the amplitude and variation rate. The proposed controller therefore generalizes the one obtained from Viel et al. (1997) which uses input constraints and nonsmooth controls. It also allows us to rewrite the closed loop dynamics (1) with (32) in a port Hamiltonian representation as seen in Proposition 1 below.

Proposition 1. *The reaction system described by* Eqs. (1) and (32) *is exponentially stabilized at the desired state* $x_d = (N_{1d}, \ldots, N_{nd}, T_d)$ *with the following state feedback control law:*

$$
T_J = T + \frac{1}{\lambda}\left\{ C_p \left[-\left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1} \sum_{i=1}^{n_c} \frac{\partial \mathcal{H}_d}{\partial N_i} \frac{dN_i}{dt} - K_T \frac{\partial \mathcal{H}_d}{\partial T}\right] \right.
$$
$$
\left. - \left(\sum_{j=1}^{n_r} (-\Delta H_{Rj}) r_j + d(T_I - T) C_{pl}\right) \right\}
$$

(34)

where $K_T > 0$ *is a tuning parameter. Furthermore, the closed loop dynamics are represented in the passive Hamiltonian format so that:*

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

(35)

where:

$$
J_d(x) = \begin{pmatrix} 0 & \cdots & 0 & \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{dN_1}{dt} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{dN_{n_c}}{dt} \\ -\left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{dN_1}{dt} & \cdots & -\left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{dN_{n_c}}{dt} & 0 \end{pmatrix}
$$

(36)

$$
R_d(x) = \begin{pmatrix} 0 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & K_T \end{pmatrix}
$$

(37)

and $\mathcal{H}_d(x)$ *is given by* (33).

Proof. By using the PBA as described in Section 2, we have $Q_d(x) = (q_{ij}(x))_{i,j=1\ldots(n_c+1)}$ and $g^\perp(x) = \text{diag}(1, \ldots, 1, 0) \in \mathbb{R}^{(n_c+1)\times(n_c+1)}$. The matching equations from (7) give the following partial differential equations:

$$
\begin{cases} q_{11}(x)\frac{\partial \mathcal{H}_d}{\partial N_1} + \cdots + q_{1n_c}(x)\frac{\partial \mathcal{H}_d}{\partial N_{n_c}} + q_{1(n_c+1)}(x)\frac{\partial \mathcal{H}_d}{\partial T} = \frac{dN_1}{dt} \\ \qquad\qquad\vdots \\ q_{n_c1}(x)\frac{\partial \mathcal{H}_d}{\partial N_1} + \cdots + q_{nn}(x)\frac{\partial \mathcal{H}_d}{\partial N_{n_c}} + q_{n_c(n_c+1)}(x)\frac{\partial \mathcal{H}_d}{\partial T} = \frac{dN_{n_c}}{dt} \end{cases}
$$

The number of equations equals n_c with $n_c \times (n_c + 1)$ unknown variables $q_{ij}(x)$. Hence this system has an infinite number of solutions. A simple solution is found using the negative definiteness of the matrix $Q_d(x)$ as follows:

(a) set $q_{ij}(x) = q_{ji}(x) = 0$ for $i, j = 1 \ldots n_c$;
(b) then set $q_{i(n_c+1)}(x) = -q_{(n_c+1)i}(x) = \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{dN_i}{dt}$ for $i = 1 \ldots n_c$;
(c) and finally choose $q_{(n_c+1)(n_c+1)}(x) = -K_T$.

It follows that $q_{i(n_c+1)}(x), i = 1 \ldots n_c$ is well defined in the limit $\frac{\partial \mathcal{H}_d}{\partial T} \to 0$ (refer to Eq. (41) below). The structure matrices $J_d(x)$ (36) and $R_d(x)$ (37) are computed by using (3). Finally, the feedback law is derived from (8) with $J_d(x)$ defined in Eq. (36), $R_d(x)$ defined in Eq. (37) and $\mathcal{H}_d(x)$ given in Eq. (33):

$$
C_p\left[-\left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{\partial \mathcal{H}_d}{\partial N_1}\frac{dN_1}{dt} - \cdots - \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1}\frac{\partial \mathcal{H}_d}{\partial N_{n_c}}\frac{dN_{n_c}}{dt} - K_T\frac{\partial \mathcal{H}_d}{\partial T}\right]
$$
$$
- \left(\sum_{j=1}^{n_r}(-\Delta H_{Rj}) r_j + d(T_I - T) C_{pl}\right) = \dot{Q}_J
$$

Using (**H2**) with $u = T_J$ leads to the feedback law (34). Let us note that the feedback law (34) is well-defined when $\mathcal{H}_d(x)$ is defined by Eq. (33). The function $\mathcal{H}_d(x)$ is positive definite and its time derivative satisfies

$$
\frac{d\mathcal{H}_d(x)}{dt} = -K_T\left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^2 < 0, \forall T \neq T_d
$$

(38)

It immediately follows by considering the partial derivative of the desired storage function $\mathcal{H}_d$ with respect to T from (33) and the boundedness of the concentrations with the help of Lemma 1, that there exists $\varsigma > 0$ so that:

$$
\frac{d\mathcal{H}_d(x)}{dt} \leqslant -\varsigma \mathcal{H}_d(x)
$$

(39)

The stability proof immediately follows invoking La Salle's invariance principle (Khalil, 2002) and (**A3**). We now develop some important limiting properties of the closed loop system to show that the control law proposed in Eq. (34) is well-defined. First, it follows from the development above that the closed loop dynamics of the temperature T with the feedback law given in Eq. (34) can be rewritten as follows:

$$\frac{dT}{dt} = -\left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1} \frac{dN_1}{dt} \frac{\partial \mathcal{H}_d}{\partial N_1} - \cdots - \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1} \frac{dN_{n_c}}{dt} \frac{\partial \mathcal{H}_d}{\partial N_{n_c}}$$
$$- K_T \frac{\partial \mathcal{H}_d}{\partial T} \tag{40}$$

Second, we note that it follows from the definition of $\mathcal{H}_d(x)$ in Eq. (33) that:

$$\frac{\partial \mathcal{H}_d}{\partial T} \to 0 \Longleftrightarrow T \to T_d$$

and,

$$\lim_{T \to T_d} \frac{\partial \mathcal{H}_d}{\partial N_i} \to 0, \quad i = 1, \dots, n_c$$

From (33) we also have:

$$\mathcal{H}_d(T = T_d, N_1, \dots, N_{n_c}) = 0$$

and

$$\frac{d\mathcal{H}_d}{dt}\Big|_{(T=T_d, N_1, \dots, N_{n_c})} = 0$$

We have shown that $\mathcal{H}_d(x)$ is a Lyapunov function with (38) for the stabilization of the reactor temperature T. As a consequence, we obtain $\lim_{T \to T_d} \frac{dT}{dt} = \lim_{\frac{\partial \mathcal{H}_d}{\partial T} \to 0} \frac{dT}{dt} = 0$ and thus we deduce from (40):

$$\begin{cases} \lim_{\frac{\partial \mathcal{H}_d}{\partial T} \to 0} \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1} \frac{dN_1}{dt} < \infty \\ \vdots \\ \lim_{\frac{\partial \mathcal{H}_d}{\partial T} \to 0} \left(\frac{\partial \mathcal{H}_d}{\partial T}\right)^{-1} \frac{dN_{n_c}}{dt} < \infty \end{cases} \tag{41}$$

The latter completes the proof. □

Remark 4. The feedback law (34) becomes similar to the one proposed by Viel and coworkers (Viel et al., 1997) when the constraints are ignored and $K_1 = \dots = K_{n_c} = 0$ in $\mathcal{H}_d(x)$ as defined by Eq. (33). In this case, the stabilization is dominated by the regulation of the thermal part in accordance with the Assumption (**A3**). In the general case ($\prod_{i=1}^{n_c} K_i \neq 0$), we may use the gains to shape the amplitude and variation rate of the control input through the presence of the material balances given by equations (33) and (34).

4.2. Asymptotic observers

We now consider a situation where only the reactor temperature T and a subset of the concentrations are measured. In this case we have to design an observer to reconstruct other missing variables within the mixture. We also need to find a method to determine how many and which concentrations need to be measured. The main feature of the proposed observer is that it is independent of the system kinetics and is called *asymptotic observers*. These *asymptotic observers* were first proposed in Dochain et al. (1992) for simplified CSTR models and developed further in Dochain et al. (2009) for more general CSTR models. However, feedback law was not considered in these contributions and there is a question whether the use of the estimated states in feedback gives stable control. In what follows we show, analytically and/or simulations, that the estimated state variables exponentially converge to their exact values with and without feedback. Let us reconsider the original system (12) and rewrite it into the following form:

$$(\Sigma) \begin{cases} \frac{dH}{dt} = d(H_I - H) + \dot{Q}_J \\ \frac{d\mathbf{N}}{dt} = d(\mathbf{N}_I - \mathbf{N}) + \mathbf{v}\mathbf{r} \end{cases} \tag{42}$$

where $\mathbf{N} = (N_1, \dots, N_{n_c})^T$ is the vector of mole numbers. $\mathbf{v} = (v_{ij})_{i=1\dots n_c, j=1\dots n_r}$ is the matrix of stoichiometric coefficients and $\mathbf{r} = (r_1, \dots, r_{n_r})^T$ is the vector composed of chemical reaction rates. The following additional assumption is made (Dochain et al., 1992; Dochain et al., 2009):

(**A4**) The reaction network (9) with $n_r < n_c$ is independent so that,

$$\text{rank}(\mathbf{v}) = n_r$$

And $(n_r - 1)$ concentrations and the reactor temperature T are assumed to be available for the online measurement.[3]

We have the following lemma.

Lemma 2. *There exists an $n_c \times n_c$ matrix Θ so that:*

$$\Theta = \begin{pmatrix} \mathbf{v}_{n_r \times n_c} \\ \mathbf{v}^{\perp}_{(n_c - n_r) \times n_c} \end{pmatrix}_{n_c \times n_c} \tag{43}$$

where the following equalities hold:

$$\mathbf{v}\mathbf{v} = \mathbb{I}_{n_r \times n_r} \tag{44}$$

and

$$\mathbf{v}^{\perp}\mathbf{v} = \mathbf{0}_{(n_c - n_r) \times n_r} \tag{45}$$

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.

Proof. The proof immediately follows using Assumption **A4**. Indeed it can be shown that the matrix Θ is directly derived by Gauss elimination. □

Example 3. Let us consider the Van de Vusse reaction system given in Example 1. Its dynamics (19) can be re-expressed as (42), where:

$$\mathbf{v} = \begin{pmatrix} -1 & 0 & -2 \\ 1 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & -1 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{r} = (r_1, r_2, r_3)^T$$

After some manipulation we have:

$$\Theta = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ 0 & 1 & 2 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{3 \times 5} \\ \mathbf{v}^{\perp}_{2 \times 5} \end{pmatrix}_{5 \times 5}$$

and Θ verifies Eqs. (44) and (45).

As a consequence of Lemma 2, we state Proposition 2.

Proposition 2. *The map from $\mathbb{R}^{n_c}$ to $\mathbb{R}^{n_c - n_r}$, $Z = \mathbf{v}^{\perp}N$, reduces the dynamics for N defined by Eq. (42) to:*

$$\frac{d\mathbf{Z}}{dt} = d(\mathbf{Z}_I - \mathbf{Z}) \tag{46}$$

where $Z_I = \mathbf{v}^{\perp}N_I$ and $\mathbf{v}^{\perp}$ are given in Eq. (43). Furthermore, the reduced dynamics are independent of the chemical reaction kinetics.

Proof. The proof immediately follows by multiplying Eq. (42) with $\mathbf{v}^{\perp}$ defined by Eq. (43) (see also Dochain et al., 1992; Dochain et al., 2009). □

---

[3] That means that n_r values are assumed to be measured.

In the remaining of the paper, we let $\mathbb{N} = \{1, \ldots, n_c\}$ be the set of indices for chemical species of the mixture described by the invariant (9) and the differential equations (42). It is worth noting that there exists a disjoint partitioning $\mathcal{I}, \mathcal{J} \subset \mathbb{N}$ with $(n_r - 1)$ and $(n_c - n_r + 1)$ elements respectively so that:

$$\begin{cases} \mathcal{I} \cap \mathcal{J} = \emptyset \\ \mathcal{I} \cup \mathcal{J} = \mathbb{N} \end{cases} \tag{47}$$

where $\mathcal{I}$ and $\mathcal{J}$ refer to the subsets of $(n_r - 1)$ measured mole numbers[4] and $(n_c - n_r + 1)$ remaining mole numbers to be estimated respectively. As a consequence, we can write from definition (14) and Proposition 2:

$$\begin{cases} H = \boldsymbol{h}_{\mathcal{I}}^T \boldsymbol{N}_{\mathcal{I}} + \boldsymbol{h}_{\mathcal{J}}^T \boldsymbol{N}_{\mathcal{J}} + \boldsymbol{h}_{ot}^T \boldsymbol{N}_{ot} \\ \boldsymbol{Z} = (\boldsymbol{v}^\perp)_{\mathcal{I}} \boldsymbol{N}_{\mathcal{I}} + (\boldsymbol{v}^\perp)_{\mathcal{J}} \boldsymbol{N}_{\mathcal{J}} \end{cases} \tag{48}$$

where $(\boldsymbol{v}^\perp)_{\mathcal{I}}$ and $(\boldsymbol{v}^\perp)_{\mathcal{J}}$ are submatrices of the matrix $\boldsymbol{v}^\perp$ formed by selecting columns corresponding to the marked mole numbers. The convergence of the estimates $\widehat{N}_j, \forall j \in \mathcal{J}$ to their exact values is shown in Proposition 3.

Proposition 3. *If the square matrix defined by*

$$\mathcal{O} = \begin{pmatrix} \boldsymbol{h}_{\mathcal{J}}^T \\ (\boldsymbol{v}^\perp)_{\mathcal{J}} \end{pmatrix}_{(n_c - n_r + 1) \times (n_c - n_r + 1)} \tag{49}$$

fulfills the following condition,

$$\text{rank}(\mathcal{O}) = n_c - n_r + 1 \tag{50}$$

then the states of the system (Σ) defined by Eq. (42) *are asymptotically reconstructed with the asymptotic observer* ($\widehat{\Sigma}$):

$$(\widehat{\Sigma}) \begin{cases} \frac{d\widehat{H}}{dt} = d(H_I - \widehat{H}) + \dot{Q}_J \\ \frac{d\widehat{\boldsymbol{Z}}}{dt} = d(\boldsymbol{Z}_I - \widehat{\boldsymbol{Z}}) \end{cases} \tag{51}$$

The convergence rate of each $\widehat{N}_j, \forall j \in \mathcal{J}$ defined from ($\widehat{\Sigma}$) to the exact value is exponential with the time constant $\tau = \frac{1}{2d}$. Furthermore, the results above hold whether the system is operated in open or closed loop.

Proof. Let us define $\boldsymbol{\epsilon}(t) = \begin{pmatrix} \epsilon_{\widetilde{H}} \\ \epsilon_{\widetilde{Z}} \end{pmatrix} = \begin{pmatrix} \widehat{H} - H \\ \widehat{\boldsymbol{Z}} - \boldsymbol{Z} \end{pmatrix} \in \mathbb{R}^{(n_c - n_r + 1)}$. By subtracting (51) and (42), we get:

$$\frac{d\boldsymbol{\epsilon}}{dt} = -d\mathbb{I}_{(n_c - n_r + 1) \times (n_c - n_r + 1)} \begin{pmatrix} \epsilon_{\widetilde{H}} \\ \epsilon_{\widetilde{Z}} \end{pmatrix} \tag{52}$$

with $d > 0$. The dynamics of $\boldsymbol{\epsilon}$ is then presented in the port Hamiltonian format (2) where $J(\boldsymbol{\epsilon}) = 0$, $R(\boldsymbol{\epsilon}) = d\mathbb{I}_{(n_c - n_r + 1) \times (n_c - n_r + 1)}$ and the Hamiltonian storage function $\mathcal{H}(\boldsymbol{\epsilon}) = \frac{1}{2}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} \geqslant 0$. $\mathcal{H}(\boldsymbol{\epsilon})$ plays a role of a Lyapunov function for the stability of the zero dynamics of $\boldsymbol{\epsilon}$ because:

$$\frac{d\mathcal{H}(\boldsymbol{\epsilon})}{dt} = -\left(\frac{\partial \mathcal{H}(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}}\right)^T R(\boldsymbol{\epsilon}) \left(\frac{\partial \mathcal{H}(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}}\right) < 0$$

Furthermore, it can be rewritten as follows:

$$\frac{d\mathcal{H}(\boldsymbol{\epsilon})}{dt} = -d\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} = -2d\mathcal{H}(\boldsymbol{\epsilon}) \Rightarrow \mathcal{H}(\boldsymbol{\epsilon}(t)) = \mathcal{H}(\boldsymbol{\epsilon}(t=0))\exp^{-\frac{t}{2d}}$$

$\mathcal{H}(\boldsymbol{\epsilon}(t))$ exponentially converges to *0* with the time constant $\tau = \frac{1}{2d}$ since $d > 0$. As a consequence, we have $\boldsymbol{\epsilon}(t) \to 0$, e.g. $\widehat{H} \to H$ and $\widehat{\boldsymbol{Z}} \to \boldsymbol{Z}$. Using Eq. (48) together with Eq. (13), we obtain:

$$\mathcal{O}(\widehat{\boldsymbol{N}}_{\mathcal{J}} - \boldsymbol{N}_{\mathcal{J}}) = 0$$

[4] It does not include the temperature.

where the matrix $\mathcal{O}$ is defined by Eq. (49). With condition (50), we conclude:

$$\widehat{\boldsymbol{N}}_{\mathcal{J}} = \boldsymbol{N}_{\mathcal{J}}$$

The estimated values $\widehat{\boldsymbol{N}}_{\mathcal{J}}$ are then calculated from the asymptotic observer ($\widehat{\Sigma}$) defined in Eq. (51) using Eqs. (48) and (13):

$$\widehat{\boldsymbol{N}}_{\mathcal{J}} = \mathcal{O}^{-1} \begin{pmatrix} \widehat{H} - \boldsymbol{h}_{\mathcal{I}}^T \boldsymbol{N}_{\mathcal{I}} - \boldsymbol{h}_{ot}^T \widehat{\boldsymbol{N}}_{ot} \\ \widehat{\boldsymbol{Z}} - (\boldsymbol{v}^\perp)_{\mathcal{I}} \boldsymbol{N}_{\mathcal{I}} \end{pmatrix} \tag{53}$$

It is important to notice that the convergence does not depend on the feedback strategy. The latter completes the proof. $\square$

Remark 5. The estimates $\widehat{\boldsymbol{N}}_{ot}$ of the states N_{ot} used in Eq. (53) are derived by using the differential Eq. (13) so that:

$$\frac{d\widehat{\boldsymbol{N}}_{ot}}{dt} = d(\boldsymbol{N}_{otI} - \widehat{\boldsymbol{N}}_{ot}) \tag{54}$$

We note that the observability matrix (49) and the full rank condition (50) can be regarded as feasibility conditions for the asymptotic observer (Moreno & Dochain, 2007). The condition (50) is fulfilled only if the reactions are independent (Dochain et al., 1992; Dochain et al., 2009), and more precisely if the states to be estimated in $\mathcal{J}$ have intrinsically been involved in the same reactions. Hence the proposed result generalizes and completes the analysis given in Dochain et al. (1992), Dochain et al. (2009). Let us illustrate this statement via the following example.

Example 4. Example 3 showed that $\mathbb{N} = \{1, 2, 3, 4, 5\}$ and

$$\boldsymbol{v}^\perp = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ 0 & 1 & 2 & 0 & 1 \end{pmatrix}$$

If we choose $\mathcal{I} = \{1, 3\}$ and $\mathcal{J} = \{2, 4, 5\}$ then we get $\mathcal{O} = \begin{pmatrix} h_2 & h_4 & h_5 \\ \frac{1}{2} & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$. We can easily check that $\mathcal{O}$ is not full rank because it is not necessarily true that $\det(\mathcal{O}) = h_2 - \frac{1}{2}h_4 + \frac{1}{2}h_5 \neq 0$ for nonisothermal reactors. Otherwise, if we choose $\mathcal{I} = \{3, 4\}, \mathcal{J} = \{1, 2, 5\}$ then we get $\mathcal{O} = \begin{pmatrix} h_1 & h_2 & h_5 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 1 & 1 \end{pmatrix}$. The latter is full rank because the species N_1, N_2 and N_5 are effectively involved in the first chemical reaction of the network (18) and thus $\det(\mathcal{O}) = \frac{1}{2}(h_1 - h_2 + h_5) = -\frac{1}{2}\Delta H_{R1} < 0$ as seen from Eq. (22).

5. Illustrative example

Let us consider a CSTR with one exothermic reaction involving 2 active chemical species A and B (e.g. $n_c = 2$ and $n_r = 1$) with the stoichiometry:

Table 1
Parameters of CSTR.

Numerical value		
c_{pA}	221.9 (J K^{-1} mol^{-1})	Heat capacity of species A
c_{pB}	128.464 (J K^{-1} mol^{-1})	Heat capacity of species B
c_{pInert}	21.694 (J K^{-1} mol^{-1})	Heat capacity of Inert
E_a	73.35 (K J mol^{-1})	Activation energy
h_{Aref}	-5.8085×10^5 (J mol^{-1})	Reference enthalpy of A
h_{Bref}	-6.6884×10^5 (J mol^{-1})	Reference enthalpy of B
$h_{Inertref}$	-3.3×10^5 (J mol^{-1})	Reference enthalpy of Inert
k_0	2.58×10^9 (s^{-1})	Kinetic constant
R	8.314 (J K^{-1} mol^{-1})	Gas constant
T_{ref}	298 (K)	Reference temperature
λ	0.75 (W K^{-1})	Heat transfer coefficient
d	0.0070 (s^{-1})	Dilution rate

$$v_A M_A \rightarrow v_B M_B \tag{55}$$

The reactor is fed by species A, B and an inert with a fixed inlet temperature T_I. The balance equations are (see also (12)):

$$\begin{cases} \frac{dN_A}{dt} = d(N_{AI} - N_A) + v_A r \\ \frac{dN_B}{dt} = d(N_{BI} - N_B) + v_B r \\ \frac{dH}{dt} = d(H_I - H) + \dot{Q}_J \end{cases} \tag{56}$$

As previously mentioned, the energy balance in Eq. (56) can be rewritten in terms of temperature as follows:

$$C_p \frac{dT}{dt} = (-\Delta H_R) r + d(T_I - T) C_{pI} + \dot{Q}_J \tag{57}$$

where $\Delta H_R = (v_B h_B(T) + v_A h_A(T)) < 0$ is the heat of reaction and $C_p = c_{pA} N_A + c_{pB} N_B + c_{pInert} N_{Inert}$ is the total heat capacity. Finally the dynamics of inert is given by:

$$\frac{dN_{Inert}}{dt} = d(N_{InertI} - N_{Inert}) \equiv 0 \tag{58}$$

The numerical values are given in Table 1 (Hoang et al., 2012).

The exothermic reaction (55) is considered with $v_A = -1$ and $v_B = 1$. The open and closed loop simulations are carried out with respect to two different initial conditions, (C1) with ($T_0 = 340$ (K), $N_{A0} = 0.04$ (mol), $N_{B0} = 0.001$ (mol)) and (C2) with ($T_0 = 300$ (K), $N_{A0} = 0.15$ (mol), $N_{B0} = 0.03$ (mol)).
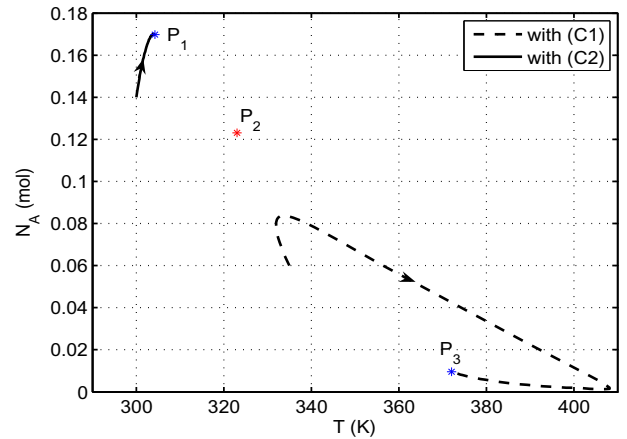

Fig. 1. The representation of the open loop phase plane.

5.1. Open loop simulation

Fig. 1 shows that the system (56) has three steady states indicated with P_1, P_2 and P_3 under the input:

$$\begin{cases} T_I = T_J = 298(K), N_{AI} = 0.18 \text{ (mol)}, \\ N_{BI} = 0(\text{mol}), N_{InertI} = 3.57 \text{ (mol)} \end{cases} \tag{59}$$

The intermediate steady state P_2 is unstable whereas P_1 and P_3 are (locally) stable. In the next subsection, we operate the reaction system at the unstable state P_2 using the feedback law defined by Eq. (34) for the jacket temperature T_J.
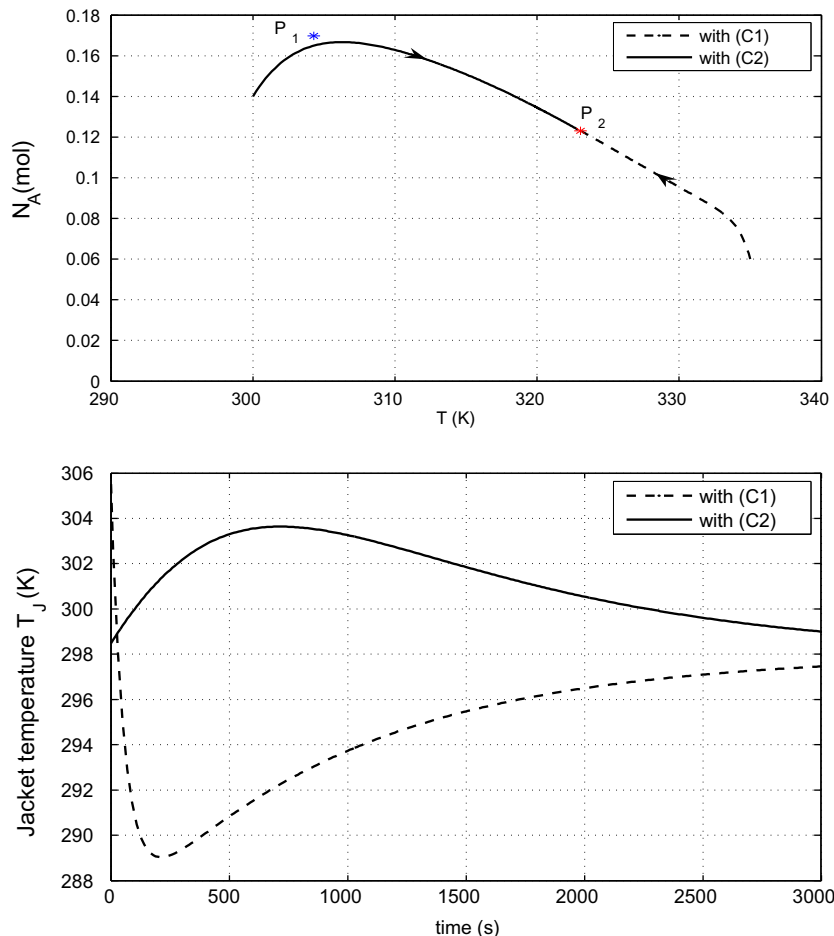

Fig. 2. Representation of the closed loop phase plane (the point P_3 outside the frame) and the feedback law T_J for two different initial conditions (C1) and (C2).
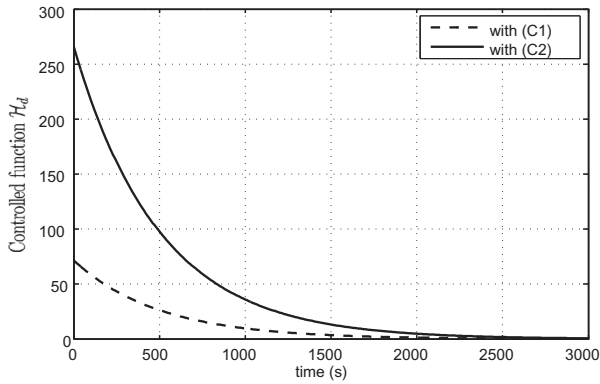
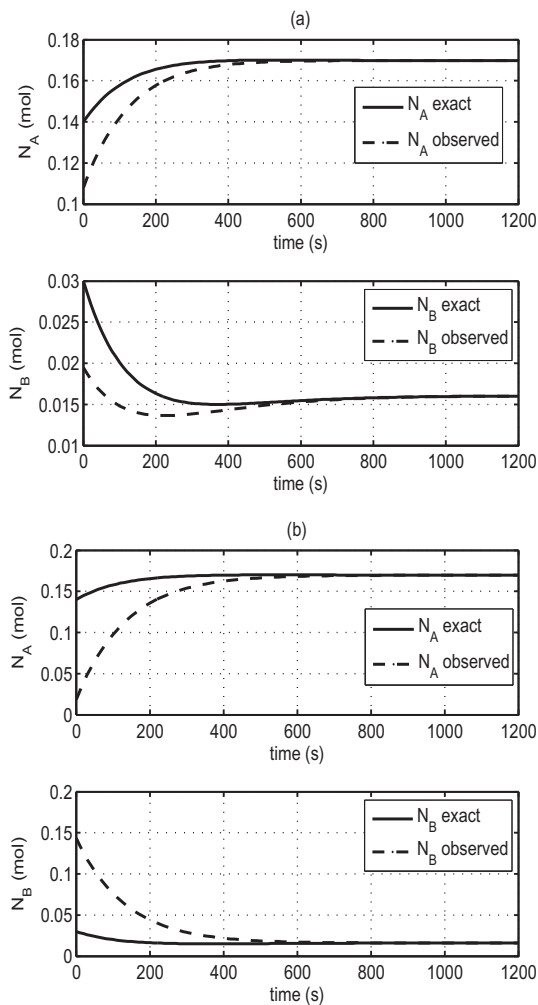**Fig. 3.** The dynamics of $\mathcal{H}_d$.

Fig. 4. N_A, N_B and their estimates in the open loop case – (a) for the initial conditions (C2) and $(\widehat{C}1)$ – (b) for initial conditions (C2) and $(\widehat{C}2)$.

5.2. Closed loop simulation

In the first case we assume that all state variables are measured. In this case we can use the state feedback law (34). We choose $K_T = 0.001$, $K_A = 0$ and $K_B = 0$ in the Hamiltonian function $\mathcal{H}_d(x)$ defined in Eq. (33). Fig. 2 shows the closed loop response with phase plane. We see, for both of the considered initial conditions, that the system converges to the desired operating point P_2.
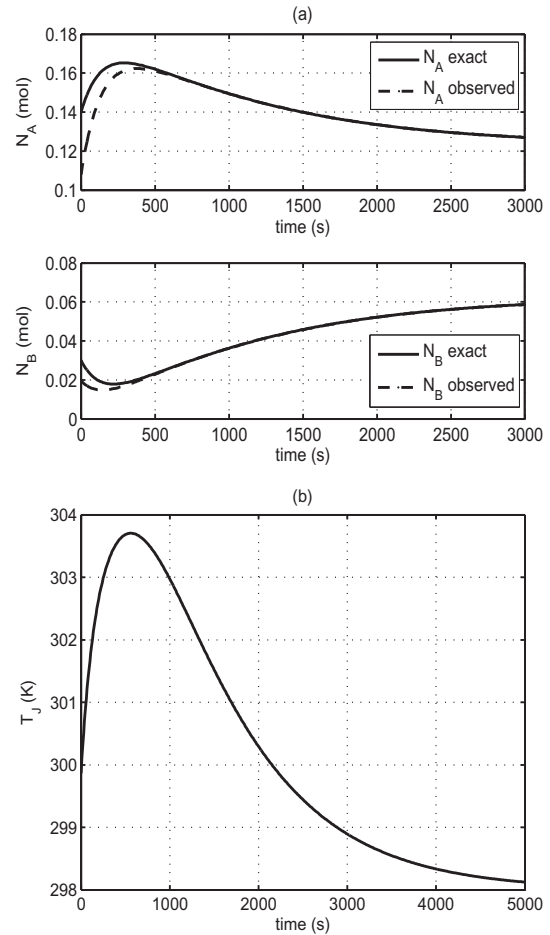

Fig. 5. N_A and its estimate with the asymptotic observer in the closed loop case – (a) for the initial conditions (C2) and $(\widehat{C}1)$ – (b) the control input T_J with the asymptotic observer.

Fig. 2 also shows that the control variable input T_J (34) is admissible in terms of amplitude and dynamics.

The Hamiltonian $\mathcal{H}_d(x)$ (33) plays the role of a global Lyapunov function for any choice of admissible initial conditions and consequently it converges to 0 as shown in Fig. 3.

5.3. Simulation with the asymptotic observer

First of all let us check that the feasibility conditions of Proposition 3 are satisfied. In our case, we have $\mathcal{I} = \emptyset$, $\mathcal{J} = \{A, B\}$ and $\boldsymbol{v} = \begin{pmatrix} v_A \\ v_B \end{pmatrix}$. Thus $(\boldsymbol{v}^\perp)_{\mathcal{J}} = (v_B - v_A)$, $\boldsymbol{h}_{\mathcal{J}}^T = (h_A(T) \ h_B(T))$ and $\det(\mathcal{O}) = -v_A h_A(T) - v_B h_B(T) = -\Delta H_R > 0$. It follows that the observability matrix $\mathcal{O}$ is full rank and the asymptotic observer is feasible.

For the sake of simplicity, the initial condition (C2) is used for the system. The initial conditions of the asymptotic observer are $(\widehat{C}1)$ with $(\widehat{H}(0) = 0.98H(T_0, N_{A0}, N_{A0}), \widehat{N}(0) = 0.75N(N_{A0}, N_{B0}))$ and $(\widehat{C}2)$ with $(\widehat{H}(0) = H(0.85T_0, N_{A0}, N_{B0}), \widehat{N}(0) = 0.95N(N_{A0}, N_{B0}))$ where the numerical values of T_0, N_{A0} and N_{B0} are given with the initial condition (C2). The open loop convergence of the estimates generated by the asymptotic observer (51) is illustrated in Fig. 4. With the initial condition (C2), the system converges to the stable point P_1. The closed loop simulations are given in Figs. 5 and 6 with the initial conditions, (C2) and $(\widehat{C}1)$, (C2) and $(\widehat{C}2)$ respectively. The stabilization at the unstable state P_2 of the controlled reaction system via the asymptotic observer is guaranteed. Furthermore, the dynamics of the control input T_J remains admissible as seen in Fig. 5(b) and Fig. 6(b).
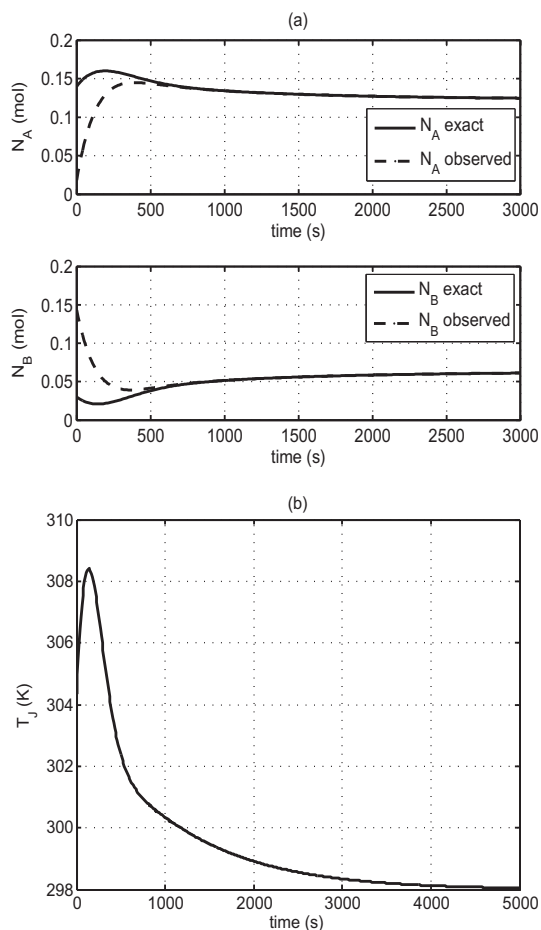
Fig. 6. N_A and its estimate with the asymptotic observer in the closed loop case – (a) for the initial conditions (C2) and $(\widehat{C2})$ – (b) the control input T_J with the asymptotic observer.

6. Conclusion

We have shown, by means of the passivity-based approach in the port Hamiltonian framework, how to synthesize a nonlinear controller for the stabilization and how to design an asymptotic observer of a class of CSTRs. The results can be applied to nonisothermal CSTRs operated under multiple steady states. The resulting state feedback developed in the paper generalizes the one proposed by Viel et al. (1997) in the sense that we do not add a constraint on the control input. The closed loop convergence of the system is theoretically shown. The use of an asymptotic observer provided the rank condition on the observability matrix. This condition is fulfilled by appropriate choice of measured states. Finally, numerical simulations show that convergence objective is satisfied for a simple case study. The state feedback law on the jacket temperature T_J is implementable and gives finite amplitude and admissible rate of variation. Open questions concern the structure of the observability matrix (with respect to traditional definition for linear systems); and the performance/robustness of the control law with respect to perturbations and parameters uncertainty.

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