Vol. 3(2), pp. 1-12, December 2024
eISSN: 2976-4009

ASEAN Journal of Process Control

Research Article

Tracking-error passivity-based control approach for the stabilization of chemical reaction systems using partially decoupled dynamics

Thanh Sang Nguyen[1]*, Ngoc Ha Hoang[2,3], Mohd Azlan bin Hussain[4]

[1] Faculty of Chemical and Food Technology, HCMC University of Technology and Education, Ho Chi Minh City, VIET NAM
[2] Institute of Research and Development, Duy Tan University, 550000 Da Nang, VIET NAM
[3] Faculty of Electrical-Electronic Engineering, Duy Tan University, 550000 Da Nang, VIET NAM
[4] Department of Chemical Engineering, Engineering faculty, Universiti Malaya, 50603 Lembah Pantai, Kuala Lumpur, MALAYSIA

*Corresponding Author: ntsang@hcmute.edu.vn

Abstract: This work aims to develop a passivity-based control method for a non-isothermal homogeneous reaction system by integrating its partially decoupled dynamics based on the concept of reaction variants/invariants with the tracking-error-based strategy in the framework of port-Hamiltonian (PH) representation. More precisely, the original reactor dynamics is transformed into an alternative model, expressed in terms of enthalpy, reaction-variant and reaction-invariant states, using a linear transformation, associated with a stoichiometric matrix. From this, it is shown that without using any state or input coordinate transformations, the transformed reactor model can be formulated into an extended class of PH systems with a unified quadratic storage function usable for control design. An irreversible first-order reaction system having multiple steady states and occurring in a continuous stirred tank reactor is utilized to illustrate the proposed control method. Simulations show that the closed-loop system is globally exponentially stabilized at the desired equilibrium point.

Keywords: Non-Isothermal Reactors, Reaction Variant and Invariants, Nonlinear System, Port-Hamiltonian Approach.

1. Introduction

In industry, continuous stirred tank reactors (CSTRs) are widely used to synthesize high-value products such as fine chemicals and polymers. From the viewpoint of mathematical modeling, they can be described by a set of ordinary differential equations (ODEs) that express material and energy balances [1, 2]. Moreover, the dynamics of CSTRs are driven by mutual interactions of physicochemical processes such as reaction kinetics and transport phenomena, thereby causing nonlinear characteristics such as steady-state multiplicity and non-minimum phase behavior [2-4]. Therefore, the set-point regulation and the stabilization of complex reaction systems at the desired equilibrium point are challenging yet interesting in process system engineering.

In recent years, the port-Hamiltonian (PH) framework for control design has been applied to regulate reaction systems in [5-9]. However, finding a suitable Hamiltonian function with structural matrices of the closed-loop systems may be difficult because it depends on the solvability of partialderivative matching equations [10, 11]. Therefore, instead of employing the original reactor model, we propose to transform it to an alternative model, expressed in terms of reaction-variant and reaction-invariant states in the sense of [12, 13] and obtained via a linear-time-invariant (LTI) transformation. It is important to note that this approach has two following advantages: (1) it reduces the necessary number of state variables to describe the system, and (2) the resulting controller relies more on the measurement rather than the information of the kinetic model, as compared to other estimator-based control approaches [14]. Due to the pertinence of this reduced model to analysis and control design, this paper shall integrate it with the tracking-error passivity-based control in the framework of PH representation, derived in [15, 16], to stabilize a non-isothermal CSTR having a steady state multiplicity behavior at the desired equilibrium point. This is the main contribution of this work.

The remaining of this paper is organized as follows. Section 2 briefly presents the mathematical model of a first-order irreversible reaction system in a CSTR and the tracking-error-based control method using an extended class of PH systems. The main results are developed in Section 3, including the control design to regulate the partially decoupled dynamics of the CSTR, expressed in terms of reaction-variant and reaction-invariant states, while simulations in Section 4 illustrate the designed controller. Finally, the conclusion is given in Section 5.

2. Preliminary

2.1. Dynamical model of a non-isothermal chemical reactor

In this work, we consider a first-order irreversible reaction, synthesizing the product B from the reactant A and taking place in a CSTR with one inlet stream and one outlet stream as shown in Figure 1. Also, its stoichiometry is given as follows [17]:

$$|v_1| A\ (S_1) \xrightarrow{r_v} v_2 B\ (S_2) \tag{1}$$

where v_1 and v_2 are the signed stoichiometric coefficients, considered to be negative for the reactant A, i.e. $v_1 < 0$, and to be positive for the product B, i.e. $v_2 > 0$. Besides, the species $I\ (S_3)$ is inert, having a role as a solvent of the reaction system; hence, its stoichiometric coefficient, denoted by v_3, is equal to zero, i.e. $v_3 = 0$. Next, the following assumptions are made throughout the paper to model the reaction system [3, 18].

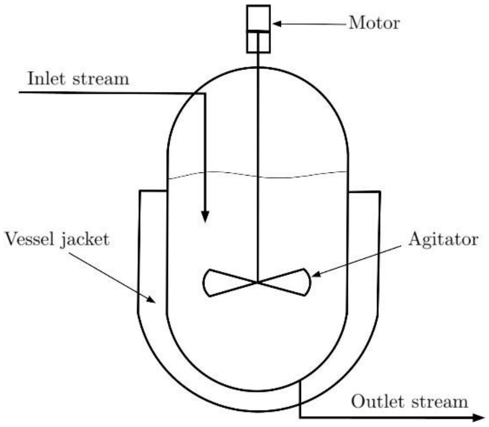

Figure 1: Schematic view of a non-isothermal chemical reactor

(A1) The mixing process inside the reactor is perfect and the reacting mixture is ideal as well as incompressible.

(A2) The CSTR operates under isobaric conditions; that is, the pressure of the reaction system remains unchanged under the pressure of the surroundings.

(A3) The volume of the reacting mixture, denoted by V, is kept unchanged, i.e. $V = \text{const.}$, leading to the operating constraint:

$$\frac{u_{in}(t)}{V\rho_{in}} = \frac{u_{out}(t)}{m(t)} = \omega(t) > 0. \tag{2}$$

(A4) The amount of heat exchanged between the vessel jacket and the reacting mixture, denoted by $q_{ex}(t)$, can be modelled as follows:

$$q_{ex}(t) = \lambda\left(T_J(t) - T(t)\right), \tag{3}$$

Where λ is the heat transfer coefficient, $T_J(t)$ and $T(t)$ are the jacket temperature and the reactor one, respectively.

(A5) The reaction rate, denoted by $\mathrm{r}_v(t)$, can be described by the mass-action law as follows:

$$\mathrm{r}_v(t) = \frac{1}{V}\mathrm{k}\left(T(t)\right)\mathrm{n}_1(t), \tag{4}$$

where the function $\mathrm{k}\left(T(t)\right)$ is expressed by the Arrhenius equation as follows:

$$\mathrm{k}\left(T(t)\right) = \mathrm{k}_0 \exp\left(\frac{-E_a}{RT(t)}\right), \tag{5}$$

with the kinetic constant k_0, the activation energy E and the ideal gas constant R.

Under Assumption (A1) – (A5), the mathematical model of the reaction system, including a set of material and energy balance equations, can be written in the following compact form:

$$\dot{\mathbf{n}}(\mathrm{t}) = \mathbf{N}^{\mathrm{T}}\mathrm{r}_v(t) + \mathbf{W}_{in}\mathrm{u}_{in}(t) - \omega(t)\mathbf{n}(t) \qquad \mathbf{n}_0 = \mathbf{n}(0), \tag{6}$$

$$\dot{H}(t) = q_{ex}(t) + \breve{h}_{in}\,\mathrm{u}_{in}(t) - \omega(t)\,H(t) \qquad H_0 = H(0), \tag{7}$$

with $\omega(t) = \dfrac{\mathrm{u}_{out}(t)}{m(t)}$, where

- $\mathbf{n}(t) = \left[\mathrm{n}_1(t) \quad \mathrm{n}_2(t) \quad \mathrm{n}_3(t)\right]^{\mathrm{T}}$ is the vector of the number of moles at the time t,
- $H(t)$ is the total enthalpy of the reacting mixture at the time t,
- $\mathbf{N} = \left[v_1 \quad v_2 \quad 0\right]$ is the constant stoichiometric matrix,
- $\mathbf{w}_{in} = \left[\mathrm{w}_{in,1} \quad \mathrm{w}_{in,2} \quad \mathrm{w}_{in,3}\right]^{\mathrm{T}}$ is the constant inlet-composition vector
- $\breve{\mathrm{h}}_{in}$ is the constant specific enthalpy of the inlet flow, calculated by $\breve{h}_{in} = \left[h_{in,1} \quad h_{in,2} \quad h_{in,3}\right]\mathbf{w}_{in}$ with $h_{in,i}$, $i = 1, 2, 3$ being the molar enthalpy of the species i evaluated at the inlet temperature T_{in},
- $\mathrm{u}_{in}(t)$ and $\mathrm{u}_{out}(t)$ are the mass flow rates of inlet and outlet flows, respectively,
- $m(t)$ is the total mass of the reacting mixture.

Remark 1: The total enthalpy $H(t)$ can be computed as follows [19, 20]:

$$H(t) = \sum_{i=1}^{3}\mathrm{n}_i(t)\,h_i(t), \tag{8}$$

where $h_i(t),\ i = 1, 2, 3$ is the component molar enthalpy of the species of each element in the outlet stream at the time t. In addition, since the reacting mixture is ideal and incompressible under Assumption (A1), $h_i(t),\ i = 1, 2, 3$ can be represented as follows:

$$h_i(t) = h_{ref,i} + c_{p,i}\left(T(t) - T_{ref}\right), \tag{9}$$

with $h_{ref,i}, c_{p,i}$ and T_{ref} being the constant reference molar enthalpy and the heat capacity of the species i and the reference temperature, respectively.

Remark 2: From the energy balance (7), the time derivatives of $T(t)$ can be expressed as follows:

$$\dot{T}(t) = \frac{q_{ex}(t) + \left(T_{in} - T(t)\right)\boldsymbol{c}_p^{\mathrm{T}}\,\mathrm{W}_{in}\,\mathrm{u}_{in}(t) - \Delta H(t)\,\mathrm{r}_v(t)}{c_P(t)}, \tag{10}$$

Where $\Delta H(t) := \mathbf{N}\boldsymbol{h}(t) = \left[\Delta\mathbf{H}_{ref}^{\mathrm{T}} + \boldsymbol{c}_p^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\left(T(t) - T_{ref}\right)\right]^{\mathrm{T}}$ with $\boldsymbol{h}(t) = \left[h_1(t) \quad h_2(t) \quad h_3(t)\right]^{\mathrm{T}}$ represents the vector of reaction enthalpies at the time t. Also, $c_P(t) := \boldsymbol{c}_p^{\mathrm{T}}\mathbf{n}(t)$ with $\boldsymbol{c}_p = \left[c_{p,1} \quad c_{p,2} \quad c_{p,3}\right]^{\mathrm{T}}$ is the time-varying heat capacity of the reacting mixture; therefore, it is always positive and bounded [21].

2.2 Tracking-error passivity-based control approach using an extended class of port-Hamiltonian models

We consider here a dynamical system that is affine in terms of the control input, and its dynamics can be given as follows:

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}(t)) + \mathbf{G}(\boldsymbol{x}(t))\boldsymbol{u}(t), \qquad \boldsymbol{x}(0) = \boldsymbol{x}_0, \tag{11}$$

where $\boldsymbol{x}(t)$ is the state vector over the operating region $D \subset \mathbb{R}^n$ and $\boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^n$ is a smooth vector-valued function concerning the vector field $\boldsymbol{x}$. Also, $\boldsymbol{u}(t) \in \mathbb{R}^m$ is the control input and $\mathbf{G}(\boldsymbol{x}) \in \mathbb{R}^{m\times n}$ are the full-rank input-to-state matrix with $m \le n$.

It is assumed that $\boldsymbol{f}(\boldsymbol{x})$ verifies a so-called separability condition [6, 9, 11], that is, it can be decomposed and expressed in the following form:

$$\boldsymbol{f}(\boldsymbol{x}) = \left[\mathbf{J}(\boldsymbol{x}) - \mathbf{R}(\boldsymbol{x})\right]\frac{\partial \mathrm{H}(\boldsymbol{x})}{\partial \boldsymbol{x}}, \tag{12}$$

where $\mathbf{J}(\boldsymbol{x})$ and $\mathbf{R}(\boldsymbol{x})$ are the $n \times n$ structural matrices, representing the skew-symmetric interconnection matrix and the symmetric damping matrix, respectively, i.e. $\mathbf{J}(\boldsymbol{x}) = -\mathbf{J}^{\mathrm{T}}(\boldsymbol{x})$ and $\mathbf{R}(\boldsymbol{x}) = \mathbf{R}^{\mathrm{T}}(\boldsymbol{x})$, while $\mathrm{H}(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}^n_{\ge 0}$ is called a Hamiltonian function. On this basis, the dynamics of $\boldsymbol{x}(t)$ (11) together with the output $\boldsymbol{y}(t) := \mathbf{G}^{\mathrm{T}}(\boldsymbol{x})\frac{\partial \mathrm{H}(\boldsymbol{x})}{\partial \boldsymbol{x}}$ can be formulated in the following form:

$$\begin{cases} \dot{x}(t) = \left[\mathbf{J}(\boldsymbol{x}) - \mathbf{R}(\boldsymbol{x})\right]\dfrac{\partial \mathrm{H}(\boldsymbol{x})}{\partial \boldsymbol{x}} + \mathbf{G}(\boldsymbol{x}(t))\boldsymbol{u}(t), \\ \boldsymbol{y}(t) = \mathbf{G}^{\mathrm{T}}(\boldsymbol{x})\dfrac{\partial \mathrm{H}(\boldsymbol{x})}{\partial \boldsymbol{x}}. \end{cases} \tag{13}$$

Clearly, if the matrix $\mathbf{R}(\boldsymbol{x})$ is positive semi-definite, i.e. $\mathbf{R}(\boldsymbol{x}) \ge 0$, the system dynamics (13) belongs to a class of *non-relaxing* PH systems, denoted by $\mathbf{H}_{e,nr}$. Additionally, the time derivatives of $\mathrm{H}(\boldsymbol{x})$ fulfills the dissipation inequality as follow:

$$\dot{\mathrm{H}}(t) = -\left[\frac{\partial \mathrm{H}(\boldsymbol{x}(t))}{\partial \boldsymbol{x}(t)}\right]^{\mathrm{T}} R(\boldsymbol{x}(t))\frac{\partial \mathrm{H}(\boldsymbol{x}(t))}{\partial \boldsymbol{x}(t)} + \boldsymbol{u}^{\mathrm{T}}(t)\boldsymbol{y}(t) \le \boldsymbol{u}^{\mathrm{T}}(t)\boldsymbol{y}(t), \tag{14}$$

which proves that the system dynamics (13) is passive with the input $\boldsymbol{u}(t)$, the output $\boldsymbol{y}(t)$ and the storage function $\mathrm{H}(\boldsymbol{x})$ [22]. On the other hand, if the matrix $\mathbf{R}(\boldsymbol{x})$ is negative semi-definite, i.e. $\mathbf{R}(\boldsymbol{x}) \le 0$, or indefinite, the system dynamics (13) belongs to a class of *relaxing* PH systems, denoted by $\mathbf{H}_{e,r}$. Moreover, $\mathbf{H}_{e,nr}$ and $\mathbf{H}_{e,r}$ are clearly two disjoint classes, that is, $\mathbf{H}_{e,nr} \cap \mathbf{H}_{e,r} = \varnothing$; therefore, their combination defines an extended class of PH systems denoted by $\mathbf{H}_e$, i.e. $\mathbf{H}_{e,nr} \cup \mathbf{H}_{e,r} = \mathbf{H}_e$, which is usable for designing a tracking-error PBC, as shown in the following lemma [15, 16, 23, 24].

Lemma 1: Assume that the system dynamics (11) can be formulated into an extended class of PH systems (13), i.e. $\boldsymbol{x}(t) \in \mathbf{H}_e$, with the quadratic Hamiltonian function $\mathrm{H}(\boldsymbol{x}(t))$ being of the following form:

$$\mathrm{H}(\boldsymbol{x}(t)) := \frac{1}{2}\boldsymbol{x}^{\mathrm{T}}(t)\boldsymbol{R}_{di}\boldsymbol{x}(t), \tag{15}$$

where $\boldsymbol{R}_{di}$ is an arbitrary constant positive-definite symmetric matrix, and the reference trajectory $\boldsymbol{x}_d(t)$ is governed by the following differential equation:

$$\dot{\boldsymbol{x}}_d(t) = \left[\mathbf{J}\left(\boldsymbol{x}(t)\right) - \mathbf{R}\left(\boldsymbol{x}(t)\right)\right]\frac{\partial \mathsf{H}(\boldsymbol{x}_d)}{\partial \boldsymbol{x}_d} + \boldsymbol{R}_I\left(\boldsymbol{x}(t)\right)\frac{\partial \mathsf{H}(e)}{\partial e} + \mathbf{G}\left(\boldsymbol{x}(t)\right)\boldsymbol{u}\left(\boldsymbol{x}(t)\right), \tag{16}$$

with $\mathsf{H}(\boldsymbol{e}) = \frac{1}{2}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{R}_{di}\boldsymbol{e}$, where $\boldsymbol{e}(t) := \boldsymbol{x}(t) - \boldsymbol{x}_d(t)$ is defined as the error state vector and $\boldsymbol{R}_I(\boldsymbol{x})$ is a symmetric matrix, i.e. $\boldsymbol{R}_I(\boldsymbol{x}) = \boldsymbol{R}_I^{\mathrm{T}}(\boldsymbol{x})$, for tuning feedback laws. Then,

i. when $\boldsymbol{x}(t) \in \mathbf{H}_{e,nr}$, there is a global exponential convergence of $\boldsymbol{x}(t)$ towards $\boldsymbol{x}_d(t)$, if $\boldsymbol{R}_I(\boldsymbol{x})$ is chosen to be positive definite, i.e.

$$\boldsymbol{R}_I(\boldsymbol{x}) \geq 0. \tag{17}$$

ii. Otherwise, when $\boldsymbol{x}(t) \in \mathbf{H}_{e,r}$, the system trajectory $\boldsymbol{x}(t)$ globally asymptotically approaches the reference trajectory $\boldsymbol{x}_d(t)$, if the following condition:

$$\boldsymbol{R}(\boldsymbol{x}) + \boldsymbol{R}_I(\boldsymbol{x}) = \left(\boldsymbol{R}(\boldsymbol{x}) + \boldsymbol{R}_I(\boldsymbol{x}) \geq 0\right)^{\mathrm{T}} \geq 0, \tag{18}$$

is satisfied

Proof: The proof can be found in [15, 16].

Remark 3: To obtain the feedback law $\boldsymbol{u}(t)$ with $\dim \boldsymbol{u} = m$, we only need to select suitably m components of $\boldsymbol{x}_d(t) \in \mathbb{R}^n$ and assign a desired trajectory, stabilized at the set-point, to them such that the resulting $m \times m$ submatrix $\mathbf{G}_d(t)$, extracted from $\mathbf{G}(\boldsymbol{x}(t))$ and having m rows with respect to m chosen elements of $\boldsymbol{x}_d(t)$, is of full-rank [15, 16].

3. Main Results

3.1 The partially decoupled dynamics of reaction system via the concept of reaction variant and invariant

It can be seen from the enthalpy balance (7) that the dynamics of $H(t)$ is independent of the reaction rate $\mathrm{r}_v(t)$ and thus it can be considered as a reaction invariant. We, therefore, propose to decompose the space of $\mathbf{n}(t)$ into two parts, including the one of reaction-variant states, denoted by $\mathrm{y}_r(t)$, and the one of reaction-invariant states, denoted by $\mathbf{y}_{iv}(t) := \left[\mathrm{y}_{iv,1}(t) \quad \mathrm{y}_{iv,2}(t)\right]^{\mathrm{T}}$, in the sense of [12, 13]. It is important to note that $\mathrm{y}_r(t)$ is a scalar quantity, and its dynamics contains information of the reaction rate $\mathrm{r}_v(t)$, while the dynamics of $\mathbf{y}_{iv}(t)$ is independent of the reaction rate $\mathrm{r}_v(t)$. Moreover, the decomposition is implemented by using a size-preserving linear transformation $\Im$, associated with the stoichiometric matrix $\mathbf{N}$, as shown in the following lemma.

Lemma 2: The transformation from the space of $\mathbf{n}(t)$ to the one of reaction-variant and reaction-invariant states, denoted by $\mathbf{y}(t)$, is expressed by:

$$\mathbf{y}(t) := \begin{bmatrix} \mathrm{y}_r(t) \\ \mathbf{y}_{iv}(t) \end{bmatrix} = \Im\mathbf{n}(t), \tag{19}$$

where the matrix $\Im$ is given by:

$$\Im = \begin{bmatrix} \frac{1}{v_1} & 0 & 0 \\ v_2 & -v_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{20}$$

Moreover, the dynamics of $\mathbf{n}(t)$, given by (6), is transformed to

$$\dot{\mathrm{y}}_r(t) = v_1\,\mathrm{k}\big(T(t)\big)\,\mathrm{y}_r(t) + \frac{\breve{w}_1}{v_1\mathrm{M}_1}\mathrm{u}_{in}(t) - \omega(t)\,\mathrm{y}_r(t), \qquad \mathrm{y}_r(0) = -\mathrm{n}_{1,0}, \tag{21}$$

$$\dot{\mathrm{y}}_{iv,1}(t) = \left(v_2\frac{\breve{w}_1}{\mathrm{M}_1} - v_1\frac{\breve{w}_2}{\mathrm{M}_2} \right)\mathrm{u}_{in}(t) - \omega(t)\,\mathrm{y}_{iv,1}(t), \qquad \mathrm{y}_{iv,1}(0) = v_2\,\mathrm{n}_{1,0} - v_1\,\mathrm{n}_{2,0}, \tag{22}$$

$$\dot{\mathrm{y}}_{iv,2}(t) = \frac{\breve{w}_3}{\mathrm{M}_3}\mathrm{u}_{in}(t) - \omega(t)\,\mathrm{y}_{iv,2}(t), \qquad \mathrm{y}_{iv,2}(0) = \mathrm{n}_{3,0}, \tag{23}$$

Proof: From (19) and (20), it is straightforward to obtain $\dot{\mathbf{y}}(t) = \Im\dot{\mathbf{n}}(t),$ which allows obtaining (21), (22), and (23) immediately

Remark 4: Since the matrix $\Im$ is non-singular, $\mathbf{n}(t)$ can be reconstructed from $\mathbf{y}(t)$ as follows:

$$\mathbf{n}(t) = \Im^{-1}\,\mathbf{y}(t), \tag{24}$$

with $\Im^{-1} = \begin{bmatrix} v_1 & 0 & 0 \\ v_2 & \dfrac{-1}{v_1} & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

It can be seen from (22) and (23) that, due to $\omega(t) > 0$, the dynamics of $\mathbf{y}_{iv}(t)$ globally exponentially converges to the equilibrium point $\bar{\mathbf{y}}_{iv}(t) := \begin{bmatrix} \bar{\mathrm{y}}_{iv,1} & \bar{\mathrm{y}}_{iv,2} \end{bmatrix}^{\mathrm{T}}$, computed as follows:

$$\bar{\mathrm{y}}_{iv,1} = \left(v_2\frac{\breve{w}_1}{\mathrm{M}_1} - v_1\frac{\breve{w}_2}{\mathrm{M}_2} \right) V\rho_{in}, \tag{25}$$

$$\bar{\mathrm{y}}_{iv,2} = \frac{\breve{w}_3}{\mathrm{M}_3} V\rho_{in}, \tag{26}$$

by using (2), (20) and (23). As a result, $\mathbf{y}_{iv}(t)$ can be excluded from the partially decoupled dynamics of the CSTR, expressed by (21), (22) and (23), to reduce the model dimension for the purpose of control design. On this basis, the reduced transformed model can be expressed in terms of the vector $\boldsymbol{x}(t) := \begin{bmatrix} \mathrm{y}_r(t) & H(t) \end{bmatrix}^{\mathrm{T}}$ as follows:

$$\dot{\mathrm{y}}_r(t) = v_1\,\mathrm{k}\big(T(t)\big)\,\mathrm{y}_r(t) + \frac{\breve{w}_1}{v_1\mathrm{M}_1}\mathrm{u}_{in}(t) - \omega(t)\,\mathrm{y}_r(t), \tag{27}$$

$$\dot{H}(t) = q_{ex}(t) + \breve{\mathrm{h}}_{in}\mathrm{u}_{in}(t) - \omega(t)H(t). \tag{28}$$

The control objective can be stated as follows. Let $\bar{\mathbf{z}} = \begin{bmatrix} \bar{\mathrm{n}}_1 & \bar{\mathrm{n}}_2 & \bar{\mathrm{n}}_3 & \bar{H} \end{bmatrix}^{\mathrm{T}}$ represent the desired equilibrium point of the reaction system (1), corresponding to the equilibrium point $\begin{bmatrix} \bar{\mathrm{y}}_r & \bar{\mathrm{y}}_{iv,1} & \bar{\mathrm{y}}_{iv,2} & \bar{H} \end{bmatrix}^{\mathrm{T}}$ of the partially decoupled dynamics. The control objective here is to design the feedback laws $\boldsymbol{u}(t) = \begin{bmatrix} \mathrm{u}_{in}(t) & q_{ex}(t) \end{bmatrix}^{\mathrm{T}}$ to stabilize the reduced partially decoupled dynamics, given by (27) and (28), at the desired equilibrium point $\bar{\boldsymbol{x}} = \begin{bmatrix} \bar{\mathrm{y}}_r & \bar{H} \end{bmatrix}^{\mathrm{T}}$.

3.1. Hamiltonian view on the partially decoupled dynamics of the non-isothermal chemical reactors

The following proposition gives the PH representation of the dynamics of $\boldsymbol{x}(t)$, given by (27) and (28).

Proposition 1: The decoupled dynamics can be formulated into a *non-relaxing* PH representation with the state vector $\boldsymbol{x}(t)$ and the quadratic Hamiltonian function $\mathrm{H}(\boldsymbol{x}) = \dfrac{1}{2}\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}$ as follows:

$$\dot{\boldsymbol{x}}(t)=\left[\mathbf{J}-\mathbf{R}(t)\right]\frac{\partial \mathrm{H}(\boldsymbol{x}_d)}{\partial \boldsymbol{x}_d}+\mathbf{G}\left(\boldsymbol{x}(t)\right)\boldsymbol{u}(t), \tag{29}$$

where the matrix $\mathbf{G}\left(\boldsymbol{x}(t)\right)$ is given by $\mathbf{G}\left(\boldsymbol{x}(t)\right)=\begin{bmatrix}\dfrac{\breve{w}_1}{v_1\mathrm{M}_1} & 0\\ \breve{\mathrm{h}}_{in} & 1\end{bmatrix}$ and the structural matrices are expressed by:

$$\mathbf{J}=\mathbf{0}_{2\times 2}\,\text{and}\;\mathbf{R}(t)=\begin{bmatrix}\omega(t)-v_1\mathrm{k}(T(t)) & 0\\ 0 & \omega(t)\end{bmatrix}. \tag{30}$$

Proof: Clearly, the dynamics of $\boldsymbol{x}(t)$, given by (27) and (28), can be formulated into (29). More importantly, the matrix $\mathbf{R}(t)$ is always positive definite owing to the physical meaning of $\mathrm{k}(T(t))$, derived from (5), and $v_1<0$, leading to $\boldsymbol{x}(t)\in\mathbf{H}_{e,nr}$. The latter completes the proof.

3.2. Controller synthesis

The feedback laws to stabilize the dynamics of $\boldsymbol{x}(t)$ at $\bar{\boldsymbol{x}}$ is designed by applying Lemma 1 for the non-relaxing PH system (29), which is shown in the following proposition.

Proposition 2: Let the reference trajectory $\boldsymbol{x}_d(t)=\left[\mathrm{y}_{r,d}(t)\quad H_d(t)\right]^{\mathrm{T}}$ be governed by

$$\dot{\boldsymbol{x}}_d(t)=\left[\mathbf{J}-\mathbf{R}(t)\right]\frac{\partial \mathrm{H}(\boldsymbol{x}_d)}{\partial \boldsymbol{x}_d}+\mathbf{R}_I\left(\boldsymbol{x}(t)-\boldsymbol{x}_d(t)\right)+\mathbf{G}\left(\boldsymbol{x}(t)\right)\boldsymbol{u}(t), \tag{31}$$

where $\mathbf{R}_I=\mathrm{diag}\left(R_{I,1},R_{I,2}\right)>0$ is the constant damping injection. Then, by using the following feedback laws, calculated by:

$$\mathrm{u}_{in}(t)=\frac{v_1\mathrm{M}_1}{\breve{w}_1}\left[K_1\left(\bar{\mathrm{y}}_r-\mathrm{y}_{r,d}(t)\right)+\left(\omega(t)-v_1\mathrm{k}\left(T(t)\right)\right)\mathrm{y}_{r,d}(t)-R_{I,1}\left(\mathrm{y}_r(t)-\mathrm{y}_{r,d}(t)\right)\right], \tag{32}$$

$$T_J(t)=T(t)+\frac{K_2\left(\bar{H}-H_d(t)\right)+\omega(t)H_d(t)-R_{I,2}\left(H(t)-H_d(t)\right)-\breve{\mathrm{h}}_{in}\mathrm{u}_{in}(t)}{\lambda}, \tag{33}$$

the system trajectory $\boldsymbol{x}(t)$ globally exponentially converges to the reference trajectory $\boldsymbol{x}_d(t)$, which can be assigned as:

$$\dot{\boldsymbol{x}}_d(t)=\mathbf{K}\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_d(t)\right), \tag{34}$$

with $\mathbf{K}=\mathrm{diag}\left(K_1,K_2\right)>0$ being a tuning matrix, if the matrix $\mathbf{R}_I$ is chosen to be positive definite, that is,

$$\mathbf{R}_I>0. \tag{35}$$

Proof: It follows immediately from Proposition 1 that the stability condition for the exponential decay of $\boldsymbol{x}(t)$ towards $\boldsymbol{x}_d(t)$, governed by (31), is given by (35) owing to $\boldsymbol{x}(t)\in\mathbf{H}_{e,nr}$. Furthermore, by assigning the dynamics of $\boldsymbol{x}_d(t)$ to the exponential profile generated by (34), the feedback laws $\mathrm{u}_{in}(t)$ and $q_{ex}(t)$ can be calculated by (32) and (33), respectively, which ensures the stabilization of $\boldsymbol{x}(t)$ at $\bar{\boldsymbol{x}}$. The latter completes the proof.

4. Simulations

For the sake of simulation, the stoichiometric coefficients v_1 and v_2 are given as $v_1=-1$ and $v_2=1$, and the reaction system (1) is initiated at one of three following conditions:

- (IC₁): $n_{1,0} = 0.06(\text{mol})$, $n_{2,0} = 0.03(\text{mol})$, $n_{3,0} = 2(\text{mol})$ and $T = 280(\text{K})$,
- (IC₂): $n_{1,0} = 0.04(\text{mol})$, $n_{2,0} = 0.001(\text{mol})$, $n_{3,0} = 2.5(\text{mol})$ and $T = 330(\text{K})$,
- (IC₃): $n_{1,0} = 0.01(\text{mol})$, $n_{2,0} = 0.01(\text{mol})$, $n_{3,0} = 3.5(\text{mol})$ and $T = 355(\text{K})$.

Moreover, the CSTR is operated with the nominal operating conditions: $u_{in} = 0.466$ (g/s) and $T_J = 290$ (K). Other operating and physical parameters of the CSTR are listed in Table 1.

Table 1. Physical and operating parameters of the first-order reaction system

Symbol	Quantity	Value	Unit
$h_{ref,1}$	Reference enthalpy of the species A	-2.7085×10^{4}	J.mol⁻¹
$h_{ref,2}$	Reference enthalpy of the species B	-1.1884×10^{5}	J.mol⁻¹
$h_{ref,3}$	Reference enthalpy of the species C	-33	J.mol⁻¹
$c_{p,1}$	Heat capacity of the species A	221.9	J.(K.mol)⁻¹
$c_{p,2}$	Heat capacity of the species B	128.46	J.(K.mol)⁻¹
$c_{p,3}$	Heat capacity of the species C	21.694	J.(K.mol)⁻¹
M_1	Molecular weight of the species A	50	g/mol
M_2	Molecular weight of the species B	50	g/mol
M_3	Molecular weight of the species C	18	g/mol
E_a	Activation energy	73350	J.mol⁻¹
R	Ideal gas constant	8.314	J.(K.mol)⁻¹
T_{ref}	Reference temperature	298.15	K
λ	Heat transfer coefficient	0.5	W/K
T_{in}	Temperature of the inlet stream	370	K
ρ_{in}	Specific density of the inlet stream	667.14	g/ℓ
V	Volume of the reacting mixture	0.1	ℓ

It is clearly shown in Figure 2 that the reaction system has three different equilibrium points, expressed by $P_i = \begin{bmatrix}\bar{n}_{1,i} & \bar{n}_{2,i} & \bar{n}_{3,i} & \bar{T}_i\end{bmatrix}$. Additionally, their values are given by:

- $P_1 = \begin{bmatrix}0.151 & 0.009 & 3.26 & 299.37\end{bmatrix}$,
- $P_2 = \begin{bmatrix}0.108 & 0.053 & 3.26 & 322.55\end{bmatrix}$,
- $P_3 = \begin{bmatrix}0.005 & 0.156 & 3.26 & 381.89\end{bmatrix}$,

which are closely similar to the values obtained in [18], thereby validating their pertinence for control design in this work. Moreover, the system trajectories starting from (IC₁) and (IC₂) approach P_1, while the trajectory starting from (IC₃) approaches P_3. Therefore, P_1 and P_3 are locally stable steady states, while P_2 is an unstable one. In practice, P_2 is the desired equilibrium point of the reaction system since it can comprimise both economic benefit and engineering constraints. However, the reactor can not be stabilized at P_2 without the feedback control. Consequently, in what follows, the feedback laws, given by (32) and (33), are used to stabilize the reactor at P_2, which is the setpoint of the closed-loop system.

To implement the closed-loop system, all state variables of the reaction system are assumed to be measurable, and the control parameters are practically tuned to support the admissibility feature of manipulated variables with respect to time [5, 25], that is,

$$\boldsymbol{u}(t=0)=\boldsymbol{u}_0 \qquad (36),$$

where $\boldsymbol{u}_0=\begin{bmatrix}\mathrm{u}_{in,0} & T_{J,0}\end{bmatrix}^{\mathrm{T}}$ is a selected constant vector at the time $t=0$, and enhance the control performance of the closed-loop system, including the transient responses of state variables and the amplitude and variation rates of manipulated variables. Therefore, with $\mathrm{u}_{in,0}=0.094$ (g/s) and $T_{J,0}=308.8(\mathrm{K})$, we can choose $R_{I,1}=2\times10^{-3}$, $R_{I,2}=10^{-3}$ and $K_1=K_2=3\times10^{-3}$. Moreover, the control performance of the closed-loop system under the proposed PBC is compared with that of under the PI control, for the design method is represented in Appendix A and the control comparamters are finely tuned to fulfill the constrain (36) with $\boldsymbol{u}_{0,\mathrm{PI}}=\begin{bmatrix}0.094 & 308.8\end{bmatrix}^{\mathrm{T}}$.

The closed-loop phase plane in Figure 3 represents that the system trajectories starting from three initial conditions globally asymptotically converge to the desired equilibrium point P_2 under the proposed PBC. Also, as shown in Figure 4, the dynamics of $\mathrm{y}_r(t)$ and $H(t)$ are globally exponentially stabilized at the desired equilibrium values, which, therefore, guarantees the convergence of $\mathbf{n}(t)$ and $T(t)$ towards the respective desired equilibrium values. Furthermore, it can be clearly seen from Figure 5 that although both two controllers can stabilize the closed-loop system at the desired equilibrium point, the time responses of $\mathrm{n}_1, \mathrm{n}_2, \mathrm{n}_3$ and T under the proposed PBC are less oscillatory than that of under the PI control. In addition, the actual control inputs: $\mathrm{u}_{in}(t)$ and $T_J(t)$ computed by the PI control give more oscillations, thereby needing more control actions, as given in Figure 6. As a result, one can conclude that the control performance is superior with the proposed PBC than PI control.

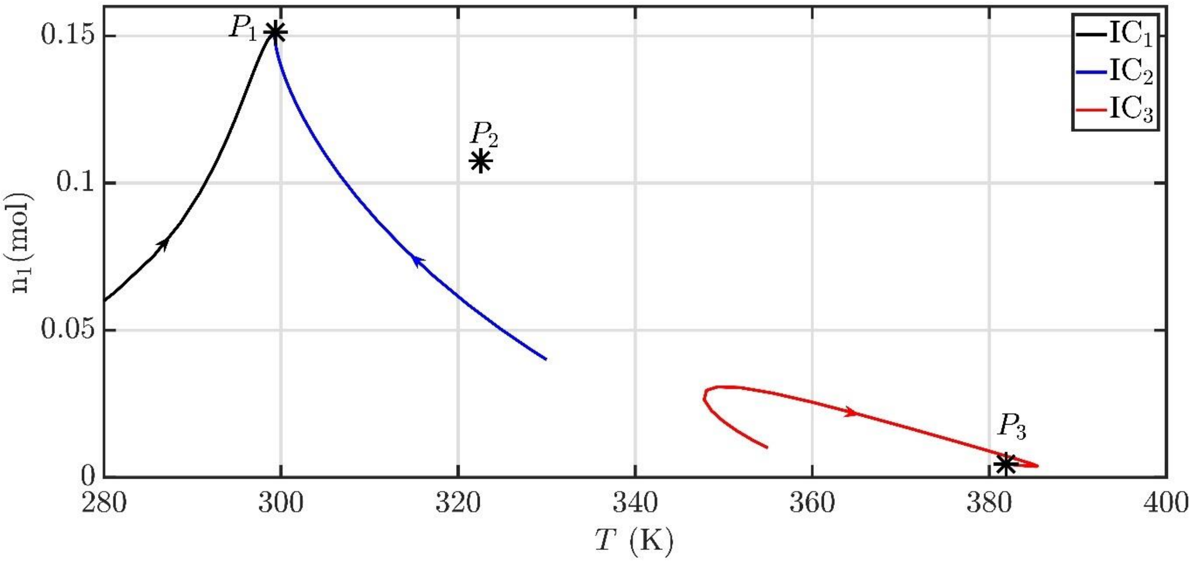

Figure 2. The representation of open-loop phase plane.

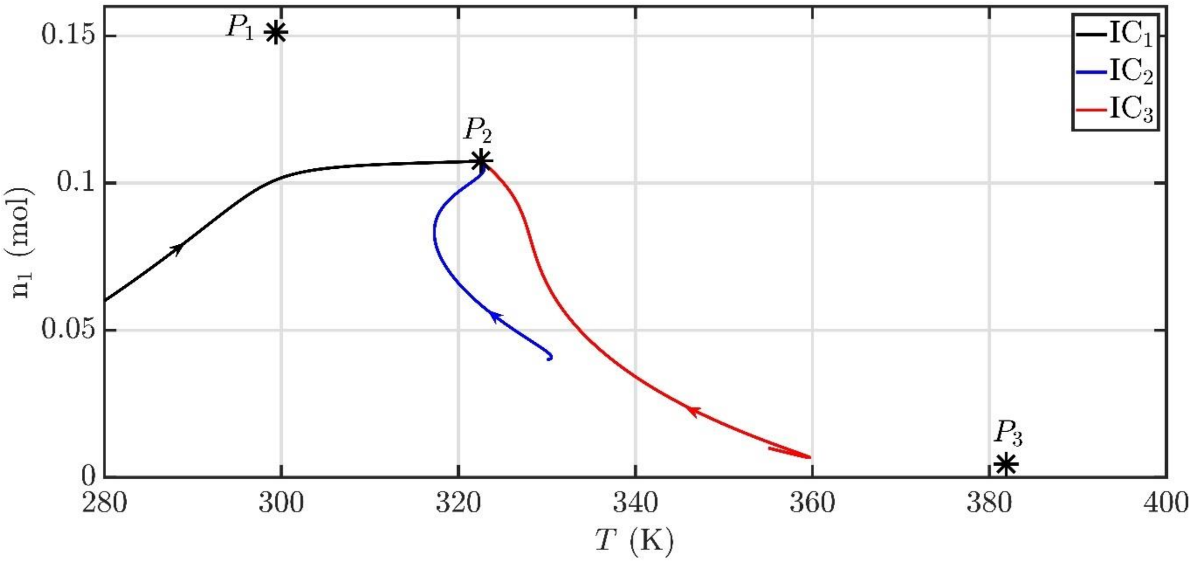

Figure 3. The representation of closed-loop phase plane.

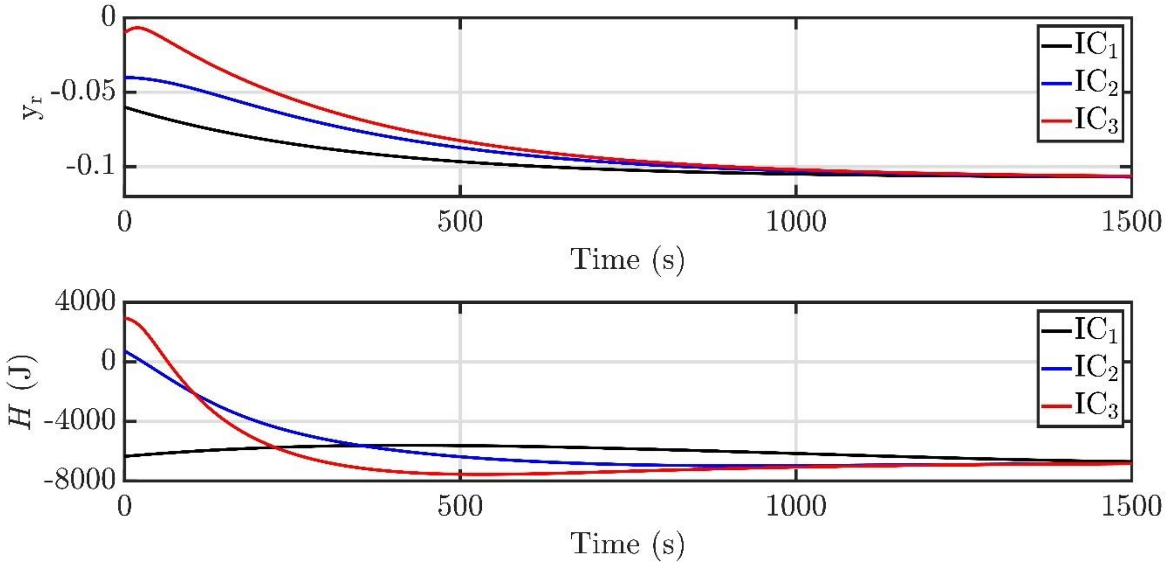

Figure 4. Dynamics of the reaction variant and the enthalpy.

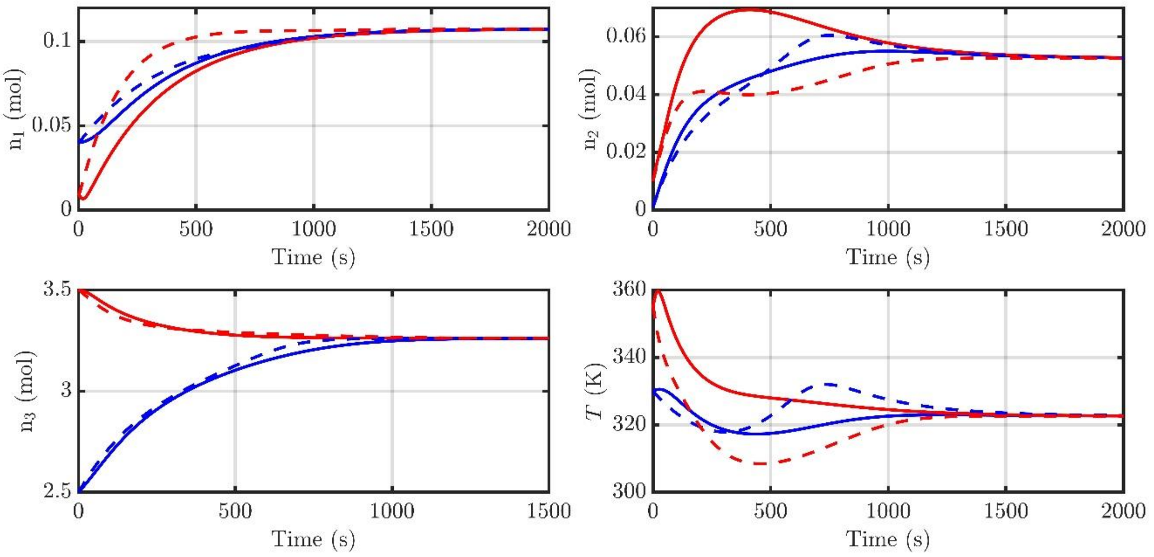

Figure 5. Time responses of the system trajectories: - (IC2) with the proposed control, - (IC3) with the proposed control, -- (IC2) with the PI control, -- (IC3) with the PI control.

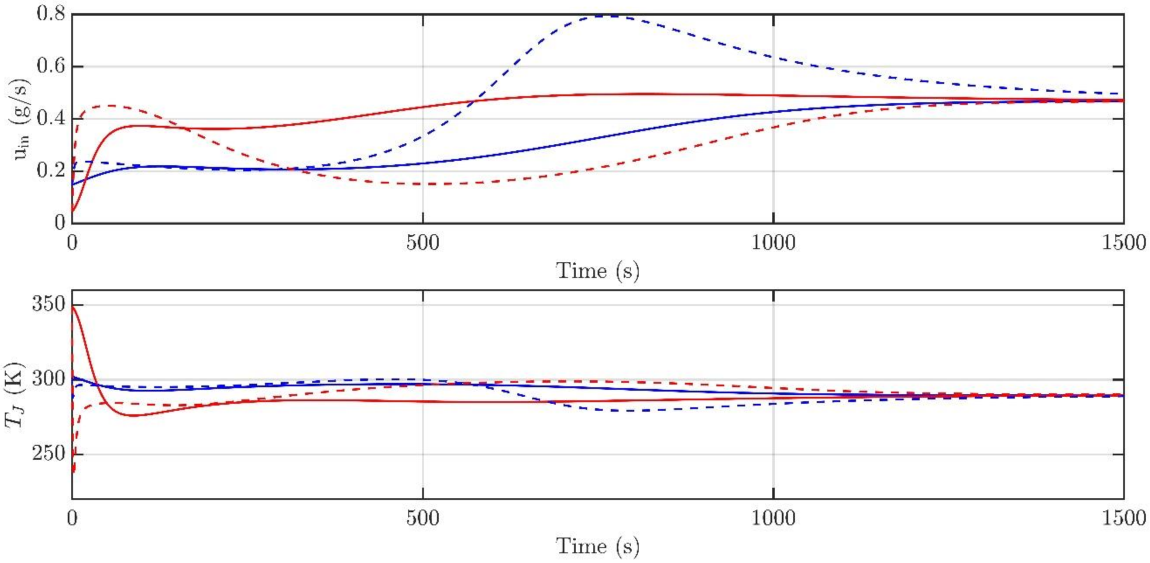

Figure 6. The control inputs: - (IC2) with the proposed control, - (IC3) with the proposed control, - - (IC2) with the PI control, -- (IC3) with the PI control.

5. Conclusions

In this work, a tracking-error PBC is designed within the framework of PH representation for the partially decoupled dynamics of a CSTR, obtained by a size-preserving linear transformation. The transformed reactor model, expressed in terms of reaction-variant and reaction-invariant states, is then formulated into a non-relaxing PH representation. The tracking-error approach addressed the stabilization problem of system trajectories at the desired equilibrium point, i.e., assigning a certain structure for the reference trajectory with an appropriate damping injection. Simulations show that the designed controller is workable. An extension of the control method to stabilize tubular reactors and multiphase-stirred tank reactors will be part of our future work.

Appendix A: PI control design

The PI controller in this research is designed by the approach derived by [26]. And, its expression is given by $u = \bar{u} + K_P\left(\bar{x} - x\right) + K_I\int_0^t\left(\bar{x} - x\right)dt$, where x and u are the output and the input, respectively. Besides, $\bar{u}$ is the nominal values, $\bar{x}$ is the set point, K_P and K_I are tuning parameteres, listed in Table A.1 for the second and the third initial conditions.

Input	$\bar{x}$	IC₂			IC₃		
		$\bar{u}$	K_P	K_I	$\bar{u}$	K_P	K_I
$u_{in,\mathrm{PI}}$	–0.1076	–16	238.46	0.65	–11.5	118.29	0.69
$q_{ex,\mathrm{PI}}$	-6.772×10^3	16000	2.13	0.01	11300	1.16	0.01

References

1. Luyben, W.L., *Process Modeling, Simulation, and Control for Chemical Engineers*. 1990, McGraw-Hill Higher Education.
2. Aris, R., *Elementary chemical reactor analysis*. 1999: Courier Corporation.
3. Favache, A. and D. Dochain, *Thermodynamics and chemical systems stability: The CSTR case study revisited.* Journal of Process Control, 2009. **19**(3): p. 371-379.
4. Freitas Filho, I.P., E.C. Biscaia, and J.C. Pinto, *Steady-state multiplicity in continuous bulk polymerization reactors—a general approach.* Chemical Engineering Science, 1994. **49**(22): p. 3745-3755.
5. Hoang, N.H., et al., *The port Hamiltonian approach to modeling and control of Continuous Stirred Tank Reactors.* Journal of Process Control, 2011. **21**(10): p. 1449-1458.

6. Hoang, N.H., et al., *Passivity-based nonlinear control of CSTR via asymptotic observers.* Annual Reviews in Control, 2013. **37**(2): p. 278-288.
7. Ramírez, H., et al., *On the passivity based control of irreversible processes: A port-Hamiltonian approach.* Automatica, 2016. **64**: p. 105-111.
8. Sira-Ramirez, H. and I. AnguloNunez, *Passivity-based control of nonlinear chemical processes.* International Journal of Control, 1997. **68**(5): p. 971-996.
9. Dorfler, F., J.K. Johnsen, and F. Allgower, *An introduction to interconnection and damping assignment passivity-based control in process engineering.* Journal of Process Control, 2009. **19**(9): p. 1413-1426.
10. Ortega, R., Z.T. Liu, and H.Y. Su, *Control via interconnection and damping assignment of linear time-invariant systems: a tutorial.* International Journal of Control, 2012. **85**(5): p. 603-611.
11. Ortega, R., et al., *Interconnection and damping assignment passivity-based control of port-controlled Hamiltonian systems.* Automatica, 2002. **38**(4): p. 585-596.
12. Asbjörnsen, O.A., *Reaction invariants in the control of continuous chemical reactors.* Chemical Engineering Science, 1972. **27**(4): p. 709-717.
13. Fjeld, M., O.A. Asbjørnsen, and K.J. Åström, *Reaction invariants and their importance in the analysis of eigenvectors, state observability and controllability of the continuous stirred tank reactor.* Chemical Engineering Science, 1974. **29**(9): p. 1917-1926.
14. Bastin, G., *On-line estimation and adaptive control of bioreactors*. Vol. 1. 2013: Elsevier.
15. Nguyen, T.S., et al., *Tracking-error control via the relaxing port-Hamiltonian formulation: Application to level control and batch polymerization reactor.* Journal of Process Control, 2019. **80**: p. 152-166.
16. Hoang, N.H., et al., *Trajectory tracking for nonlinear systems using extended quadratic port-Hamiltonian models without input and state coordinate transformations.* Systems & Control Letters, 2022. **167**: p. 105325.
17. Hoang, N.H., D. Rodrigues, and D. Bonvin, *Revisiting the concept of extents for chemical reaction systems using an enthalpy balance.* Computers & Chemical Engineering, 2020. **136**: p. 106652.
18. Hoang, N.H., et al., *Thermodynamics based stability analysis and its use for nonlinear stabilization of the CSTR.* Computers & Chemical Engineering, 2013. **58**: p. 156-177.
19. Sandler, S.I., *Chemical, biochemical, and engineering thermodynamics*. 2017: John Wiley & Sons.
20. Hoang, N.H. and D. Dochain, *On an evolution criterion of homogeneous multi-component mixtures with chemical transformation.* Systems & Control Letters, 2013. **62**(2): p. 170-177.
21. Nguyen, T.S., et al., *Output regulation via trajectory tracking for chemical reactors with jacket dynamics.* Computers & Chemical Engineering, 2023. **169**: p. 108071.
22. Bao, J. and P.L. Lee, *Process Control - The Passive Systems Approach*. 1st ed. Advances in Industrial Control, ed. A.i.I. Control. 2007: Springer-Verlag London.
23. Nguyen, T.S., N.H. Hoang, and M.A. Hussain, *Tracking error plus damping injection control of non-minimum phase processes.* IFAC-PapersOnLine, 2018. **51**(18): p. 643-648.
24. Nguyen, T.S., et al., *Tracking-error-based control of a chemical reactor using decoupled dynamic variables.* IFAC-PapersOnLine, 2019. **52**(7): p. 74-79.
25. Nguyen, T.S., et al., *A perturbed Port-Hamiltonian approach for the stabilization of homogeneous reaction systems via the control of vessel extents.* Computers & Chemical Engineering, 2021. **154**: p. 107458.
26. Alvarez-Ramirez, J. and H. Puebla, *On classical PI control of chemical reactors.* Chemical Engineering Science, 2001. **56**(6): p. 2111-2121.