Preprints of the 21st IFAC World Congress (Virtual)
Berlin, Germany, July 12-17, 2020

Control of reaction systems using decoupled dynamics via perturbed Hamiltonian formulation

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Abstract: This work proposes a novel control strategy to stabilize the dynamics of a homogeneous reactor, described by the extents of reaction and inlet streams with the inclusion of heat balance. Specifically, we formulate this transformed model into a perturbed port-Hamiltonian (PH) structure, where the vector of reaction rates is expressed as a matched/unmatched and time-varying disturbance. Then, together with the tracking-error-based control method for the stabilization, two different configurations to compensate such disturbance, including a feed-forward law and a dynamic feedback one, are designed such that the error system asymptotically converges to the set point and preserves the PH representation by assigning an appropriate damping injection. A complex reaction system is used to illustrate the approach.

Keywords: Tracking-error-based control, extent of reaction, disturbance compensation.

1. INTRODUCTION

Chemical reactors play a key role in synthesizing commercial products such as polymer and fine chemical from raw materials. The operation of these reacting systems is driven by reaction kinetics and transport phenomena. Hence, a mathematical model, expressing the mass balance of each component and the heat balance of reactor, is usually highly nonlinear, thereby giving rise to abnormal behaviors such as multiple steady states and non-minimum phase characteristic (Hoang *et al.*, 2013). Therefore, numerous model-based controllers have been designed to handle nonlinear characteristics of reacting systems for the stabilization at the desired set-point. However, applications of these control strategies are somehow limited due to the intrinsic nonlinearity of mathematical descriptions, caused by interactions of various processes inside reactors. For example, the feedback linearization method via a diffeomorphism is not capable of dealing with non-minimum phase systems due to unstable zero dynamics (Khalil, 2002). In fact, the control design and the system analysis of reacting systems would become simpler if effects of different physical/chemical processes on each chemical state could be separated because it could allow controlling and analyzing each rate process individually. In other words, we wish to model a reacting system in a new state presentation where each state variable only depends on a single rate process (Rodrigues *et al.*, 2015).

The concept of vessel extents for reactions and inlet/outlet streams were initially proposed by Amrhein *et al.* (2010) [1] to decompose the dynamics of a isothermal homogeneous reactor via a multi-step procedure but still to maintain the physical meaning of state variables, which is the amount of material with respect to each rate process that is not left the vessel. This interesting transformed model was then extended for a non-isothermal reactor via a linear transformation and studied for the model reduction, optimal estimations of reaction kinetics and the data reconciliation (Rodrigues *et al.*, 2015). For the purpose of control design, Marquez-Ruiz *et al.* (2018, 2019) considered the vessel-extent-based decoupled dynamics as a linear parameter-varying (LPV) system, where the vector of reaction kinetics constitutes an internal disturbance. In this framework, two control configurations, namely a model-predictive control scheme and a combination of a feedback law for the stabilization and a feed-forward law for the disturbance rejection, were proposed to calculate control algorithms.

This paper focusses on the use of the concept of vessel extent transformation and the tracking-error-based control method, given by Nguyen *et al.* (2019), to derive a novel control strategy. Specifically, the vessel-extent-based decoupled dynamics of a general non-isothermal homoge-

⋆ The first author is supported by Japan International Cooperation Agency (JICA) and University of Malaya (UM) via the AUN/Seed-Net scholarship. The third author acknowledges the support of The Viet Nam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.99-2019.385.

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[1] This nice work has been considered as a generalisation of the concept of reaction variants and invariants (Asbjørnsen and Fjeld, 1970). Control of chemical reactors in the subspace of reaction and control variants can be found in Hammarström (1979).

neous reactor is viewed as a perturbed PH representation where the vector of reaction rates is expressed as an matched/unmatched disturbance. Noting that such disturbance is time-varying; thus previous approaches to reject the constant disturbance for control systems (Ortega and Romero, 2012; Donaire and Junco, 2009; Ferguson *et al.*, 2017), can not be applied. Hence, two novel strategies, including a feed-forward law and a dynamic feedback one, to compensate such disturbance are contributed so that the error system can approach asymptotically the set point and preserve the PH representation by assigning a suitable damping injection.

The paper is organized as follows. Section 2 briefly review the tracking-error-based control via the usage of PH representation. In Section 3, the Hamiltonian view on the extents-based decoupled dynamics of a non-isothermal homogeneous reactor is represented. Also, the controller design method and its illustration for Van de Vusse reaction system modeled with the continuous stirred tank reactor (CSTR) are given in Section 4 and 5, respectively.

2. AN OVERVIEW OF THE TRACKING-ERROR-BASED CONTROL APPROACH

Consider here a dynamical system that is affine in terms of the control input $\boldsymbol{u}$ and its (nonlinear) dynamics can be represented as follows :

$$\dot{\boldsymbol{x}} = \mathrm{F}(\boldsymbol{x}) + \mathrm{G}(\boldsymbol{x})\boldsymbol{u}, \quad \boldsymbol{x}(t=0) = \boldsymbol{x}_0 \tag{1}$$

where $\boldsymbol{x} = \boldsymbol{x}(t)$ is the state vector in the operating region $\mathbb{D} \in \mathbb{R}^n$ and $\boldsymbol{u} \in \mathbb{R}^m$ expresses the control input. Additionally, $\mathrm{F}(\boldsymbol{x})$ and $\mathrm{G}(\boldsymbol{x})$ are smooth (nonlinear) functions with respect to the vector field $\boldsymbol{x}$. We assume that the dynamics (1) can be formulated in the PH representation with dissipation as follows :

$$\begin{cases} \dot{\boldsymbol{x}} = \Big[J(\boldsymbol{x}) - R(\boldsymbol{x})\Big]\dfrac{\partial \mathcal{H}(\boldsymbol{x})}{\partial \boldsymbol{x}} + \mathrm{G}(\boldsymbol{x})\boldsymbol{u} \\ \boldsymbol{y} = \mathrm{G}(\boldsymbol{x})^\top \dfrac{\partial \mathcal{H}(\boldsymbol{x})}{\partial \boldsymbol{x}} \end{cases} \tag{2}$$

where $\boldsymbol{y}$ is the output vector. Also, $J(\boldsymbol{x})$ and $R(\boldsymbol{x})$ are the $n \times n$ skew-symmetric interconnection matrix (i.e., $J(\boldsymbol{x}) = -J^\top(\boldsymbol{x})$) and the $n \times n$ symmetric and positive semi-definite damping matrix (i.e., $R(\boldsymbol{x}) = R^\top(\boldsymbol{x}) \geq 0$), respectively. The Hamiltonian $\mathcal{H}(\boldsymbol{x}) : \mathbb{R}^n \longrightarrow \mathbb{R}_+$ is the storage function of the system (Ortega and Romero, 2012).

Let $\boldsymbol{x}_d$ be a reference trajectory passing through a set-point and assume that the dynamics (1) can be written into the PH formulation with respect to an *a priori* quadratic storage function :

$$\mathcal{H}(\boldsymbol{x}) := \frac{1}{2}\boldsymbol{x}^\top R_{di}\boldsymbol{x} \tag{3}$$

where R_{di} is an arbitrary positive definite and symmetric (constant) matrix. Nguyen *et al.* (2019) proposed a certain structure for $\boldsymbol{x}_d$ by

$$\dot{\boldsymbol{x}}_d = \Big[J(\boldsymbol{x}) - R(\boldsymbol{x})\Big]\frac{\partial \mathcal{H}(\boldsymbol{x}_d)}{\partial \boldsymbol{x}_d} + R_I(\boldsymbol{x})\frac{\partial \mathbb{H}(\boldsymbol{e})}{\partial \boldsymbol{e}} + \mathrm{G}(\boldsymbol{x})\boldsymbol{u} \tag{4}$$

where $\boldsymbol{e} = \boldsymbol{x} - \boldsymbol{x}_d$ is the error state vector, $\mathbb{H}(\boldsymbol{e}) = \frac{1}{2}\boldsymbol{e}^\top R_{di}\boldsymbol{e}$ and $R_I(\boldsymbol{x})$ is a positive definite symmetric matrix (or the damping injection). With this, it allows to implement the tracking-error-based control approach by finding $R_I(\boldsymbol{x})$ in conjunction with a matrix constraint.

The PH formulation with a quadratic storage function of the nonlinear system (1) is needed prior to adopting tracking-error-based control approach. However, this challenging issue is not theoretically obvious as discussed in Nguyen *et al.* (2019). In this work, we shall show that this issue can be handled easily for a large class of nonlinear systems, namely homogeneous reaction systems, by a structural way on the basis of a transformed model that is based on the concept of extents as shown in next sections.

3. DECOUPLED DYNAMICS OF HOMOGENEOUS REACTORS USING VESSEL EXTENTS

Given a homogeneous reactor where R chemical transformations are occurring irreversibly among S species. This reactor is operated with p feed inlets and one outlet.

3.1 Mathematical model

The material balance for this reactor is expressed by a following set of ordinary differential equations (ODEs) :

$$\dot{\mathbf{n}} = \mathbf{N}^\top \mathbf{r}_v + \mathbf{W}_{in}\mathbf{u}_{in} - \frac{\mathrm{u}_{out}}{m}\mathbf{n} \tag{5}$$

where $\mathbf{n}$ is a S-dimensional vector of number of moles with the initial condition $\mathbf{n}(t=0) = \mathbf{n}_0$; $\mathbf{N}$ is the $R \times S$ stoichiometric matrix; $\mathbf{u}_{in}$ is a p-dimensional vector of mass flow rate; $\mathbf{W}_{in} = M_w^{-1}\varpi_{in}$ is a $S \times p$-inlet-composition matrix with M_w being a diagonal matrix of molecular weights and $\varpi_{in} = [\boldsymbol{\varpi}_{in,1}, \boldsymbol{\varpi}_{in,2}, \ldots, \boldsymbol{\varpi}_{in,p}]$ with $\boldsymbol{\varpi}_{in,j}$ the weight fraction vector of the j^{th} inlet; u_{out} is outlet flow; m is the mass of the mixture; and $\mathbf{r}_v$ is a R-dimensional vector of the reaction rates. Note that $\dfrac{\mathrm{u}_{out}}{m}$ corresponds to the inverse of the reactor residence time.

Together with the material balance (5), the heat balance can be written as follows (Rodrigues *et al.*, 2015) :

$$\dot{Q} = \left(-\Delta\mathbf{H}_{ref}\right)^\top \mathbf{r}_v + q_{ex} + \check{\mathbf{T}}_{in}^\top \mathbf{u}_{in} - \frac{\mathrm{u}_{out}}{m}Q \tag{6}$$

where $Q = mC_p(T - T_{ref})$ expresses the heat of the mixture with C_p and T being the mass specific heat capacity and the reactor temperature, respectively; $\Delta\mathbf{H}_{ref}$ is a R-dimensional vector of the reaction enthalpies at some reference temperature T_{ref}; q_{ex} is the rate of heat exchanged between the jacket and the mixture; and $\check{\mathbf{T}}_{in} = \big[\check{T}_{in,1}, \ldots, \check{T}_{in,p}\big]$. Also, $\check{T}_{in,j}$ is the constant specific heat of j^{th} inlet stream and is equal to $C_{p,in,j}(T_{in,j} - T_{ref})$ with $C_{p,in,j}$ and $T_{in,j}$ being the mass specific heat capacity and the temperature of the corresponding inlet, respectively.

3.2 Hamiltonian view on the decoupled model

Rodrigues *et al.* (2015) proposed a linear transformation to decompose the material balance (5) into four different parts, including the R-dimensional vector of vessel extents of reaction $\mathbf{x}_r(t)$, the p-dimensional vector of vessel extents of inlet flows $\mathbf{x}_{in}(t)$, the vessel extent of initial conditions $\mathrm{x}_{ic}(t)$ being a scalar and the orthogonal remaining part $\mathbf{x}_{iv}(t)$ with the dimension $q = S - R - p - 1 \geq 0$, so-called the invariants. This full-rank linear transformation is expressed as follows :

$$\left[\mathbf{x}_r \ \mathbf{x}_{in} \ \mathrm{x}_{ic} \ \mathbf{x}_{iv}\right]^\top = \mathcal{T}\mathbf{n} := \left[\mathbf{N}^\top \ \mathbf{W}_{in} \ \mathbf{n}_0 \ \mathbf{P}\right]^{-1}\mathbf{n} \tag{7}$$

where $\mathbf{P}$ is the null space of matrix $\begin{bmatrix}\mathbf{N}^\top & \mathbf{W}_{in} & \mathbf{n}_0\end{bmatrix}^\top$ with the dimension of p, i.e., $\begin{bmatrix}\mathbf{N}^\top & \mathbf{W}_{in} & \mathbf{n}_0\end{bmatrix}^\top \mathbf{P} = \mathbf{0}_{(R+p+1)\times q}$.

An alternative mathematical model of (5) is then obtained (Rodrigues *et al.*, 2015; Hoang *et al.*, 2020) :

$$\dot{\mathbf{x}}_r = \mathbf{r}_v - \theta \mathbf{x}_r, \qquad \mathbf{x}_r(t=0) = 0 \tag{8}$$

$$\dot{\mathbf{x}}_{in} = \mathbf{u}_{in} - \theta \mathbf{x}_{in}, \qquad \mathbf{x}_{in}(t=0) = 0 \tag{9}$$

$$\dot{\mathrm{x}}_{ic} = -\theta \mathrm{x}_{ic}, \qquad \mathrm{x}_{ic}(t=0) = 1 \tag{10}$$

$$\mathbf{x}_{iv} = \mathbf{0}_q \tag{11}$$

where θ is computed by $\frac{\mathrm{u}_{out}}{m}$. In this work, the above decoupled dynamics is completed with the inclusion of the heat balance, given by (6), to describe the reactor dynamics.

It can be clearly seen from (11) and (10) that $\mathbf{x}_{iv}$ is always zero and the dynamics of x_{ic} will be exponentially stable at origin if θ is bounded or a persistently exciting signal; therefore, the considered dynamics can be stabilized at the desired steady state if the convergence of the vector field $[\mathbf{x}_r^\top, \mathbf{x}_{in}^\top, Q]^\top$ towards its desired equilibrium point $[\mathbf{x}_r^{*\top}, \mathbf{x}_{in}^{*\top}, Q^*]^\top$ is guaranteed. Indeed, this extended model can be viewed as a perturbed PH formulation without the interconnection matrix [2], where the vector of the reaction rates $\mathbf{r}_v$ is a time-varying and matched/unmatched disturbance, as follows :

$$\begin{bmatrix}\dot{\mathbf{x}}_r \\ \dot{\mathbf{x}}_{in} \\ \dot{Q}\end{bmatrix} = -\begin{bmatrix}\theta\mathbf{I}_R & \mathbf{0} & 0 \\ \mathbf{0} & \theta\mathbf{I}_p & 0 \\ \mathbf{0} & \mathbf{0} & \theta\end{bmatrix}\begin{bmatrix}\mathbf{x}_r \\ \mathbf{x}_{in} \\ Q\end{bmatrix} + \begin{bmatrix}\mathbf{0} & 0 \\ \mathbf{I}_p & \mathbf{0} \\ \check{\mathbf{T}}_{in}^\top & 1\end{bmatrix}\begin{bmatrix}\mathbf{u}_{in} \\ q_{ex}\end{bmatrix} + \begin{bmatrix}\mathbf{I}_R \\ \mathbf{0}_p \\ -\Delta\mathbf{H}_{ref}^\top\end{bmatrix}\mathbf{r}_v \tag{12}$$

where $\mathbf{I}$ and $\mathbf{0}$ are the identity and zero matrices, respectively. Note that Eq. (12) holds for general non-isothermal homogeneous reactors, described by (5) and (6).

Noting from Eq.(8) that the steady state of $\mathbf{x}_r^*$ is given by

$$\mathbf{x}_r^* = \frac{\mathbf{r}_v^*}{\theta^*} \tag{13}$$

where $\mathbf{r}_v^*$ and θ^* are the steady-state reaction kinetics and outlet stream, respectively.

Control Objective: We aim to derive a control strategy to stabilize the system (12) at the desired equilibrium point $[\mathbf{x}_r^{*\top}, \mathbf{x}_{in}^{*\top}, Q^*]^\top$ with $\boldsymbol{u} = [\mathbf{u}_{in}^\top, q_{ex}]^\top$ as control inputs by adopting the tracking-error-based approach together with handling the disturbance, caused by $\mathbf{r}_v$.

4. MAIN RESULTS

From Eq. (12), we re-express the perturbed PH system with the output [3]

$$\begin{cases}\begin{bmatrix}\dot{\boldsymbol{x}}_1 \\ \dot{\boldsymbol{x}}_2\end{bmatrix} = -\begin{bmatrix}R_1 & \mathbf{0} \\ \mathbf{0} & R_2\end{bmatrix}\dfrac{\partial \mathrm{H}(\boldsymbol{x})}{\partial \boldsymbol{x}} + \begin{bmatrix}\boldsymbol{d}_1(\boldsymbol{x}) \\ \boldsymbol{d}_2(\boldsymbol{x}) + \mathrm{g}(\boldsymbol{x})\boldsymbol{u}\end{bmatrix} \\ \boldsymbol{y} = \left[\mathrm{x}_{in,1} + \check{T}_{in,1}Q, \ldots, \mathrm{x}_{in,p} + \check{T}_{in,p}Q, Q\right]^\top\end{cases} \tag{14}$$

where $\boldsymbol{x}$ is partitioned with two different parts as $[\boldsymbol{x}_1^\top, \boldsymbol{x}_2^\top]^\top$ where $\boldsymbol{x}_1 = \mathbf{x}_r$ and $\boldsymbol{x}_2 = \left[\mathbf{x}_{in}^\top, Q\right]^\top$ with $n = R + p + 1$ and $m = p + 1$; $\boldsymbol{u} \triangleq \boldsymbol{v} + \boldsymbol{w}$, is the input variable, where $\boldsymbol{w}$ is used for the reference tracking and $\boldsymbol{v}$ is used for the disturbance compensation; $R_1 = \theta\mathbf{I}_R$ and $R_2 = \theta\mathbf{I}_{p+1}$ are symmetric and positive definite matrices. $\boldsymbol{d}_1(\boldsymbol{x})$ and $\boldsymbol{d}_2(\boldsymbol{x})$ describe the time-varying unmatched and matched disturbances, respectively and the storage energy function $\mathrm{H}(\boldsymbol{x})$ is of a quadratic form, i.e.

$$\mathrm{H}(\boldsymbol{x}) := \frac{1}{2}\boldsymbol{x}^\top\boldsymbol{x} \tag{15}$$

It is important to note that $\mathrm{g}(\boldsymbol{x})$ in (14) is invertible. To solve the control problem, the structures of $\boldsymbol{d}_1(\boldsymbol{x})$ and $\boldsymbol{d}_2(\boldsymbol{x})$ will be specified by the following two assumptions :

Assumption 1. The unmatched disturbance $\boldsymbol{d}_1(\boldsymbol{x})$ can be factorized in the following form :

$$\boldsymbol{d}_1(\boldsymbol{x}) = F_d(\boldsymbol{x})\bar{\boldsymbol{d}}_1 \tag{16}$$

where $F_d(\boldsymbol{x}) = \mathrm{diag}[F_{1d}(\boldsymbol{x}), F_{2d}(\boldsymbol{x}), \ldots, F_{Rd}(\boldsymbol{x})]$ is a $R\times R$ positive definite diagonal matrix and $\bar{\boldsymbol{d}}_1$ is the constant R-dimensional column vector.

Assumption 2. The matched disturbance $\boldsymbol{d}_2(\boldsymbol{x})$ can be factorized in the following form :

$$\boldsymbol{d}_2(\boldsymbol{x}) = G_d(\boldsymbol{x})\bar{\boldsymbol{d}}_2 \tag{17}$$

where $G_d(\boldsymbol{x})$ is an arbitrary $m \times m$ matrix and $\bar{\boldsymbol{d}}_2$ is the constant m-dimensional column vector.

For the sake of clarity, we let $\boldsymbol{x^*} \triangleq [\boldsymbol{x}_1^{*\top}, \boldsymbol{x}_2^{*\top}]^\top$ denote the desired equilibrium point of the perturbed PH system (14). Propositions 1–3 below show that the system trajectory $\boldsymbol{x}_2$ will track the desired dynamic reference trajectory $\boldsymbol{x}_{2d}$ where the dynamics of $\boldsymbol{x}_{2d}$ is assigned to pass through $\boldsymbol{x}_2^*$ while $\boldsymbol{x}_1$ follows up $\boldsymbol{x}_1^*$ as time goes to infinity.

4.1 Tracking error controller plus a feed-forward law

The following proposition proposes the use of a feed-forward law for the matched disturbance rejection $\boldsymbol{d}_2(\boldsymbol{x})$ while the effect of $\boldsymbol{d}_1(\boldsymbol{x})$ is compensated by assigning a certain damping injection of reference trajectory.

Proposition 1. Let us assume that the reference trajectory $\boldsymbol{x}_d = [\boldsymbol{x}_{1d}, \boldsymbol{x}_{2d}]^\top$ is governed by

$$\begin{bmatrix}\dot{\boldsymbol{x}}_{1d} \\ \dot{\boldsymbol{x}}_{2d}\end{bmatrix} = -\begin{bmatrix}R_1 & \mathbf{0} \\ \mathbf{0} & R_2\end{bmatrix}\frac{\partial \mathrm{H}(\boldsymbol{x}_d)}{\partial \boldsymbol{x}_d} + \begin{bmatrix}R_{I1} & \mathbf{0} \\ \mathbf{0} & R_{I2}\end{bmatrix}\frac{\partial \mathbb{H}(\boldsymbol{e})}{\partial \boldsymbol{e}} + \begin{bmatrix}\mathbf{0} \\ \mathrm{g}(\boldsymbol{x})\boldsymbol{w}\end{bmatrix} \tag{18}$$

where $\boldsymbol{e} = [\boldsymbol{e}_1, \boldsymbol{e}_2]^\top = \boldsymbol{x} - \boldsymbol{x}_d$ is the error state vector, $\mathbb{H}(\boldsymbol{e})$ is defined by $\mathbb{H}(\boldsymbol{e}) = \frac{1}{2}\boldsymbol{e}^\top\boldsymbol{e}$, $R_{I1} = \mathrm{diag}(R_{I1,1}, \ldots, R_{I1,R})$ and $R_{I2} = \mathrm{diag}(R_{I2,1}, \ldots, R_{I2,p+1})$ are symmetric matrices. If the feed-forward law $\boldsymbol{v}$ for the matched disturbance rejection is computed as follows

$$\boldsymbol{v} = -\mathrm{g}(\boldsymbol{x})^{-1}\boldsymbol{d}_2(\boldsymbol{x}) \tag{19}$$

then the system trajectory $\boldsymbol{x}_2$ will converge asymptotically towards the reference trajectory $\boldsymbol{x}_{2d}$ while the difference between $\boldsymbol{x}_1$ and $\boldsymbol{x}_{1d}$ will approach $\bar{\boldsymbol{d}}_1$ as the equilibrium point asymptotically if the damping injections R_{I1} and R_{I2} are appropriately assigned such that :

$$R_1 + R_{I1} = F_d(\boldsymbol{x}) \succ 0 \tag{20}$$

$$\Big(R_2 + R_{I2}\Big) = \Big(R_2 + R_{I2}\Big)^\top \succ 0 \tag{21}$$

Proof. From (15), it is straightforward to show that :

$$\left[\frac{\partial \mathrm{H}(\boldsymbol{x})}{\partial \boldsymbol{x}} - \frac{\partial \mathrm{H}(\boldsymbol{x}_d)}{\partial \boldsymbol{x}_d}\right] = \frac{\partial \mathbb{H}(\boldsymbol{e})}{\partial \boldsymbol{e}} := \boldsymbol{e} \tag{22}$$

[2] From a physics-based viewpoint, this feature is obvious because the various rate processes are decoupled.

[3] The output $\boldsymbol{y}$ is strongly related to the temperature, therefore, it can be easily measured as long as the extents of the p inlet streams and the component mole heat capacities together with the molar numbers of all species are available (Hoang *et al.*, 2020).

By subtracting (18) from (14) and applying (22), the dynamics of the error state vector $\boldsymbol{e}$ is achieved as follows :

$$\dot{\boldsymbol{e}} = -\begin{bmatrix} R_1 + R_{I1} & \mathbf{0} \\ \mathbf{0} & R_2 + R_{I2} \end{bmatrix} \frac{\partial \mathbb{H}(\boldsymbol{e})}{\partial \boldsymbol{e}} + \begin{bmatrix} \boldsymbol{d}_1(\boldsymbol{x}) \\ \boldsymbol{d}_2(\boldsymbol{x}) \end{bmatrix} + \begin{bmatrix} \mathbf{0} \\ \mathrm{g}(\boldsymbol{x})\boldsymbol{v} \end{bmatrix} \quad (23)$$

Then, by substituting the feed-forward law $\boldsymbol{v}$ (19) for (23), the disturbance $\boldsymbol{d}_2(x)$ is canceled and the dynamics of (23) becomes :

$$\dot{\boldsymbol{e}} = -\begin{bmatrix} R_1 + R_{I1} & \mathbf{0} \\ \mathbf{0} & R_2 + R_{I2} \end{bmatrix} \frac{\partial \mathbb{H}(\boldsymbol{e})}{\partial \boldsymbol{e}} + \begin{bmatrix} F_d(\boldsymbol{x}) \\ \mathbf{0} \end{bmatrix} \bar{\boldsymbol{d}}_1 \quad (24)$$

Let us define $\boldsymbol{e}_{1d} = \boldsymbol{e}_1 - \bar{\boldsymbol{d}}_1$.
As the matrix $F_d(\boldsymbol{x})$ is a positive definite and diagonal matrix, thereby existing a matrix R_{I1} such that the condition (20) is met, then (24) becomes :

$$\begin{bmatrix} \dot{\boldsymbol{e}}_{1d} \\ \dot{\boldsymbol{e}}_2 \end{bmatrix} = -\begin{bmatrix} R_1 + R_{I1} & \mathbf{0} \\ \mathbf{0} & R_2 + R_{I2} \end{bmatrix} \begin{bmatrix} \boldsymbol{e}_{1d} \\ \boldsymbol{e}_2 \end{bmatrix} \quad (25)$$

By applying the conditions (20) and (21), the dynamics of (25) preserves the PH representation with the following storage function :

$$\Psi(\boldsymbol{e}_{1d}, \boldsymbol{e}_2) = \frac{1}{2}\boldsymbol{e}_{1d}^\top \boldsymbol{e}_{1d} + \frac{1}{2}\boldsymbol{e}_2^\top \boldsymbol{e}_2 > 0 \quad (26)$$

Moreover, the time derivative of Ψ is obtained as follows :

$$\dot{\Psi} = -\left[\frac{\partial \Psi}{\partial \boldsymbol{e}_{1d}}\right]^\top [R_1 + R_{I1}] \left[\frac{\partial \Psi}{\partial \boldsymbol{e}_{1d}}\right] - \left[\frac{\partial \Psi}{\partial \boldsymbol{e}_2}\right]^\top [R_2 + R_{I2}] \frac{\partial \Psi}{\partial \boldsymbol{e}_2} < 0 \quad (27)$$

The last inequality is satisfied due to (20) and (21). Moreover, because $\Psi(\boldsymbol{e}_{1d}, \boldsymbol{e}_2)$ is bounded below by the origin, it can be used as a Lyapunov function candidate according to LaSalle's theorem (Khalil, 2002). Consequently, the trajectories of dynamics (25) converge asymptotically to the equilibrium point $(\boldsymbol{e}_{1d}^*, \boldsymbol{e}_2^*) = (\mathbf{0}, \mathbf{0})$, implying that

$$\lim_{t\to\infty} \boldsymbol{x}_2 = \lim_{t\to\infty} \boldsymbol{x}_{2d} \quad (28)$$

$$\lim_{t\to\infty} \boldsymbol{x}_1 = \lim_{t\to\infty} \boldsymbol{x}_{1d} + \bar{\boldsymbol{d}}_1 \quad (29)$$

The latter concludes the proof. □

4.2 Tracking error controller plus a dynamic feedback law

Together with the feed-forward law (19), the impact of $\boldsymbol{d}_2(\boldsymbol{x})$ is also compensated by a dynamic feedback law, given by the following proposition.

Proposition 2. Consider the perturbed PH system (14) and the reference trajectory $\boldsymbol{x}_d$ (18) under the dynamic feedback law $\boldsymbol{v}$, written in the following form :

$$\begin{cases} \dot{\boldsymbol{\eta}} = G_d^\top(\boldsymbol{x}) \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2} - K_D(\boldsymbol{\eta} - \bar{\boldsymbol{d}}_2) \\ \boldsymbol{v} = -\mathrm{g}(\boldsymbol{x})^{-1} G_d(\boldsymbol{x}) \boldsymbol{\eta} \end{cases} \quad (30)$$

where $\boldsymbol{\eta} \in \mathbb{R}^m$, $m = p+1$, is the state vector, $K_D \in \mathbb{R}^{m\times m}$ is a positive definite (constant) matrix for tuning control parameters, $\boldsymbol{d}_2(\boldsymbol{x})$ meets Assumption 2 and the function $\mathcal{H}_{cl}(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta}) : \mathbb{R}^R \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}_+$ is defined by :

$$\mathcal{H}_{cl}(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta}) = \Psi(\boldsymbol{e}_{1d}, \boldsymbol{e}_2) + \frac{1}{2}\boldsymbol{\eta}^\top \boldsymbol{\eta} \quad (31)$$

with $\boldsymbol{e}_{1d} = \boldsymbol{x}_1 - \boldsymbol{x}_{1d} - \bar{\boldsymbol{d}}_1$, $\boldsymbol{e}_2 = \boldsymbol{x}_2 - \boldsymbol{x}_{2d}$ and $\Psi(\boldsymbol{e}_{1d}, \boldsymbol{e}_2)$, given in (26). Then the extended dynamics of closed-loop system, described by $\boldsymbol{e}_{1d}, \boldsymbol{e}_2$ and $\boldsymbol{\eta}$, will have an equilibrium point at $(\boldsymbol{e}_{1d}^*, \boldsymbol{e}_2^*, \boldsymbol{\eta}^*) = (\mathbf{0}, \mathbf{0}, \bar{\boldsymbol{d}}_2)$. In other words, the system trajectory $\boldsymbol{x}_2$ will converge asymptotically towards the reference profile $\boldsymbol{x}_{2d}$ while the discrepancies between $\boldsymbol{x}_1$ and $\boldsymbol{x}_{1d}$ will approach $\bar{\boldsymbol{d}}_1$ as the equilibrium point asymptotically if the conditions (20) and (21) are met.

Proof. Because the structure of $\boldsymbol{x}_d$ (18) is unchanged, the dynamics of error state vector $\boldsymbol{e}$ will be similar to (23). Consequently, this dynamics under the regulation of (30) and the condition (20) is rendered as :

$$\begin{bmatrix} \dot{\boldsymbol{e}}_{1d} \\ \dot{\boldsymbol{e}}_2 \\ \dot{\boldsymbol{\eta}} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \boldsymbol{d}_2(\boldsymbol{x}) \\ K_D \bar{\boldsymbol{d}}_2 \end{bmatrix} + \left\{ \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -G_d(\boldsymbol{x}) \\ \mathbf{0} & G_D^\top(\boldsymbol{x}) & \mathbf{0} \end{bmatrix} - \begin{bmatrix} R_1 + R_{I1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & R_2 + R_{I2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & K_D \end{bmatrix} \right\} \begin{bmatrix} \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_{1d}} \\ \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2} \\ \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{\eta}} \end{bmatrix} \quad (32)$$

Let the right-hand side of (32) equalize to zero, we obtain :

$$\begin{bmatrix} -(R_1 + R_{I1}) \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_{1d}} \\ -(R_2 + R_{I2}) \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2} - G_d(\boldsymbol{x}) \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{\eta}} + \boldsymbol{d}_2(\boldsymbol{x}) \\ G_d(\boldsymbol{x})^\top \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2} - K_D \dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{\eta}} + K_D \bar{\boldsymbol{d}}_2 \end{bmatrix} = \mathbf{0} \quad (33)$$

It can be clearly seen that the first identity is met because of $\left.\dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_{1d}}\right|_{\boldsymbol{e}_{1d}=\mathbf{0}} = \mathbf{0}_R$ while the second and third identities are satisfied provided that $\boldsymbol{\eta} = \bar{\boldsymbol{d}}_2$ and $\left.\dfrac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2}\right|_{\boldsymbol{e}_{2d}=\mathbf{0}} = \mathbf{0}_{p+1}$ thanks to Assumption 2. As a result, $(\boldsymbol{e}_{1d}^*, \boldsymbol{e}_2^*, \boldsymbol{\eta}^*) = (\mathbf{0}, \mathbf{0}, \bar{\boldsymbol{d}}_2)$ is an equilibrium point of (32).

Next, we define a Lyapunov function $\Omega(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta})$ for the stability analysis of closed-loop system (32) as follows :

$$\Omega(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta}) = \mathcal{H}_{cl}(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta}) - \left.\left(\frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{\eta}}\right)^\top\right|_{\boldsymbol{\eta}^*} (\boldsymbol{\eta} - \boldsymbol{\eta}^*) - \mathcal{H}_{cl}(\boldsymbol{e}_{1d}^*, \boldsymbol{e}_2^*, \boldsymbol{\eta}^*) > 0 \quad (34)$$

where $\mathcal{H}_{cl}(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta})$ is given in (31).

Admittedly, the quadratic function $\mathcal{H}_{cl}$ has an isolated minimum at $(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta}) = (\mathbf{0}, \mathbf{0}, \mathbf{0})$; hence, it is indeed a strictly convex function. As a result, $\Omega(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta})$ (34) is also bounded from below by origin (Jayawardhana *et al.*, 2007). On the other hand, the time derivative of $\Omega(\boldsymbol{e}_{1d}, \boldsymbol{e}_2, \boldsymbol{\eta})$ is obtained as follows :

$$\begin{aligned} \dot{\Omega} = &-\left(\frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_{1d}}\right)^\top (R_1 + R_{I1}) \frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_{1d}} - \left(\frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2}\right)^\top (R_2 + R_{I2}) \frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2} \\ &+ \left(\frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2}\right)^\top [\boldsymbol{d}_2(\boldsymbol{x}) + \mathrm{g}(\boldsymbol{x})\boldsymbol{v}] + \left(\boldsymbol{\eta}^\top - \bar{\boldsymbol{d}}_2^\top\right) G_d^\top(\boldsymbol{x}) \frac{\partial \mathcal{H}_{cl}}{\partial \boldsymbol{e}_2} \\ &- \left(\boldsymbol{\eta}^\top - \bar{\boldsymbol{d}}_2^\top\right) K_D (\boldsymbol{\eta} - \bar{\boldsymbol{d}}_2) \end{aligned} \quad (35)$$

By applying the condition (21) and the feedback law $\boldsymbol{v}$ (30) for (35), we obtain

$$\dot{\Omega} < -\left(\boldsymbol{\eta} - \bar{\boldsymbol{d}}_2\right)^\top K_D \left(\boldsymbol{\eta} - \bar{\boldsymbol{d}}_2\right) < 0 \quad (36)$$

The last inequality is satisfied due to the positive definite condition of K_D. Consequently, La Salle's invariance principle is invoked to guarantee the globally asymptotic stabilization of the error system (23) at the desired equilibrium point under the control of the dynamic feedback (30) (Khalil, 2002). The latter concludes the proof. □

The asymptotic stabilization of the system trajectory $\boldsymbol{x}_1$ to $\boldsymbol{x}_1^*$ is not explicitly shown in Propositions 1 and 2, thus this issue will be addressed by the following proposition.

Proposition 3. The convergence of $\boldsymbol{x}_1$ towards $\boldsymbol{x}_1^*$ is guaranteed and independent of the factorization of $\boldsymbol{d}_1(x)$ of Assumption 1 if and only if

$$\boldsymbol{x}_1^* \equiv \boldsymbol{x}_{1d}^* + \bar{\boldsymbol{d}}_1 \tag{37}$$

where $\boldsymbol{x}_{1d}^*$ is the equilibrium point of $\boldsymbol{x}_{1d}$ given by (18).

Proof. First of all, it can be verified that the equilibrium point $\boldsymbol{x}_1^*$ of the perturbed PH system (14) fulfills

$$\boldsymbol{x}_1^* = R_1^{*-1}\boldsymbol{d}_1^* \tag{38}$$

On the other hand, it can be shown from (18) that $\boldsymbol{x}_{1d}^*$ is given by

$$\boldsymbol{x}_{1d}^* = R_1^{*-1}R_{I1}^*\bar{\boldsymbol{d}}_1 \tag{39}$$

where R_1^* and R_{I1}^* are the matrices corresponding to R_1 and R_{I1} calculated at the desried equilibrium point $\boldsymbol{x}^*$. From this, one derives:

$$\boldsymbol{x}_{1d}^* + \bar{\boldsymbol{d}}_1 = R_1^{*-1}\left(R_1^* + R_{I1}^*\right)\bar{\boldsymbol{d}}_1 \tag{40}$$

Because the matrix R_{I1} is chosen to fulfill the condition (20) at all the time, Eq. (40) therefore becomes:

$$\boldsymbol{x}_{1d}^* + \bar{\boldsymbol{d}}_1 = R_1^{*-1}F_d^*\bar{\boldsymbol{d}}_1 = R_1^{*-1}\boldsymbol{d}_1^* \tag{41}$$

Eq. (37) immediately follows thanks to Eqs. (38) and (41). Furthermore, note that it is possible to do so only if Eq. (37) is valid, that is, the only-if condition holds. □

Remark 1. Two proposed control configurations in Proposition 1 and 2 share the same method to compensate the effect of unmatched disturbance $\boldsymbol{d}_1(\boldsymbol{x})$, i.e. by assigning a certain structure for R_{I1} to meet the condition (20), but while the effect of $\boldsymbol{d}_2(\boldsymbol{x})$ is cancelled directly by the feed forward law $\boldsymbol{v}$ (19) in the first configuration, the second one rejects gradually its effect via the dynamics of $\boldsymbol{\eta}$ (30).

5. ILLUSTRATIVE EXAMPLE

5.1 The decoupled dynamics via the extent transformation

We consider the synthesis of cyclopentenol from cyclopendaiene by sulfuric acid-catalyzed addition of water in a CSTR. The following stoichiometry is expressed for $R = 3$ reactions and $S = 6$ components, including 5 active species and sulfuric acid as a catalyst (Hoang *et al.*, 2013) :

$$C_5H_6(A) \xrightarrow[+H_2O(E)]{k_1} C_5H_7O(B) \xrightarrow[+H_2O(E)]{k_2} C_5H_8(OH)_2(C)$$

$$2C_5H_6(A) \xrightarrow{k_3} C_{10}H_{12}(D)$$

where the catalyst (H_2SO_4) is denoted by F. Also, the stoichiometric matrix $\mathbf{N}$ is given as follows :

$$\mathbf{N} = \begin{bmatrix} -1 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 1 & 0 & -1 & 0 \\ -2 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \tag{42}$$

The CSTR is initially operated with two inlets, i.e. $\mathbf{u}_{in} = [\mathrm{u}_{in,1}, \mathrm{u}_{in,2}]^\top$, where $\mathrm{u}_{in,1}$ and $\mathrm{u}_{in,2}$ are 12000 and 24000 (g/h), respectively, and one outlet with the assumption that $\mathrm{u}_{in,1} + \mathrm{u}_{in,2} = \mathrm{u}_{out} = const.$ Additionally, $\mathbf{W}_{in}$ is chosen as

$$\mathbf{W}_{in}^\top = \begin{bmatrix} \frac{0.3}{66} & 0 & 0 & 0 & \frac{0.7}{18} & 0 \\ 0 & 0 & 0 & 0 & \frac{0.925}{18} & \frac{0.075}{98} \end{bmatrix} \text{(mol/g)} \tag{43}$$

Other physical parameters and operating conditions can be found in (Hoang *et al.*, 2013). Then, we can calculate $\check{\mathbf{T}}_{in} = [364.34, 419.60]^\top$ (J/g).

5.2 Controller design

To apply Propositions 1 and 2 for control design, the reference trajectory $\boldsymbol{x}_d$ is derived as follows :

$$\dot{\boldsymbol{x}}_d = -\begin{bmatrix} \theta\mathbf{I}_3 & 0 \\ \mathbf{0} & \theta\mathbf{I}_3 \end{bmatrix}\boldsymbol{x}_d + \begin{bmatrix} R_{I1} & \mathbf{0} \\ \mathbf{0} & R_{I2} \end{bmatrix}\begin{bmatrix} \boldsymbol{e}_1 \\ \boldsymbol{e}_2 \end{bmatrix} + \begin{bmatrix} \mathbf{0} \\ \mathrm{g}(\boldsymbol{x}) \end{bmatrix}\boldsymbol{w} \tag{44}$$

where $R_{I2} = \mathrm{diag}(R_{I2,1}, R_{I2,2}, R_{I2,3})$, $\mathrm{g}(\boldsymbol{x}) = \begin{bmatrix} \mathbf{I}_2 & \mathbf{0} \\ \check{\mathbf{T}}_{in}^\top & 1 \end{bmatrix}$ and $\boldsymbol{w} = [w_{\mathrm{u}_{in,1}}, w_{\mathrm{u}_{in,2}}, w_{q_{ex}}]^\top$.

Then, the unmatched disturbance $\boldsymbol{d}_1(\boldsymbol{x}) = \mathbf{r}_v$ can be factorized in the following form to meet Assumption 1 :

$$\boldsymbol{d}_1(\boldsymbol{x}) = \mathbf{r}_v = \underbrace{\begin{bmatrix} \alpha_1 r_{v1} & 0 & 0 \\ 0 & \alpha_2 r_{v2} & 0 \\ 0 & 0 & \alpha_3 r_{v3} \end{bmatrix}}_{F_d(\boldsymbol{x})\succ 0} \underbrace{\begin{bmatrix} \frac{1}{\alpha_1} \\ \frac{1}{\alpha_2} \\ \frac{1}{\alpha_3} \end{bmatrix}}_{\bar{\boldsymbol{d}}_1} \tag{45}$$

where $\alpha_i, i = 1, 2, 3$ are positive tuning parameters. Then, the matrix R_{I1} is computed by :

$$R_{I1} = \begin{bmatrix} \alpha_1 r_{v1} - \theta & 0 & 0 \\ 0 & \alpha_2 r_{v2} - \theta & 0 \\ 0 & 0 & \alpha_3 r_{v3} - \theta \end{bmatrix} \tag{46}$$

that satisfies the condition (20). Moreover, the matched disturbance $\boldsymbol{d}_2(\boldsymbol{x})$ can be expressed in the following form to meet Assumption 2 :

$$\boldsymbol{d}_2(\boldsymbol{x}) = \begin{bmatrix} \mathbf{0} \\ \left(-\Delta\mathbf{H}_{ref}\right)^\top \mathbf{r}_v \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(-\Delta\mathbf{H}_{ref}\right)^\top \frac{\mathbf{r}_v}{k_{01}} \end{bmatrix}}_{G_d(\boldsymbol{x})} \underbrace{\begin{bmatrix} \mathbf{0} \\ k_{01} \end{bmatrix}}_{\bar{\boldsymbol{d}}_2} \tag{47}$$

where k_{01} is the kinetic constant of the first reaction. Note also that the derivations of $F_d(\boldsymbol{x})$ in (45) and $G_d(\boldsymbol{x})$ in (47) are not unique.

Next, the inverse of $\mathrm{g}(\boldsymbol{x})$ is derived as follows :

$$\mathrm{g}(\boldsymbol{x})^{-1} = \begin{bmatrix} \mathbf{I}_2 & \mathbf{0} \\ -\check{\mathbf{T}}_{in}^\top & 1 \end{bmatrix} \tag{48}$$

Thus, the feed-forward law $\boldsymbol{v} = [v_{\mathrm{u}_{in,1}}, v_{\mathrm{u}_{in,2}}, v_{q_{ex}}]^\top$ (19) is calculated by using (47) and (48) :

$$\boldsymbol{v} = -\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\check{T}_{in,1} & -\check{T}_{in,2} & 1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ \left(-\Delta\mathbf{H}_{ref}\right)^\top \mathbf{r}_v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \left(\Delta\mathbf{H}_{ref}\right)^\top \mathbf{r}_v \end{bmatrix} \tag{49}$$

On the other hand, the dynamic feedback law $\boldsymbol{v}$ (30) is obtained by using (47) and (48) :

$$\begin{cases} \dot{\boldsymbol{\eta}} = \begin{bmatrix} \dot{\eta}_{\mathrm{u}_{in,1}} \\ \dot{\eta}_{\mathrm{u}_{in,2}} \\ \dot{\eta}_{q_{ex}} \end{bmatrix} = \begin{bmatrix} -K_{D1}\eta_{\mathrm{u}_{in,1}} \\ -K_{D2}\eta_{\mathrm{u}_{in,2}} \\ (-\Delta\mathbf{H}_{ref})^\top \frac{\mathbf{r}_v}{k_{01}} e_Q - K_{D3}(\eta_{q_{ex}} - k_{01}) \end{bmatrix} \\ \boldsymbol{v} = \left[v_{\mathrm{u}_{in,1}}, v_{\mathrm{u}_{in,2}}, v_{q_{ex}}\right]^\top = \left[0, 0, (\Delta\mathbf{H}_{ref})^\top \frac{\mathbf{r}_v}{k_{01}}\eta_{q_{ex}}\right]^\top \end{cases} \tag{50}$$

where $e_Q = Q - Q_d$ and $K_{Di}, i = 1, 2, 3$ are components of the matrix K_D.

In what follows, for sake of simplicity, we will keep $\mathrm{u}_{in,2}$ as a constant and we will use $\mathrm{u}_{in,1}$ and q_{ex} as manipulated variables. Then, the dynamics of $\mathrm{x}_{ind,1}$ and Q_d are assigned as $\dot{\mathrm{x}}_{ind,1} = K_1(\mathrm{x}_{in,1}^* - \mathrm{x}_{ind,1})$ and $\dot{Q}_d = K_2(Q^* - Q_d)$, respectively, for reference tracking. Then, the tracking-error-based controller is achieved from (44) as follows :

$$w_{\mathrm{u}_{in,1}} = \frac{K_1(\mathrm{x}^*_{in,1} - \mathrm{x}_{ind,1}) + \frac{\mathrm{u}_{in,2}}{m}\mathrm{x}_{ind,1} - R_{I2,1}(\mathrm{x}_{in,1} - \mathrm{x}_{ind,1})}{1 - \frac{\mathrm{x}_{ind,1}}{m}} \quad (51)$$

$$w_{q_{ex}} = K_2(Q^* - Q_d) - R_{I2,3}\,(Q - Q_d) + \theta Q_d - \check{\mathbf{T}}_{in}^{\top}\mathbf{u}_{in} \quad (52)$$

The actual controllers: $\mathrm{u}_{in,1}$ and q_{ex} are then calculated by $\mathrm{u}_{in,1} = w_{u_{in,1}} + v_{\mathrm{u}_{in,1}}$ and $q_{ex} = w_{q_{ex}} + v_{q_{ex}}$. Noting that $v_{\mathrm{u}_{in,1}}$ and $v_{q_{ex}}$ are extracted from either (49) or (50).

5.3 Simulation results for the control system

The applicability of proposed control strategy to stabilize the vessel-extent-based decoupled dynamics is illustrated by simulations with two initial conditions: (IC_1) $[\mathbf{n}_0\ T_0]$ = [1.4 1.6 11 0.4242 447 5.102 410] and (IC_2) $[\mathbf{n}_0\ T_0]$ = [0.8 0.4 9 0.2697 470 5.102 300]. From considered operating conditions, given by Hoang *et al.* (2013), the optimal steady state is computed by $[\mathbf{n}^*\ T^*]$ = [6.60 3.35 3.48 0.87 461.91 5.102 367.34]. In practice, this state is chosen as a set point of control system, leading to x^*_{r1} = 6.83 mol, x^*_{r2} = 3.48 mol, x^*_{r3} = 0.87 mol, $\mathrm{x}^*_{in,1}$ = 3333 (g) and Q^* = 2838.9 (kJ/h). We select $\alpha_1 = \alpha_2 = 1$ and $\alpha_3 = 10$ in (46) while $K_1, K_2, R_{I2,1}$ and $R_{I2,3}$ in (51) and (52) are chosen as $K_1 = K_2 = 4.45$ and $R_{I2,1} = R_{I2,3} = 8$. Additionally, K_{D3} in (50) is chosen as 5. Fig. 1 shows that trajectories of decoupled

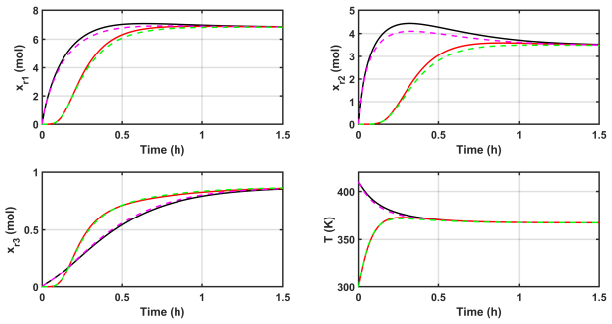

Fig. 1. Closed-loop trajectories of output (−: (IC_1) with the feed-forward law; −−: (IC_1) with the dynamic feedback law; −: (IC_2) with the feed-forward law and −−: (IC_2) with the dynamic feedback law).

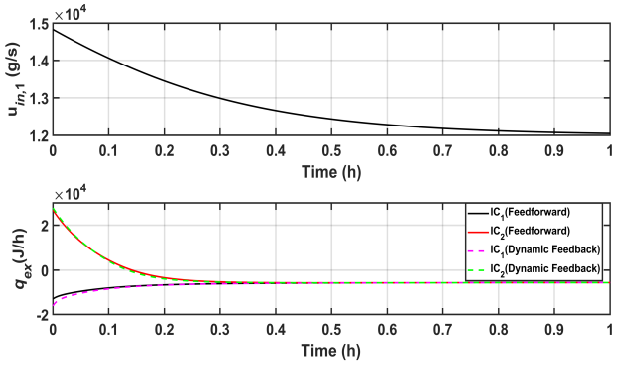

Fig. 2. Control input.

dynamics: $\mathrm{x}_{r1}, \mathrm{x}_{r2}, \mathrm{x}_{r3}$ and T, converge to the desired equilibrium point for both initial conditions by using either feed-forward law or dynamic feedback one for disturbance rejection. Furthermore, the representation of the control inputs, namely $\mathrm{u}_{in,1}$ and q_{ex} in Fig. 2, are physically admissible in terms of their dynamics and amplitudes. Finally, Fig. 3 presents the closed loop responses of the molar number of species A and B of the reaction system as expected.

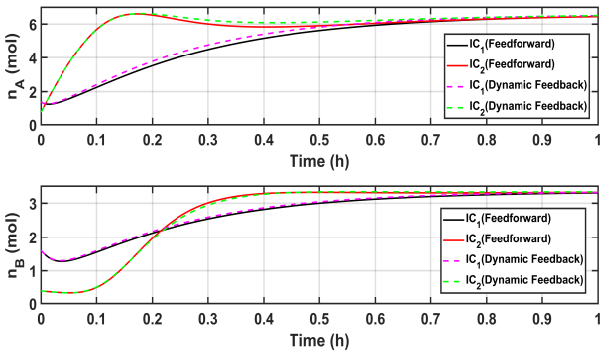

Fig. 3. The controlled variables of the reaction system.

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