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Tracking error plus damping injection control of non-minimum phase processes

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Abstract: This work proposes a passivity-based approach to deal with the output-tracking-error problem for a large class of nonlinear chemical processes including non-minimum phase systems. More precisely, in that framework, the system dynamics is firstly written into the relaxing (pseudo) port-Hamiltonian representation which does not necessarily require the positive semi-definite property of the damping matrix. Then, a reference trajectory associated with a certain structure passing through a desired equilibrium point (i.e., the set-point) is chosen so that the error dynamics can be globally asymptotically stabilized at the origin thanks to the assignment of an appropriate damping injection. This method is subsequently illustrated for a benchmark of multiple reactions systems, namely Van de Vusse reaction system. The numerical simulations show the applications of the proposed approach.

Keywords: Port-Hamiltonian framework, chemical process systems, non-minimum phase system, passivity, tracking error.

1. INTRODUCTION

The (nonlinear) dynamics of chemical process systems usually exhibits the abnormal behaviors (such as the input/output multiplicity or chaos and limit cycle, etc.) caused by the highly nonlinear characteristics of reaction kinetics, constitutive equations of transport phenomena and thermal effects (Melo *et al.* (2001); Favache and Dochain (2010); Aris (2013); Hoang *et al.* (2013a)). In fact, these behaviors give rise to the internal instability and restrict the systems themselves to reach their desirable performance if they are operated without the feedback laws (Åström (2000)). Hence, during the last few decades, numerous advanced control strategies have been proposed to tackle this theoretically difficult but interesting challenges. Generally speaking, the controllers are capable of canceling the intrinsic nonlinearities of the system and stabilizing it at a desired set-point. However, several issues related to the applicability of developed control methods for a wide range of nonlinear systems, especially the non-minimum phase ones, remain open (see e.g., feedback passivation (Byrnes *et al.* (1991); Sepulchre *et al.* (1997))). This is due to the fact that their unstable zero dynamics cannot be (asymptotically) stabilized by the traditional strategies such as the feedback linearization technique (Khalil (2002)).

Among the advanced control strategies applied to the control of non-minimum phase systems (such as model predictive control (MPC) (Panjapornpon *et al.* (2006)), the physics/energy-based strategy (Ydstie and Alonso (1997); Favache and Dochain (2010); Alvarez *et al.* (2011); Hoang *et al.* (2011a,b, 2013a,b)), the adaptive backstepping controller (Dochain (1992); Gopaluni *et al.* (2003)), the sliding mode control (Chen and Peng (2006)) and others (Niemiec and Kravaris (2003); Kravaris and Mousavere (2007))), the passivity-based approach (PBA) is recognized as a systematic and useful tool for control design and it can be used in different ways (see e.g., Ortega *et al.* (2002)). In addition, in (Sira-Ramírez and Angulo-Núnez (1997); Sira-Ramírez (1998)), the authors proposed another method which is the so-called feedback passivation design, for the single-input-single-output (SISO) or multi-input-multi-output (MIMO) systems. The proposed method was of great interest, yet for instance paid by considering the systems with (slightly) minimum phase behavior and/or the relative degree one only (Byrnes *et al.* (1991); Sepulchre *et al.* (1997)).

The main objective of this work is to extend the results proposed by (Sira-Ramírez and Angulo-Núnez (1997); Sira-Ramírez (1998); Nguyen *et al.* (2018)) to the control of a typical non-minimum phase system of chemical engineering, namely the Van de Vusse reaction system (Chen *et al.* (1995); Antonelli and Astolfi (2003); Ramírez *et al.* (2009); Kuntanapreeda and Marusak (2012)). The contributions of this paper are twofold :

- Firstly, to circumvent the feedback passivation obstacle that seems to be impossible due to non-minimum phase characteristics, the nonlinear dynamical system is directly formatted into a (pseudo) Port-Hamiltonian (PH) representation in a direct and understandable way. This resulting representation [1] is of ultimate importance, but paid possibly by losing some structural properties.

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[1] This belongs to the so-called relaxing pseudo PH models due to thermodynamically consistent features (Hoang *et al.* (2015)).

- Then, once the relaxing PH model of the system dynamics is derived, the (generalized) passivity plus tracking-error-based control strategy is applied to achieve the global asymptotic stabilization thanks to an appropriate damping injection.

This paper is organized as follow. Section 2 gives a brief overview of the PH representation of an affine nonlinear system. Section 3 is devoted to the generalizations of the passivity plus tracking-error-based controller. The illustrations of the proposed approach for the stabilization of the (non-minimum phase) Van de Vusse reaction system are given in section 4. The numerical simulations are carried out in section 5 to illustrate the theoretical developments.

2. THE PORT-HAMILTONIAN REPRESENTATION OF NONLINEAR SYSTEMS

Throughout the paper, the nonlinear dynamical system which is affine in the input u is considered as follows :

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

where $x = x(t)$ is the state vector in the operating region $\mathbb{D} \in \mathbb{R}^n$, $f(x) \in \mathbb{R}^n$ expresses the smooth (nonlinear) function with respect to the vector field x. The input-state map and the control input are represented by $g(x) \in \mathbb{R}^{n\times m}$ and $u \in \mathbb{R}^m$, respectively.

Assume that if the function $f(x)$ verifies the so-called separability condition (Dörfler *et al.* (2009); Ramírez *et al.* (2009); Favache *et al.* (2011); Hudon *et al.* (2015); Guay and Hudon (2016); Hoang *et al.* (2017)), that is, $f(x)$ can be decomposed and expressed as the product of some (interconnection and damping) structure matrices and the gradient of the generalized Hamiltonian storage function with respect to the state variables, i.e. :

$$f(x) = [J(x) - R(x)]\,\frac{\partial \mathbb{H}(x)}{\partial x} \tag{2}$$

where $J(x)$ and $R(x)$ are the $n \times n$ skew-symmetric interconnection matrix (i.e., $J(x) = -J^\top(x)$) and the $n\times n$ symmetric and positive semi-definite damping matrix (i.e. $R(x) = R^\top(x) \geq 0$), respectively while $\mathbb{H}(x) : \mathbb{R}^n \longrightarrow \mathbb{R}$ represents the storage function of the system, then the original dynamics described by (1) is said to be a PH representation (Van der Schaft (2000); Ortega *et al.* (2002)). Equation (1) is then rewritten as follows :

$$\begin{cases} \dot{x} = [J(x) - R(x)]\,\dfrac{\partial \mathbb{H}(x)}{\partial x} + g(x)u \\ y = g(x)^\top \dfrac{\partial \mathbb{H}}{\partial x} \end{cases} \tag{3}$$

where y is the output.

It can be clearly seen that the time derivative of the storage function $\mathbb{H}(x)$ satisfies the inequality below

$$\frac{d\mathbb{H}(x)}{dx} = -\left[\frac{\partial \mathbb{H}(x)}{\partial x}\right]^\top R(x)\frac{\partial \mathbb{H}(x)}{\partial x} + u^\top y \leq u^\top y \tag{4}$$

From a physical point of view, this implies that the total amount of energy supplied from external source is always greater than the increase in the energy stored in the system. Also, equality in (4) holds only if the damping matrix $R(x)$, that is strongly related to the dissipation term, is equal to 0. Hence, the PH system (3) is passive with input u and output y corresponding to the storage function $\mathbb{H}(x)$. We shall not elaborate any further on the PH representation here and refer the readers to (Ortega *et al.* (2002); Dörfler *et al.* (2009); Van der Schaft (2000); Hoang *et al.* (2017)) for more information.

Remark 1. The storage function $\mathbb{H}(x)$ is possibly equal to the total energy function for electromechanical systems or the generalized energy function for physicochemical systems (such as entropy production, etc. (Hoang *et al.* (2014); Hoang and Dochain (2016); Hoang *et al.* (2017))). Other choices with no physical significance for the storage function $\mathbb{H}(x)$ are also made (Sira-Ramírez (1998); Ramírez *et al.* (2009); Dörfler *et al.* (2009)).

For the cases of biochemical processes we are concerned with here, the formulation described by (3) refers to the so-called pseudo PH representation (i.e., the structure matrices depend not only on the state variables x but also the co-state variables $\frac{\partial \mathbb{H}(x)}{\partial x}$) (Hangos *et al.* (2001); Eberard *et al.* (2007); Dörfler *et al.* (2009); Ramírez *et al.* (2009); Favache *et al.* (2011); Hoang *et al.* (2011b); Ramírez *et al.* (2013); Hoang *et al.* (2017)). Furthermore, in some cases, the damping matrix R can also be relaxed (i.e., this does not necessarily require the positive semi-definiteness of damping matrix R) due to thermodynamically consistent properties of the system, the resulting representation is then called the relaxing pseudo PH models (Hoang *et al.* (2015)). Even if the structural properties are violated, such relaxing pseudo PH models can be considered further for the control design in the framework of the passivity plus tracking-error-based control. This is one of the main contributions of this paper.

3. A GENERALIZATION OF THE PASSIVITY PLUS TRACKING-ERROR-BASED CONTROLLER

Let x_d be the reference trajectory passing through the (desired) set-point. The following proposition proposes a dynamic structure for x_d that allows to implement the control design. The proposed developments generalize the results given in (Sira-Ramírez and Angulo-Núnez (1997); Sira-Ramírez (1998)).

Proposition 1. Assume that :

(i) there exists a relaxing PH model (3) of the nonlinear dynamical system (1) and the storage energy function $\mathbb{H}(x)$ is of a quadratic form, i.e.,

$$\mathbb{H}(x) := \frac{1}{2} x^\top R_{di} x \tag{5}$$

where R_{di} is an arbitrary positive definite symmetric (constant) matrix;

(ii) the reference trajectory x_d is governed by

$$\dot{x}_d = \Big[J(x) - R(x)\Big]\frac{\partial \mathbb{H}(x_d)}{\partial x_d} + R_I(x)\frac{\partial \mathbb{H}(e)}{\partial e} + g(x)u \tag{6}$$

where $e = x - x_d$ is the error state vector and $R_I(x)$ is a positive definite symmetric matrix.

Then, the system trajectory x globally asymptotically converges to the reference trajectory x_d if and only if the damping injection $R_I(x)$ is appropriately assigned so that the following condition holds :

$$\Big(R(x) + R_I(x)\Big) = \Big(R(x) + R_I(x)\Big)^\top > 0 \tag{7}$$

Proof. From (5), it is straightforward to show that :

$$\Big(\frac{\partial \mathbb{H}(x)}{\partial x} - \frac{\partial \mathbb{H}(x_d)}{\partial x_d}\Big) = \frac{\partial \mathbb{H}(e)}{\partial e} := R_{di} e \tag{8}$$

On the other hand, the time derivative of the storage function $\mathbb{H}(e)$ is expressed as follows :

$$\dot{\mathbb{H}}(e) = \left[\frac{\partial \mathbb{H}(e)}{\partial e}\right]^{\top} \dot{e} \tag{9}$$

with the error state vector dynamics described by[2] :

$$\dot{e} = \Big\{J(x) - [R(x) + R_I(x)]\Big\} \frac{\partial \mathbb{H}(e)}{\partial e} \tag{10}$$

where the first entry of (3), equations (6) and (8) have been used. As a consequence of (10), (9) becomes :

$$\begin{aligned}\dot{\mathbb{H}}(e) &= \left[\frac{\partial \mathbb{H}(e)}{\partial e}\right]^{\top} \Big\{J(x) - [R(x) + R_I(x)]\Big\} \frac{\partial \mathbb{H}(e)}{\partial e} \\ &= -\left[\frac{\partial \mathbb{H}(e)}{\partial e}\right]^{\top} [R(x) + R_I(x)] \frac{\partial \mathbb{H}(e)}{\partial e} < 0 \end{aligned} \tag{11}$$

Strict inequality (11) holds thanks to (7). Since $\mathbb{H}(e)$ is bounded from below by 0, the error dynamics can be stabilized globally at the origin by invoking La Salle's invariance principle (Khalil (2002)). The latter concludes the proof. ☐

Remark 2. The exponential convergence property of the system trajectory x towards the reference one x_d (i.e., $\lim_{t\to\infty} e = 0$) can be obtained only if $R(x) = R(x)^{\top} \geq 0$ (i.e., for non-relaxing PH systems). Indeed, by (8) and (11) one derives :

$$\dot{\mathbb{H}}(e) \leq -e^{\top} R_{di} R_I(x) R_{di} e \tag{12}$$

Hence,

$$\dot{\mathbb{H}}(e) \leq -2 \frac{\lambda_{\inf}}{\beta_{\sup}} \mathbb{H}(e) \tag{13}$$

where

$$\begin{cases} \lambda_{\inf} = \inf \Big(\mathrm{eig}\left(R_{di} R_I(x) R_{di}\right)\Big) > 0 \\ \beta_{\sup} = \sup \Big(\mathrm{eig}\left(R_{di}\right)\Big) > 0 \end{cases} \tag{14}$$

Remark 3. In order to derive the feedback laws for u ($\dim(u) = m$), only m components of x_d need to be chosen appropriately prior to assigning their desired trajectories (including the set-point) so that the corresponding $m \times m$ submatrix obtained from $g(x)$ is of full rank. In other words, this guarantees the solvability of the linear system (6) with the unknown u (i.e., the degree of freedom of (6) equals 0).

4. APPLICATION TO THE (NON-MINIMUM PHASE) VAN DE VUSSE REACTION SYSTEM

We consider the synthesis of cyclopentenol (main product) from cyclopentadiene (material) by sulfuric acid-catalyzed addition of water in a dilute solution taking place in a continuous stirred tank reactor (Luyben (1990)). The stoichiometric equations are given as follows (Ramírez *et al.* (2009); Hoang *et al.* (2013a)) :

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

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

4.1 The mathematical model

Based on the material and energy balance equations, the (reduced-order) mathematical model of Van de Vusse reaction system described by a set of ODEs is written as follows (Ramírez *et al.* (2009); Hoang *et al.* (2013b)) :

$$\begin{cases} \dot{x}_1 = -k_1 x_1 - 2k_3 x_1^2 + (x_{10} - x_1)\, u_1 \\ \dot{x}_2 = k_1 x_1 - k_2 x_2 - x_2 u_1 \\ \dot{x}_3 = \dfrac{-\Delta H_1 k_1 x_1 - \Delta H_2 k_2 x_2 - \Delta H_3 k_3 x_1^2}{\rho C_p} \\ \qquad\qquad + (x_{30} - x_3)\, u_1 + \dfrac{u_2}{\rho C_p} \end{cases} \tag{15}$$

where x_1 and x_2 are the concentrations of cyclopentadiene (denoted by A) and cyclopentenol (denoted by B), respectively while x_3 represents the reactor temperature (denoted by T). Physically, all theses states are positive and characterise the so-called positive system (Hoang *et al.* (2013b)).

Also, $k_i, i = 1, 2, 3$ are the reaction kinetics and governed by the Arrhenius law as below.

$$k_i\,(T) = k_{i0} \exp\left(\frac{E_i}{RT}\right) \tag{16}$$

All process parameters and their numerical values are listed in Appendices A and B.

4.2 The analysis of non-minimum phase behavior and optimization of the reaction system

Let $P^e = (x_1^e, x_2^e, x_3^e)$ be an equilibrium point of the system (15), the computations leads to the mathematical expressions of P^e as below

$$\begin{cases} x_1^e &= \dfrac{-\left(k_1\left(x_3^e\right) + u_1\right) + \sqrt{\left(k_1\left(x_3^e\right) + u_1\right)^2 + 8k_3\left(x_3^e\right) x_{10} u_1}}{4k_3\left(x_3^e\right)} \\ &\equiv f_1(x_3^e) \\ x_2^e &= \dfrac{k_1\left(x_3^e\right)}{k_2\left(x_3^e\right) + u_1} x_1^e \end{cases} \tag{17}$$

where x_3^e is one positive solution of the following nonlinear equation.

$$\begin{aligned} u_2 = &\left[\Delta H_1 k_1\left(x_3^e\right) + \Delta H_2 \frac{k_1\left(x_3^e\right) k_2\left(x_3^e\right)}{k_2\left(x_3^e\right) + u_1}\right] f_1\left(x_3^e\right) \\ &+ \Delta H_3 k_3\left(x_3^e\right) f_1^2\left(x_3^e\right) - \left(x_{30} - x_3^e\right) u_1 \rho C_p \equiv f_3\left(x_3^e\right) \end{aligned} \tag{18}$$

In (Dochain (1992)), the author showed that for the Van de Vusse reaction system if all the zeros of the transfer function of the linearized system (derived at an equilibrium point) have a strictly negative real part, then the nonlinear process is minimum phase at that equilibrium point. And, if some of them have a strictly positive real part, then the process is non-minimum phase. Let us recheck quickly this result, we assume the reactor is initially operated corresponding to $u_1 = 19.52$ (1/h) and $u_2 = -500$ (kJ/(l.h)). The equilibrium point P^e is then calculated by $P^e = (1.25, 0.86, 404.7)$. In this case, the transmission zero of the linearized system from u_2 to x_2 is found to be + 89.11. Hence, the Van de Vusse reaction system belongs to a class of non-minimum phase systems.

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[2] Obviously, the dynamics of the error state vector e is naturally formatted in a PH structure.

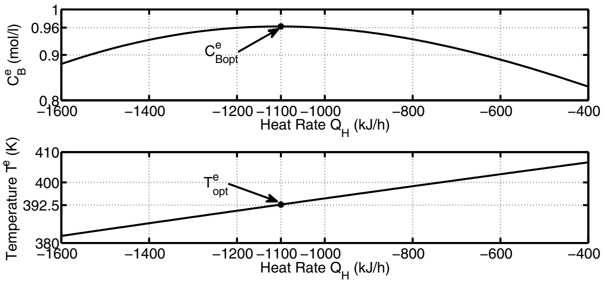

Fig. 1. Optimization steady-sate concentration of main product

In practice, the reaction system (15) is usually operated so that the concentration of primary product at the equilibrium point (x_2^e) reaches the optimal solution, i.e ($x^e_{2\mathrm{opt}}$). Hence, the constrained optimization problem of this system can be stated from (17) and (18) as follows :

$$\max_{u_2} x_2^e\,(x_3^e) \tag{19}$$

$$\text{subject to}\, f_3(x_3^e) = u_2 \text{ and } x^e_{3\min} \le x_3^e \le x^e_{3\max}$$

Figure 1 shows that the steady-state concentration of cyclopentenol (x_2^e) reaches the maximum value $x^e_{2\mathrm{opt}} = 0.96$ (mol/l) corresponding to $x^e_{3\mathrm{opt}} = 392.67$ (K) when the rate of heat exchanged between the jacket and reactor is equal to -1100 (kJ/(l.h)). During the rest of this paper, the optimal equilibrium point $P^e_{\mathrm{opt}} = (1.87, 0.96, 392.67)$ will be used as the set-point of the reaction system (15) for the purpose of control design.

4.3 The control design

Our control objective is to stabilize the reactor at the optimal equilibrium point $P^e_{\mathrm{opt}} = (1.87, 0.96, 392.67) \equiv (x^e_{1\mathrm{opt}}, x^e_{2\mathrm{opt}}, x^e_{3\mathrm{opt}})$ using the dilution rate u_1 and the rate of heat exchanged between the jacket and the reactor u_2 as the control inputs.

In order to apply Proposition 1 to design the tracking-error-based controller, the nonlinear dynamics (15) is firstly written into the PH representation (3) with a certain quadratic storage function (5). However, it is not likely to the isothermal case[3], the PH representation of the non-isothermal system dynamics with a quadratic storage function cannot be found apparently due to the nonlinearity of thermal effects. Hence, the relaxing (pseudo) PH formulation is needed for the control design. For sake of simplicity, the new state variable is introduced (see also (Ramírez *et al.* (2009))).

$$\bar{x}_3 = -\frac{\rho C_p}{\Delta H_3} x_3 \tag{20}$$

From this, the set of ODEs described the non-isothermal reactor dynamics (15) can be re-written into the relaxing PH formulation with the quadratic storage function $\mathbb{H}(x) = \frac{1}{2}\left(x_1^2 + x_2^2 + \bar{x}_3^2\right)$ as below[4]

$$\dot{x} = [J(x) - R(x)]\,\frac{\partial \mathbb{H}(x)}{\partial x} + g(x)u \tag{21}$$

where :

$$g(x) = \begin{bmatrix} x_{10} - x_1 & 0 \\ -x_2 & 0 \\ -\dfrac{\rho C_p}{\Delta H_3}\left(x_{30} + \dfrac{\Delta H_3}{\rho C_p}\bar{x}_3\right) & -\dfrac{1}{\Delta H_3} \end{bmatrix}, \tag{22}$$

$$u = [u_1, u_2]^\top, \tag{23}$$

$$J(x) = \begin{bmatrix} 0 & a_1 & b_1 \\ -a_1 & 0 & 0 \\ -b_1 & 0 & 0 \end{bmatrix} \tag{24}$$

where :

$$a_1 = -\frac{k_1}{2} + \frac{k_3 x_1 \bar{x}_3}{2x_2} + \frac{\Delta H_2}{\Delta H_3}\frac{k_2 \bar{x}_3}{2x_1} \tag{25a}$$

$$b_1 = -k_3 x_1 - \frac{\Delta H_2}{\Delta H_3}\frac{k_2 x_2}{x_1} \tag{25b}$$

and,

$$R(x) = \begin{bmatrix} d_1 & e_1 & 0 \\ e_1 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} \tag{26}$$

where :

$$d_1 = k_1 + 2k_3 x_1; \quad d_2 = k_2; \quad d_3 = -\frac{\Delta H_1}{\Delta H_3}\frac{k_1 x_1}{\bar{x}_3} \tag{27a}$$

$$e_1 = -\frac{k_1}{2} - \frac{k_3 x_1 \bar{x}_3}{2x_2} - \frac{\Delta H_2}{\Delta H_3}\frac{k_2 \bar{x}_3}{2x_1} \tag{27b}$$

Hence the assigned mathematical expression of the state vector $x_d = (x_{d1}, x_{d2}, \bar{x}_{d3})$ where $\bar{x}_{d3} = -\frac{\rho C_p}{\Delta H_3} x_{d3}$ is given as below,

$$\begin{aligned} \dot{x}_{d1} = &- d_1 x_{d1} + (a_1 - e_1)x_{d2} + b_1 \bar{x}_{d3} \\ &+ R_{1I}(x_1 - x_{d1}) + (x_{10} - x_1)u_1 \end{aligned} \tag{28}$$

$$\begin{aligned} \dot{x}_{d2} = &(-a_1 - e_1)x_{d1} - d_2 x_{d2} + R_{2I}(x_2 - x_{d2}) \\ &- x_2 u_1 \end{aligned} \tag{29}$$

$$\begin{aligned} \dot{\bar{x}}_{d3} = &- b_1 x_{d1} - d_3 \bar{x}_{d3} + R_{3I}(\bar{x}_3 - \bar{x}_{d3}) \\ &- \frac{\rho C_p}{\Delta H_3}\left(x_{30} + \frac{\Delta H_3}{\rho C_p}\bar{x}_{d3}\right)u_1 - \frac{u_2}{\Delta H_3} \end{aligned} \tag{30}$$

where a_1 and b_1 are the elements of matrix $J(x)$ (24) while d_1, d_2, d_3 and e_1 are the components of matrix $R(x)$ (26). Also, R_{1I}, R_{2I} and R_{3I} represent the positive elements of $R_I(x) = \mathrm{diag}(R_{1I}, R_{2I}, R_{3I})$.

We can check easily that the positive semi-definite condition of matrix $R(x)$ (26) is not met, this structure belongs to relaxing (pseudo) PH representation. The global asymptotic stabilization of the controlled dynamics is achieved since the condition defined in (7) holds. Indeed, in the case of $R(x)$ (26), an example of $R_I(x)$ is proposed below[5],

$$R_I(x) = \begin{bmatrix} R_{1I} & 0 & 0 \\ 0 & R_{2I} & 0 \\ 0 & 0 & R_{3I} \end{bmatrix} = R_I(x)^\top \tag{31}$$

where R_{1I} and R_{2I} are calculated as follows :

$$R_{1I} = \frac{k_3 x_1 \bar{x}_3}{2x_2} + \frac{\Delta H_2}{\Delta H_3}\frac{k_2 \bar{x}_3}{2x_1} + \alpha > 0 \tag{32}$$

$$R_{2I} = 2k_3 x_1 + \frac{k_3 x_1 \bar{x}_3}{2x_2} + \frac{\Delta H_2}{\Delta H_3}\frac{k_2 \bar{x}_3}{2x_1} + \alpha > 0 \tag{33}$$

with α as an additional positive scalar to be chosen, while $R_{3I} \ge 0$ is an arbitrary tuning parameter. From this, the

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[3] Such a PH representation can be derived easily.

[4] Without loss of generality and when no confusion results, the same notation x for the novel state vector, i.e., $x = (x_1, x_2, \bar{x}_3)$ is also used.

[5] The positive semi-definiteness property holds since $\Delta H_2 < 0$ and $\Delta H_3 < 0$ (See Appendix B).

Table 1. The initial conditions

	x_1^0 (mol/l)	x_2^0 (mol/l)	x_3^0 (K)
SSI	2.1	0.8	403
SSII	1.5	1.0	360

symmetric matrix $\Big(R(x)+R_I(x)\Big)$ is positive semi-definite since its principal minors determinants are positive :

$$\begin{cases} \Delta_1 = d_1 + R_{1I} > 0 \\ \Delta_2 = (d_1 + R_{1I})(d_2 + R_{2I}) - e_1^2 > 0 \\ \Delta_3 = R_{3I}\Delta_2 > 0 \end{cases} \tag{34}$$

In what follows, x_{d2} and $\bar{x}_{d3}$ are assigned as $\dot{x}_{d2} = K_1\left(x^e_{2\text{opt}} - x_{d2}\right)$ and $\dot{\bar{x}}_{d3} = K_2\left(\bar{x}^e_{3\text{opt}} - \bar{x}_{d3}\right)$, respectively, where K_1 and K_2 are the gains of the controller; $\bar{x}^e_{3\text{opt}} = -\frac{\rho C_p}{\Delta H_3} x^e_{3\text{opt}}$. From (29) and (30), the internal dynamic controller can be obtained as below.

$$\begin{aligned} u_1 =& \frac{-1}{x_2}\Big[K_1\left(x^e_{2\text{opt}} - x_{d2}\right) + (a_1 + e_1)\,x_{d1} + d_2 x_{d2} \\ & - R_{2I}\left(x_2 - x_{d2}\right)\Big] \end{aligned} \tag{35}$$

$$\begin{aligned} u_2 =& -\Delta H_3\Bigg[K_2\left(\bar{x}^e_{3\text{opt}} - \bar{x}_{d3}\right) + b_1 x_{d1} + d_3\bar{x}_{d3} \\ & - R_{3I}\left(\bar{x}_3 - \bar{x}_{d3}\right) + \frac{\rho C_p}{\Delta H_3}\left(x_{30} + \frac{\Delta H_3}{\rho C_p}\bar{x}_3\right)u_1\Bigg] \end{aligned} \tag{36}$$

5. NUMERICAL SIMULATIONS

In this section, the numerical simulations are conducted to illustrate the proposed feedback laws (35) and (36) of the non-isothermal reactor. We choose $K_1 = K_2 = 5$ and $R_{3I} = 5$ in the equations of controllers (35) and (36) while α in (32) is selected to be 15. Moreover, the reactor (15) is operated in two different initial conditions listed in Table 1. Obviously, Fig. 2(a) and 2(b) show that the system trajectories x_2 and x_3 converge to the desired steady state $x^e_{2\text{opt}}$ and $x^e_{3\text{opt}}$, respectively for both of the considered initial conditions. Additionally, the dynamics of control inputs including u_1 and u_2 given in Fig. 3(a) and 3(b), respectively are physically admissible in terms of amplitude and dynamics. Hence, the proposed control algorithms can stabilize the reaction system at the optimal equilibrium point P^e_{opt}.

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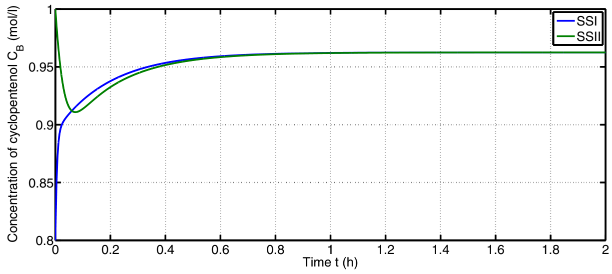
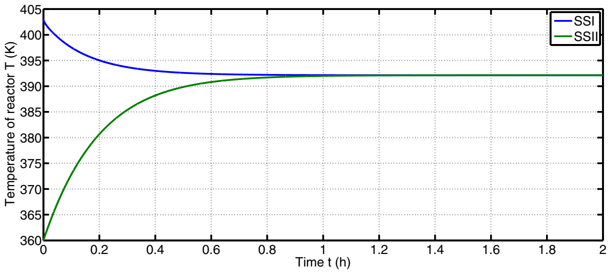
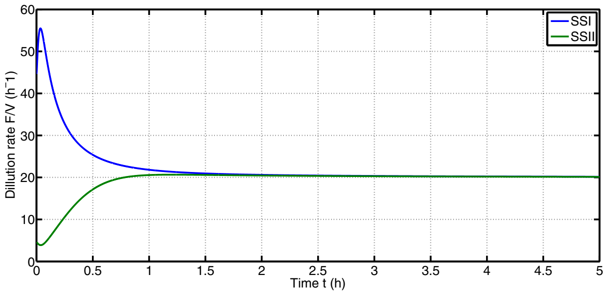


(a) Concentration of cyclopentenol.

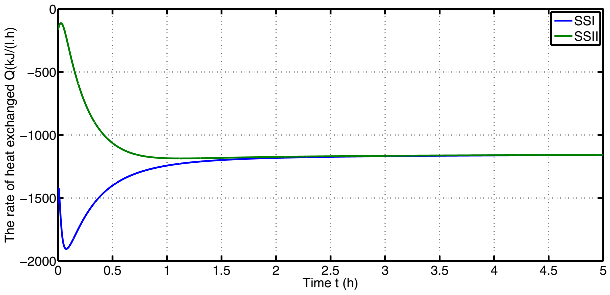


(b) Reactor temperature.

Fig. 2. Closed-loop system's response



(a) Dillution rate u_1.



(b) Rate of heat exchanged between jacket and reactor u_2.

Fig. 3. The control inputs

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Appendix A. NOMENCLATURE

Symbol	Quantity
u_1	Dilution rate
u_2	Heat removal
ρ	Density of reacting mixture
C_p	Heat capacity of reacting mixture
$\Delta H_i, i = 1, 2, 3$	Heat of ith reaction
$E_i, i = 1, 2, 3$	Activation energy of ith reaction
R	Ideal gas constant

Appendix B. PHYSICAL AND OPERATING PARAMETERS

Symbol	Unit	Value	Symbol	Unit	Value
x_{10}	mol/l	5	k_{10}	h	1.287×10^{12}
x_{30}	K	403.15	k_{20}	h	1.287×10^{12}
ρ	kg/l	0.9342	k_{30}	$\frac{\text{l}}{\text{mol.h}}$	9.403×10^{9}
C_p	kJ/(kg.K)	3.01			
ΔH_1	kJ/mol	4.20	$\frac{E_1}{R}$	K	-9758.3
ΔH_2	kJ/mol	-11.00	$\frac{E_2}{R}$	K	-9758.3
ΔH_3	kJ/mol	-41.85	$\frac{E_3}{R}$	K	-8560.0