

# A passivation approach to the control design of non-passive nonlinear system

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This work proposes a tracking error passivity-based multivariable control via feedback passivation for a class of free-radical polymerization systems in a continuously stirred tank reactor (CSTR). Firstly, this system dynamics with high nonlinearity is passivized by input coordinate transformations, the resulting passive system is then re-written into a canonical form strongly related to the so-called Port Control Hamiltonian structure. Actually, this representation allows to show the physical meanings of system dynamics such as dissipative, non-dissipative terms and supply rate. From this, a feedback controller based on tracking error is designed for the globally exponential stabilization at an arbitrarily chosen reference trajectory passing the desired equilibrium point. The theoretical developments are then illustrated for polystyrene polymerization system in the CSTR. The numerical simulations show that the trajectories of styrene polymerization system considered as an illustrative example of FRP system converges globally exponentially to the imposed trajectories.

**Keywords** : Free-radical polymerization, polystyrene, passivity-based control, feedback passivation, tracking error, multivariable system

## INTRODUCTION

Free-radical polymerization (FRP) reactors play a key role to synthesize many different types of plastic such as polystyrene, polymethylmethacrylate and polyvinyl chloride, etc. (Matyjaszewski & Davis, 2002; Meyer & Keurentjes, 2005). Therefore, together with the experimental researches (Lederle & Hübner, 2017), the studies into the optimal operation and control design of these chemical processes

have attracted much attention of practitioners and researchers over the year. In fact, it is not easy to stabilize globally the FRP system at a desired equilibrium point with an affordable performance due to the highly nonlinear characteristics caused by the reaction kinetics and transport phenomena, etc. In fact, these characteristics result in the abnormal dynamical behaviors namely stable/unstable multiple steady states, limit cycle and bifurcation under some certain

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operating conditions (Freitas Filho, Biscaia, & Pinto, 1994; Jaisinghani & Ray, 1977; Melo, Biscaia Jr, & Pinto, 2003; Russo & Bequette, 1998). To tackle the challenge issue, many proposed control strategies were applied to eliminate the highly nonlinear characteristics and allow to stabilize the system dynamics at the desired equilibrium point such as model predictive control (MPC) (Hidalgo & Brosilow, 1990), intelligent control<sup>1</sup> (Ghasem, Sata, & Hussain, 2007; Hosen, Hussain, & Mjalli, 2011; Hosen et al., 2014) and backstepping controller (Biswas & Samanta, 2013), the input/output linearization technique (Assala, Viel, & Gauthier, 1997; Viel, Busvelle, & Gauthier, 1995), etc. Although all of these control strategies are of great interest, they rely heavily on mathematical tools in general and do not consider the energy's aspects of system dynamics.

Among the control designs, the passivity-based control (PBC)<sup>2</sup> is recognized as a systematical and useful design tools. Actually, although this control strategy has been successfully applied to control for electrical and mechanical systems (Ortega, Van der Schaft, Mareels, & Maschke, 2001; Petrovic, Ortega, & Stankovic, 2001; Sira-Ramírez, Perez-Moreno, Ortega, & Garcia-Esteban, 1997), it has been rarely utilized for control study of chemical processes because the links between stability theory and energy of a reacting system has been poorly understood (Favache & Dochain, 2009;

Hoang, Couenne, Jallut, & Le Gorrec, 2012; Hoang, Couenne, Le Gorrec, Chen, & Ydstie, 2013). Hence, this issue has become an interesting topic in the control community recently and some attempts have been made. For instances, the design methodology of interconnection and damping assignment passivity-based control (IDA-PBC)<sup>3</sup> is proposed to stabilize asymptotically a nonlinear chemical process including  $n$  chemical reactants and  $m$  reactions taking place in a continuous stirred tank reactor (CSTR) in (Hoang, Couenne, Le Gorrec, et al., 2013; Ramírez, Sbarbaro, & Ortega, 2009). Besides, the PBCs based on the thermodynamic perspectives are considered for the stabilization of some process systems (Hoang, Couenne, Jallut, & Le Gorrec, 2011; Ydstie, 2002; Ydstie & Alonso, 1997). In this paper, another PBC, which established by the feedback passivation plus tracking error is proposed for the stabilization of FRP system in CSTR at the desired steady state. More precisely, firstly, the original nonlinear system is rendered strictly input/output passive system by the use of input coordinate transformations. Then, the resulting passive system is re-written into the canonical form strongly related to the port-control Hamiltonian structure. In fact, this representation enables to show the physical meanings of the system dynamics including dissipative, non-dissipative terms and supply rate. Finally, the feedback controller through tracking error is subsequently derived. In that respect, this

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<sup>1</sup> The intelligent control strategies include the fuzzy logic, artificial neural network and generic algorithm.

<sup>2</sup> The PBC is established by the passivity theory via the pioneering works of Willems (1972).

<sup>3</sup> We refer the readers to (Ortega, Van der Schaft, Maschke, & Escobar, 2002) and references cited therein for the rigorous definitions and further discussion of IDA-PBC strategy.

work is an extended version of control design method which was achieved by Sira-Ramírez and AnguloNunez (1997) as the multi input multi output (MIMO) chemical process system is considered for the practical implementation in the unit operation of chemical engineering (Nguyen, Hoang, & Hussain, 2017b). Although the PBC via input coordinate transformation plus tracking error was applied successful for a class of single input single output (SISO) systems, the theoretical developments for MIMO system are still not obvious owing to the complexity of mathematical model, etc.

The paper is organized as follow. The section 2.1 reviews briefly the fundamentals of passivity theory and then the section 2.2 provides the main theoretical results of this article through propositions. In section 3 and section 4, the theoretical developments are then illustrated by considering the polystyrene production process in CSTR as a main case study and the Van de Vusse reaction system as an additional case study. The numerical simulations are given in section 5. Finally, the conclusion is shown in section 6.

## CONTROL STUDY

### Fundamental of Passive System and PBC

Firstly, let us consider a nonlinear system described by a set of ordinary differential equations (ODEs) as follows,

$$\dot{x} = f(x) + g(x)u, \quad y = h(x) \quad (1)$$

where  $x$  is the state vector on the operating region  $\chi \subset \mathbb{R}^n$ ;  $u$  is control input and the scalar function  $y$  is the output function of the system. The vector-valued (nonlinear) functions  $f(x)$  and  $g(x)$  are assumed to be smooth vector fields in  $\chi$ .

**Definition 1** (Bao & Lee, 2007).

The system (1) is said to be dissipative regarding to the supply rate  $s(u, y)$  if there exists a storage function  $V(x): \chi \rightarrow \mathbb{R}^+$ , then the inequality below is hold for all  $x \in \chi$  and for all  $t_1 > t_0$  input functions  $u$ ,

$$V(x(t_1)) - V(x(t_0)) \leq \int_{t_0}^{t_1} s(u(t), y(t)) dt \quad (2)$$

where  $x(t_0) = x_0$  and  $x(t_1)$  are the initial condition and the solution of system dynamics (1) at time  $t_1$ , respectively. If  $V(x)$  is differential for  $x \in \chi$ , the inequality (2) is equivalent to

$$\dot{V}(x) \leq s(u(t), y(t)) \quad (3)$$

From the physical viewpoint, the inequality (4) shows that the rate of increase in the storage function  $V(x(t))$  is always no greater than the supply rate. Besides, there exists dissipation terms which dissipate a part of the system's energy. In the case, the dissipation term is equal to zero, the dissipative system conserves all energy with any supplied energy function.

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**Definition 2** (Bao & Lee, 2007).

The nonlinear system (1) is said to be passive if it is dissipative with respect to the supply rate  $s(u, y) = u^T y$ .

Obviously, the passive system is a special case of dissipative system when the supply rate is considered as the scalar product of input  $u$  and output  $y$ . If the inequalities (2) and (3) hold strictly with respect to the supply rate  $s(u, y) = u^T y$ , the passive system is called a strictly passive system.

**Definition 3** (Bao & Lee, 2007; Khalil, 2002).

A passive system is output strictly passive if  $s(u, y) = u^T y - \gamma\phi(y)$  where  $\gamma$  is arbitrary strictly positive constant. Also, system is input strictly passive if  $s(u, y) = u^T y - \delta\phi(u)$  where  $\delta$  is arbitrary strictly positive constant.

**Passivity – Based Multivariable Control Via Feedback Passivation**

Sira-Ramírez and AnguloNunez (1997) proposed a systematic approach to passivize a nonlinear system via an input coordinate transformation. This method was also applied successfully in several physical and chemical processes (Chou & Wu, 2007; Riverol, 2001; Szederkényi, Kristensen, Hangos, & Bay Jørgensen, 2002) but was limited for the SISO system. Hence, the aim of paper is to extend the method of feedback passivation via a natural decomposition of  $f(x)$  for a class of MIMO system and then apply to design the multivariable control. In fact, the interesting issue is solved by following the control

design methodology, which are realized as the main contributions of paper, as follows. First of all, we assume that there exists a natural decomposition of  $f(x)$ , i.e.

$$f(x) = f_I(x) + f_d(x) + f_{nd}(x) \quad (4)$$

such that

- $L_{f_I(x)}V(x) = 0$ ,
- $L_{f_d(x)}V(x) \leq 0$ ,
- $L_{f_{nd}(x)}V(x)$  is sign-undefined in  $\chi$ .

Actually,  $f_I(x)$ ,  $f_d(x)$  and  $f_{nd}(x)$  are considered as the invariant, dissipative and non-dissipative term of  $f(x)$ . Besides, the notion  $L_{f(x)}V(x)$  is the Lie derivative of  $V(x)$  along  $f(x)$  and it is defined as follow (Khalil, 2002),

$$L_{f(x)}V(x) = \frac{\partial V(x)}{\partial x} f(x) = \sum_{i=1}^n \frac{\partial V(x)}{\partial x_i} f_i(x) \quad (5)$$

where  $n$  is the number of rows of vector  $f(x)$ .

After the natural decomposition of  $f(x)$  (4) is proposed, the nonlinear system (1) can achieve the passivation by following proposition.

**Proposition 1**

The nonlinear system (1) is transferred to a strictly output passive system with respect to storage function  $V(x)$  by two input coordinate transformations  $u_1$  and  $u_2$  defined below under conditions  $L_{g_1(x)}V(x) \neq 0$  and  $L_{g_2(x)}V(x) \neq 0$  for all  $x \in \chi$ .

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$$u_1 = \frac{h_1(x)}{L_{g_1(x)}V(x)}v_1 - \gamma_1 \frac{h_1^2(x)}{L_{g_1(x)}V(x)} - \frac{L_{f_{nd,1}(x)}V(x)}{L_{g_1(x)}V(x)} \quad (6)$$

$$u_2 = \frac{h_2(x)}{L_{g_2(x)}V(x)}v_2 - \gamma_2 \frac{h_2^2(x)}{L_{g_2(x)}V(x)} - \frac{L_{f_{nd,2}(x)}V(x)}{L_{g_2(x)}V(x)} \quad (7)$$

With  $f_{nd}(x) = f_{nd,1}(x) + f_{nd,2}(x)$ <sup>4</sup>, where  $v_1$  and  $v_2$  are the new inputs. Also,  $\gamma_1$  and  $\gamma_2$  are arbitrary positive scalars.

### Proof

The detailed proof can be found in (Nguyen, Hoang, & Hussain, 2018).

The original nonlinear system (1) becomes a strictly output-passive system with new inputs  $v = [v_1, v_2]$  which is also called an internal dynamic input control and the old output  $h(x) = [h_1, h_2]$ .

### Remark 1

A nonlinear system can achieve the passivation by the different ways which depend on input coordinate transformations. In (Fossas, Ros, & Sira-Ramírez, 2004; Sira-Ramírez, 1998), authors proposed other methods but all of them are just valid if the conditions  $L_{g(x)}V(x) \neq 0 \forall x \in \mathcal{X}$  is hold in general.

A passive system guarantees that the energy stored inside the system is always no greater than energy supplied by the external source. Based the features, we can propose a systematic procedure of control design via the use of physical meaning of the dissipative term. The following

proposition enables to re-write the resulting passive system to a canonical form and show the nature of dissipative term.

### Proposition 2

A passive system with inputs  $v = [v_1, v_2]$  and output  $h(x) = [h_1, h_2]$  is represented by the canonical form defined as follows,

$$\dot{x} = -R(x) \frac{\partial V}{\partial x} + J(x) \frac{\partial V}{\partial x} + M(x)v \quad (8)$$

where  $R(x)$  and  $J(x)$  are a positive diagonal symmetric matrix and a skew-symmetric matrix, respectively, defined as follows,

$$f_d(x) - g_1(x)\gamma_1 \frac{h_1^2(x)}{L_{g_1(x)}V(x)} \quad (9)$$

$$-g_2(x)\gamma_2 \frac{h_2^2(x)}{L_{g_2(x)}V(x)} = -R(x) \frac{\partial V}{\partial x}$$

$$f_l(x) + f_{nd}(x) - g_1(x) \frac{L_{f_{nd,1}(x)}V(x)}{L_{g_1(x)}V(x)} \quad (10)$$

$$-g_2(x) \frac{L_{f_{nd,2}(x)}V(x)}{L_{g_2(x)}V(x)} = -J(x) \frac{\partial V}{\partial x}$$

Also,

$$\left[ g_1(x) \frac{h_1(x)}{L_{g_1(x)}V(x)} \quad g_2(x) \frac{h_2(x)}{L_{g_2(x)}V(x)} \right] = M(x) \quad (11)$$

<sup>4</sup> Note also that if it is difficult to identify both  $f_{nd,1}(x)$  and  $f_{nd,2}(x)$ , we can choose arbitrarily one components which is equal to zero and another component is equal to  $f_{nd}(x)$ .

*Proof*

The detailed proof can be found in (Nguyen et al., 2017a, 2017b).

*Remark 2*

The canonical form of passive structure defined by **Proposition 2** is equivalent to the well-known port-Hamiltonian structure (Ortega et al., 2002). But this expression is just valid if the conditions  $L_{g_1(x)}V(x) \neq 0$  and  $L_{g_2(x)}V(x) \neq 0$  hold  $\forall x \in \mathcal{X}$ . Actually, it is shown that these conditions can be fulfilled by using an appropriate storage function as seen in the remaining of the paper.

From Propositions 1 and 2, the method of feedback passivation through the natural decomposition of  $f(x)$  was extended for the MIMO system with 2 inputs and 2 outputs. In fact, this method can be totally generalized for a MIMO system with  $m$  inputs and  $m$  outputs. This extension is, therefore, considered one of main contributions of this work. The following proposition proposes a PBC based on tracking error. More precisely, an arbitrarily reference trajectory  $x_d$  is chosen such that its time evolution converges asymptotically to the desired equilibrium point while the system trajectory  $x$  tracks  $x_d$  exponentially when time goes to infinity.

**Proposition 3**

If the storage energy function  $V(x)$  of the passive system in Propositions 1 and 2 is a positive quadratic function, i.e.  $V(x) = x^T R_d x$  where  $R_d$  is a positive semi-definite matrix, then the system trajectory converges exponentially to the reference trajectory chosen as below,

$$\begin{aligned} \dot{x}_d = & -R(x) \frac{\partial V(x_d)}{\partial x_d} + J(x) \frac{\partial V(x_d)}{\partial x_d} \\ & + R_l \frac{\partial V(e)}{\partial e} + M(x)v \end{aligned} \quad (12)$$

where  $x_d$  is an arbitrarily chosen reference trajectory. Matrices  $R(x)$ ,  $J(x)$  and  $M(x)$  are calculated by using (9), (10) and (11), respectively, while  $R_l$  is an arbitrarily chosen positive constant matrix.

*Proof*

The detailed proof can be found in (Nguyen, Hoang, & Hussain, 2018).

*Remark 3*

The Proposition 3 proposed a different reference trajectory compared to the reference trajectory in (Fossas et al., 2004). In fact, the reference trajectory (12) enables to show explicitly the physical meanings of the auxiliary system related to the vector field  $x_d$  (i.e., the interconnection and damping injection terms). On the other hand, this also simplifies considerably the complexity of the controller design in case of MIMO systems.

*Remark 4*

Once the reference trajectory  $x_d$  (12) is assigned, the internal control input  $v = [v_1, v_2]$  is derived by substituting  $x_d$  to (12). However, just some components of  $x_d$  can be chosen (Sira-Ramírez & AnguloNunez, 1997) due to the constraint of the degree of freedom of system (18). The actual control input  $u = [u_1, u_2]^T$  is subsequently computed by the

**Table 1:** Styrene polymerization's physical parameters

Reaction rate	Unit
$k_d = 1.58 \times 10^{15} \exp\left(\frac{-1.28 \times 10^5}{RT}\right)$	$s^{-1}$
$k_i = 2.184 \cdot 10^3 \exp\left(\frac{-1.15 \times 10^5}{RT}\right)$	$l \cdot mol^{-2} \cdot s^{-1}$
$k_p = 1.051 \times 10^7 \exp\left(\frac{-2.954 \times 10^4}{RT}\right)$	$l \cdot mol^{-1} \cdot s^{-1}$
$k_{tc} = 6.275 \times 10^8 \exp\left(\frac{-7.026 \times 10^3}{RT}\right)$	$l \cdot mol^{-1} \cdot s^{-1}$
$k_{td} = 0$	$l \cdot mol^{-1} \cdot s^{-1}$
$k_{tm} = 2.31 \times 10^6 \exp\left(\frac{-5.3 \times 10^4}{RT}\right)$	$l \cdot mol^{-1} \cdot s^{-1}$

combination of input coordinate transformations (7), (8) and  $v = [v_1, v_2]^T$ .

### CASE STUDY 1: THE POLYSTYRENE PRODUCTION PROCESS IN CSTR

#### Mathematical Model of Polymerization Production Process in CSTR

The FRP reaction taking place in the CSTR plays a key role in the petrochemical industry to produce many different types of polymers, especially polystyrene. The feed including monomer, initiator and solvent is fed into CSTR and the growth of monomer molecules into polymer occurs under constraints of free-radical's mechanism (Jaisinghani & Ray, 1977). In this paper, the polystyrene polymerization process system in the CSTR is concerned.

In fact, the monomer styrene is fed to CSTR and the reaction system is initiated by initiator (AIBN) which is also fed to the reactor (Russo & Bequette, 1998). Based on the material and energy balance equations, mathematical model of styrene FRP reactor

can be written as below,

$$\begin{aligned}
 \frac{dC_M}{dt} &= \frac{Q_{mF}}{V} C_{MF} - \frac{Q_{mF} + Q_{ml}}{V} C_M \\
 &\quad - (k_p + k_{tm}) C_M C_R - 2fk_d C_I, \\
 \frac{dC_I}{dt} &= \frac{Q_{ml}}{V} C_{IF} - \frac{Q_{mF} + Q_{ml}}{V} C_I - k_d C_I, \\
 \frac{dT}{dt} &= \frac{Q_{mF} + Q_{ml}}{V} \left( \frac{c_{pF}}{c_p} T_F - T \right) \\
 &\quad + \frac{UA}{\rho V c_p} (T_J - T) - \frac{k_p C_M \Delta H}{\rho c_p} C_R,
 \end{aligned} \tag{13}$$

Where  $f$  is the efficiency factor of initiator;  $C_M$ ,  $C_I$  and  $C_S$  are the concentrations of styrene, initiator (AIBN) and solvent in the CSTR, respectively while  $k_d$ ,  $k_i$ ,  $k_p$ ,  $k_{tc}$  and  $k_{tm}$  are reaction rates in the free-radical's mechanism and given by the Arrhenius law in **Table 1** (Assala et al., 1997; Viel et al., 1995). In (13),  $C_R$  derives the concentration of free-radical species and is defined by

$$C_R = \sqrt{\frac{f k_d C_I}{k_{tc} + k_{td}}} \quad (14)$$

We refer the readers to the appendix A and appendix B for the nomenclature and the operating parameter of the styrene polymerization reactor.

### Control Problem Statement

Under certain operating conditions, it is shown that the reaction system (13) exists three different steady states<sup>5</sup> which can be divided into three different groups according to their monomer conversion rate  $\alpha = 1 - C_M/C_{MF}$ . In fact, the low-conversion steady state is asymptotically stable, but it is no economic benefits because just a few monomers are converted into polymer chain. On the other hand, although the high-conversion steady state is also asymptotically state, it causes some practical challenging problems, namely the catastrophic solidification due to the high viscosity of the reacting mixture. Therefore, from a practical viewpoint, we propose to operate the reactor at the medium conversion that is unstable but gives acceptable process performance.

### Application of PBC for the Polystyrene Production Process in CSTR

In this section, the control strategy, which is discussed in section 2.2, is applied to design the controller for the exponential stabilization of reactor temperature and concentration of initiator at unstable-open-loop point. Firstly, jacket temperature  $T_j$

and feed rate of initiator (AIBN)  $Q_{mi}$  are chosen as manipulated variables. For the sake of convenience, let us note that

$$Q_2 = \frac{Q_{mi}}{V} \quad (15)$$

and  $Q_2$  is used instead of  $Q_{mi}$  without any confusion.

For controller synthesis, the system dynamics (13) is represented as (1) by the state vector  $x = (C_M, C_I, T) = (x_1, x_2, x_3)$ ,

$$f(x) = \begin{bmatrix} Q_1 x_{1F} - Q x_1 - (k_p + k_{tm}) C_M C_R - 2 f k_d x_2 \\ Q(-x_2) - k_d x_2 \\ Q(x_{4F} - x_4) - A x_4 - C C_R k_p x_1 \end{bmatrix}$$

$$g_1(x) = \begin{bmatrix} 0 \\ x_{2F} \\ 0 \end{bmatrix}, \quad g_2(x) = \begin{bmatrix} 0 \\ 0 \\ A \end{bmatrix}, \quad u_1 = Q_2 \text{ and}$$

$$u_2 = T_j, \quad \text{where } A = \frac{UA}{\rho V c_p}, \quad Q_1 = \frac{Q_{mF}}{V},$$

$$Q = Q_1 + Q_2, \quad C = \frac{\Delta H}{\rho c_p} \quad \text{and}$$

$$x_F = (C_{MF}, C_{IF}, \frac{c_{pF}}{c_p} T_F)^T = (x_{1F}, x_{2F}, x_{3F})^T.$$

*Remark 5:*

Note that the operating region  $\chi = \{x / x_i > 0, i \in \{1, 2, 3\}\}$  is a positive invariant set, i.e.,  $\forall x(t=0) \in \chi$ , then  $x(t) \in \chi$  (Blanchini, 1999). Of course, this property results from the (total) mass conservation and the positive definiteness condition of the (absolute) temperature. A general analysis of this concern can be found in (Antonelli & Astolfi, 2003; Hoang, Couenne, Le Gorrec, et al., 2013; Viel, Jadot,

<sup>5</sup> A nonlinear system existing different steady state under certain conditions exhibits the steady-state multiplicity behavior

(Khalil, 2002). And such expected behavior causes the instability of the system dynamics in the practical operation.

& Bastin, 1997).

The quadratic function  $V(x) = \frac{1}{2} \sum_{i=1}^3 x_i^2$  is chosen as a storage function<sup>6</sup> of the passive system.

Clearly,  $L_{g_1(x)}V(x) = x_2 x_{2F} \neq 0$  and  $L_{g_2(x)}V(x) = Ax_3 \neq 0$  are hold in the operating region  $\chi$  because of the physical meanings of  $x_1, x_2$  and  $x_3$ . Hence, the system (12) can be passivized by two input coordinate transformations by following Proposition 1. Firstly, a natural decomposition of  $f(x)$  is given as below,

$$f_d(x) = \begin{bmatrix} -Qx_1 - (k_p + k_{im})x_1 C_R - 2f k_d x_2 \\ -Qx_2 - k_d x_2 \\ -Qx_3 - Ax_3 \end{bmatrix} \quad (16)$$

$f_{nd,1}(x) = 0$  and

$$f_{nd,2}(x) = \begin{bmatrix} Q_1 x_{1F} \\ 0 \\ Qx_{3F} - k_p x_1 C C_R \end{bmatrix} \quad (17)$$

In fact, the function  $f_I(x)$  is not available because no function  $f_I(x)$  can be found to satisfy the property  $L_{f_I(x)}V(x) = 0; \forall x \in \chi$ . Then, two input coordination transformations are defined,

$$u_1 = \frac{1}{x_{2F}} v_1 - \frac{\gamma_1 x_2}{x_{2F}} \quad (18)$$

$$u_2 = \frac{1}{A} v_2 - \frac{\gamma_1 x_3}{A} - \frac{Qx_{1F} x_1 + (Qx_{3F} - k_p x_1 C C_R) x_3}{Ax_3} \quad (19)$$

Consequently, the initial nonlinear system (13) achieves the strictly-output passivation with new input  $v = [v_1, v_2]$  and output  $y = h(x) = [x_2, x_3]$ .

Next, the resulting passive system is rewritten into the canonical form by following proposition 2 as follow,

$$\dot{x} = -R(x) \frac{\partial V}{\partial x} + J(x) \frac{\partial V}{\partial x} + M(x)v \quad (20)$$

where the matrix  $R(x)$  and  $J(x)$  are given as below,

$$R(x) = \begin{bmatrix} Q + (k_p + k_{im})x_1 C_R - 2f k_p x_2 & 0 & 0 \\ 0 & Q + k_d - \gamma_1 \frac{x_1^2}{x_2^2} & 0 \\ 0 & 0 & Q + A + \gamma_2 \end{bmatrix} \quad (21)$$

$$J(x) = \begin{bmatrix} 0 & \frac{Q_1 x_{1F}}{x_2} & 0 \\ -\frac{Q_1 x_{1F}}{x_2} & 0 & \frac{Q_1 x_{1F} x_1}{x_2 x_3} \\ 0 & -\frac{Q_1 x_{1F} x_1}{x_2 x_3} & 0 \end{bmatrix} \quad (22)$$

$$M(x) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (23)$$

After rewriting the resulting passive system into the canonical form, the reference trajectory  $x_d$ , which is used for the tracking-error of the system trajectory, is derived by following Proposition 3 and is shown as follows,

$$\dot{x}_{1d} = -R_1 x_{1d} + \frac{Qx_{1F}}{x_2} x_{d1} + R_{d1} (x_1 - x_{1d}) \quad (24)$$

<sup>6</sup> In this case, the storage function  $V(x)$  is chosen as a quadratic function of state variable  $x$ . In many chemical process

systems,  $V(x)$  can be chosen by the considerations of thermodynamic perspectives (Hoang et al., 2011; Hoang & Dochain, 2013).

$$\begin{aligned} \dot{x}_{2d} = & -R_2 x_{2d} - \frac{Q x_{1F}}{x_2} x_{1d} + \frac{Q x_1 x_{1F}}{x_2 x_3} x_{3d} \\ & + R_{d2} (x_2 - x_{2d}) + \frac{x_2}{x_1} u_1 \end{aligned} \quad (25)$$

$$\dot{x}_{3d} = -R_3 x_{3d} - \frac{Q x_1 x_{1F}}{x_2 x_3} x_{3d} + R_{d3} (x_3 - x_{3d}) + u_2 \quad (26)$$

Let us assign  $x_{2d}$  and  $x_{3d}$  as  $\dot{x}_{2d} = K_{T1} (x_2^e - x_{2d})$  and  $\dot{x}_{3d} = K_{T2} (x_3^e - x_{3d})$ , respectively with  $K_{T1}$  and  $K_{T2}$  are turning parameters. It is straightforward to see that  $x_{2d}(t)$  and  $x_{3d}(t)$  goes to  $x_2^e$  and  $x_3^e$  when time goes to infinity, respectively. From (25) and (26), the two internal dynamic controllers can be obtained immediately,

$$\begin{aligned} u_1 = & R_2 x_{2d} + \frac{Q x_{1F}}{x_2} x_{1d} - \frac{Q x_1 x_{1F}}{x_2 x_3} x_{3d} \\ & - R_{d2} (x_2 - x_{2d}) + K_1 (x_2^e - x_{2d}) \end{aligned} \quad (27)$$

$$\begin{aligned} u_2 = & R_3 x_{3d} + \frac{Q x_1 x_{1F}}{x_2 x_3} x_{2d} - R_{d3} (x_3 - x_{3d}) \\ & + K_2 (x_3^e - x_{3d}) \end{aligned} \quad (28)$$

Finally, the actual control input  $(Q_2, T_f)$  are calculated by (18), (19), (27) and (28).

$$\begin{aligned} u_1 = & \frac{1}{x_{2F}} \left[ R_2 x_{2d} + \frac{Q x_{1F}}{x_2} x_{1d} - \frac{Q x_1 x_{1F}}{x_2 x_3} x_{3d} \right. \\ & \left. - R_{d2} (x_2 - x_{2d}) + K_{T1} (x_2^e - x_{2d}) \right] \\ & - \frac{\gamma_1 x_1^2}{x_{2F} x_2} \end{aligned} \quad (29)$$

$$\begin{aligned} u_2 = & \frac{1}{A} \left[ R_3 x_{3d} + \frac{Q x_1 x_{1F}}{x_2 x_3} x_{2d} - R_{d3} (x_3 - x_{3d}) \right. \\ & \left. + K_{T2} (x_3^e - x_{3d}) \right] - \frac{\gamma_1 x_3}{A} \\ & - \frac{Q x_{1F} x_1 + (Q x_{3F} - k_p x_1 C_Y) x_3}{A x_3} \end{aligned} \quad (30)$$

In this paper, the polystyrene production process in CSTR is used as a main illustrative example of FRP process for the exponential stabilization. Furthermore, this research work aims to extend the proposed control strategy to the Van de Vusse reaction system which exhibits the non-minimum phase behavior. The following section will present briefly the application of proposed PBC strategy for this system.

## CASE STUDY 2: THE VAN DE VUSSE REACTION SYSTEM

### Mathematical Model of the Van de Vusse Reaction System

For the case study 2, let us consider the Van de Vusse reaction system<sup>7</sup> which is a typical non-minimum phase reaction system, its mathematical model is given as follow,

$$\begin{aligned} \dot{x}_1 = & -k_1 x_1 - k_3 x_1^2 + (x_{10} - x_1) u_1 \\ \dot{x}_2 = & k_1 x_1 - k_2 x_2 + x_2 u_1 \\ \dot{x}_3 = & \frac{(-\Delta H_1) k_1 x_1 + (-\Delta H_2) k_2 x_2 + (-\Delta H_3) k_3 x_1^2}{\rho C_\rho} \\ & + \frac{u_2}{\rho C_\rho} + (x_{30} - x_3) u_1 \end{aligned} \quad (31)$$

<sup>7</sup> The process of synthesis of cyclopentenol from cyclopentadiene in CSTR is considered as the Van de Vusse reaction system (Chen, Kremling, & Allgöwer, 1995).

**Table 2.** Nomenclature of the Van de Vusse system

Quantity	Symbol	Units
Inlet temperature of feed	$T$	K
Heat capacity of the reacting mixture in CSTR	$c_p$	kJ/(kg.K)
Average density of mixture in CSTR	$\rho$	kg/l
Temperature of CSTR	$T$	K
Enthalpy of reactions	$\Delta H_1, \Delta H_2$ and $\Delta H_3$	kJ/mol
Activation energy of reactions	$E_1, E_2$ and $E_3$	kJ/mol
Reaction kinetic constants	$k_{01}, k_{02}$ and $k_{03}$	$h^{-1}$ and l/(mol.h)

where  $x_1, x_2$  and  $x_3$  represent the concentration of cyclopentadiene, the concentration of cyclopentenol and the reactor temperature, respectively. Additionally, the reaction rates  $k_i, i = 1, 2, 3$  obey the Arrhenius law, i.e.

$$k_i = k_i(x_3) = \exp\left(\frac{E_i}{R x_3}\right) \text{ (with } E_i < 0 \text{) while}$$

the  $u_1$  and  $u_2$  expressing the dilution rate and the heat flow rate, respectively, are used as manipulated variables, i.e. control inputs. The physical meaning of other symbols can be found in **Table 2**.

*Remark 6:*

In (Ramírez et al., 2009), (32) can be rewritten into the (pseudo) port-Hamiltonian representation as follow

$$\dot{x} = -R(x) \frac{\partial V}{\partial x} + J(x) \frac{\partial V}{\partial x} + M(x)u \quad (32)$$

$$R(x) = \begin{bmatrix} 0 & -k_1 x_1 & -k_3 x_1^2 \\ k_1 x_1 & 0 & -\frac{\Delta H_2}{\Delta H_3} k_2 x_2 \\ k_3 x_1^2 & \frac{\Delta H_2}{\Delta H_3} k_2 x_2 & 0 \end{bmatrix} \quad (33)$$

$$J(x) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \left(1 - \frac{\Delta H_1}{\Delta H_2}\right) k_2 x_2 & 0 \\ 0 & 0 & -\frac{\Delta H_1}{\Delta H_3} k_1 x_1 \end{bmatrix} \quad (34)$$

and

$$M(x) = \begin{bmatrix} x_{10} - x_1 & 0 \\ -x_2 & 0 \\ \frac{\rho C_p}{(-\Delta H_3)} \left(x_{30} + \frac{\Delta H_3}{\rho C_p} x_3\right) & \frac{1}{(-\Delta H_3)} \end{bmatrix} \quad (35)$$

where  $k_i = k_i(\bar{x}_3) = \exp\left(\frac{E_i \rho C_p}{R(\Delta H_3) \bar{x}_3}\right)$ ,

$\frac{\Delta H_2}{\Delta H_3} < 1$  and  $-\frac{\Delta H_1}{\Delta H_3} > 0$ . Hence, the

Hamiltonian storage function is

$$H(x) = x_1 + x_2 + x_3 \quad (36)$$

Obviously, the (pseudo) port-Hamiltonian structure of the non-minimum phase reacting system is equivalent to the canonical form (13) but the representation is achieved without using the input coordinate transformations, i.e. the internal

input  $v$  in which  $u = \alpha(x)v + \beta(x)$  is equal to zero. In this case, the storage function of the system is the sum of all state variables, not a quadratic function, so the feedback laws based on the tracking error in proposition 3 cannot be implemented properly.

### Control Problem Statement

The Van de Vusse reaction system under operation without control exhibits the non-minimum phase system. Such unexpected behavior causes the internal instability of the system because of unstable zero dynamics (Khalil, 2002). From the practical viewpoint, an inverse response behavior of output can be observed when the operators or practitioners increase the input. Consequently, it results in the input multiplicity behavior, i.e. the system can be still stabilized with a desired setpoint but it will cost more raw materials and/or need a greater heat flow rate for the inputs (Kuhlmann & Bogle, 1997). In fact, the control design and the asymptotical stabilization of non-minimum phase systems in general and the Van de Vusse reaction system in particular have become a challenging issue for few decades and many attempts have been made (Engell & Klatt, 1993; Niemiec & Kravaris, 2003). In this research, the issue is addressed by the proposed PBC strategy in section 2.2.

### Application of PBC for the Van de Vusse Reaction System

In this section, the proposed control strategy is applied to design feedback laws for the exponential stabilization of the reactor temperature  $T$  and concentration of cyclopentadiene  $x_1$ . Firstly, the dilution

rate  $u_1$  and the heat flow rate  $u_2$  are chosen as the manipulated variables.

For controller synthesis, the system dynamics (31) is represented as (1) by the state vector  $x = (x_1, x_2, x_3)$ ,

$$f(x) = \begin{bmatrix} -k_1x_1 - k_3x_1^2 \\ +k_1x_1 - k_2x_2 \\ \frac{(-\Delta H_1)k_1x_1 + (-\Delta H_2)k_2x_2 + (-\Delta H_3)k_3x_1^2}{\rho C_p} \end{bmatrix}$$

$$g(x) = [g_1 \quad g_2] = \begin{bmatrix} x_{10} - x_1 & 0 \\ x_2 & 0 \\ x_{30} - x_3 & \frac{1}{\rho C_p} \end{bmatrix},$$

$$y = h(x) = [x_2, x_3] \quad \text{and} \quad u = [u_1 \quad u_2].$$

Secondly, the quadratic function  $V(x) = \frac{1}{2} \sum_{i=1}^3 x_i^2$  is also chosen as a storage function of passive system. Then, the natural decomposition of  $f(x)$  is given as follow,

$$f_d(x) = \begin{bmatrix} -k_1x_1 - k_3x_1^2 \\ -k_2x_2 \\ -\frac{\Delta H_1}{\rho C_p} k_1x_1 \end{bmatrix} \quad (37)$$

$$f_{nd,1}(x) = 0 \quad \text{and}$$

$$f_{nd,2}(x) = \begin{bmatrix} 0 \\ 0 \\ \frac{-\Delta H_2k_2x_2 - \Delta H_3k_3x_1^2}{\rho C_p} \end{bmatrix} \quad (38)$$

Actually, the function  $f_I(x)$  is not available in this case because no function  $f_I(x)$  can be found to satisfy the property  $L_{f_I(x)}V(x) = 0; \forall x \in \mathcal{X}$ . Then, by following

proposition 1, two input coordination transformations are defined as follow,

$$u_1 = \frac{x_2}{\Phi} v_1 - \gamma_1 \frac{x_2^2}{\Phi} \quad (39)$$

$$u_2 = \rho C_p v_2 - \gamma_2 x_3 \rho C_p - \frac{k_1 x_1 x_2}{x_3} \rho C_p + \Delta H_2 k_2 x_2 + \Delta H_3 k_3 x_1^2 \quad (40)$$

where

$$\Phi = L_{g_1} V(x) = x_1 (x_{10} - x_1) + x_2^2 + x_3 (x_{30} - x_3)$$

Next, the representation of the resulting passive system is rewritten into the canonical form by following proposition 2 as follow,

$$\dot{x} = -R(x) \frac{\partial V}{\partial x} + J(x) \frac{\partial V}{\partial x} + M(x) v \quad (41)$$

where

$$J(x) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{k_1 x_1}{x_3} \\ 0 & -\frac{k_1 x_1}{x_3} & 0 \end{bmatrix} \quad (42)$$

$$R = \begin{bmatrix} k_1 + k_3 x_1 + \frac{x_2^2 (x_{10} - x_1)}{x_1 \Phi} \gamma_1 & 0 & 0 \\ 0 & k_2 + \frac{x_2^2}{\Phi} \gamma_1 & 0 \\ 0 & 0 & \frac{\Delta H_1}{\rho C_p} k_1 x_1 + \frac{x_2^2 (x_{30} - x_3)}{x_3 \Phi} \gamma_1 + \gamma_2 x_3 \end{bmatrix} \quad (43)$$

$$M(x) = \begin{bmatrix} \frac{x_2}{\Phi} (x_{10} - x_1) & 0 \\ \frac{x_2^2}{\Phi} & 0 \\ \frac{x_2}{\Phi} (x_{30} - x_3) & 1 \end{bmatrix} \quad (44)$$

It is similar to the case study 1, after rewriting the structure of resulting passive system into the canonical form, a multivariable control based on the tracking error is proposed by the proposition 3. The explicit formulas of feedback laws and the simulation studies of the system will be presented in another research.

## SIMULATIONS

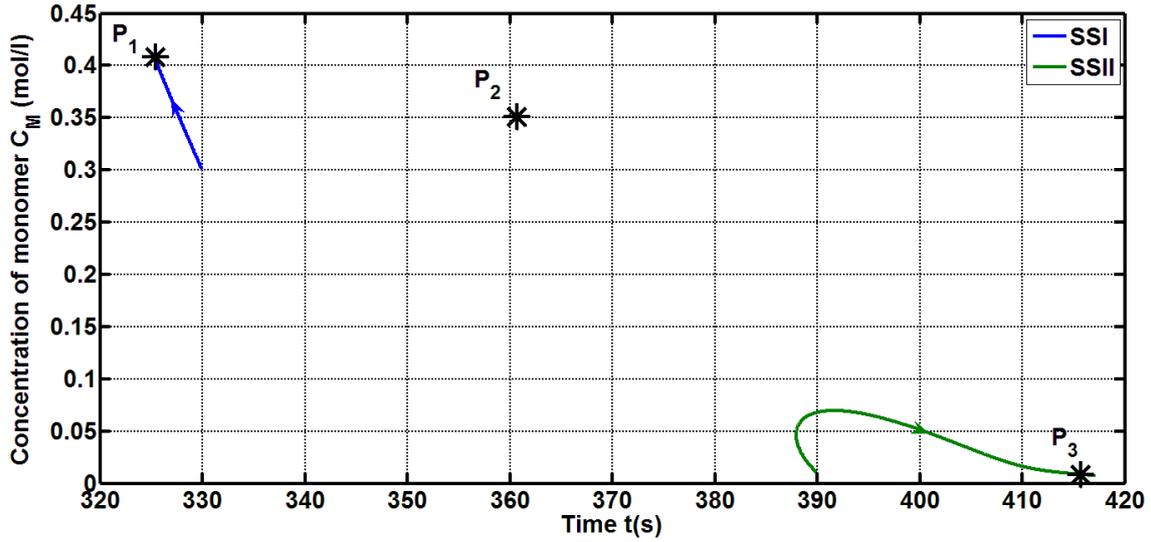
### Open – Loop Response

First of all, the styrene polymerization reactor is operated without control to show the multiplicity behavior. In fact, two different initial conditions applied for numerical simulations are given by in **Table 3**.

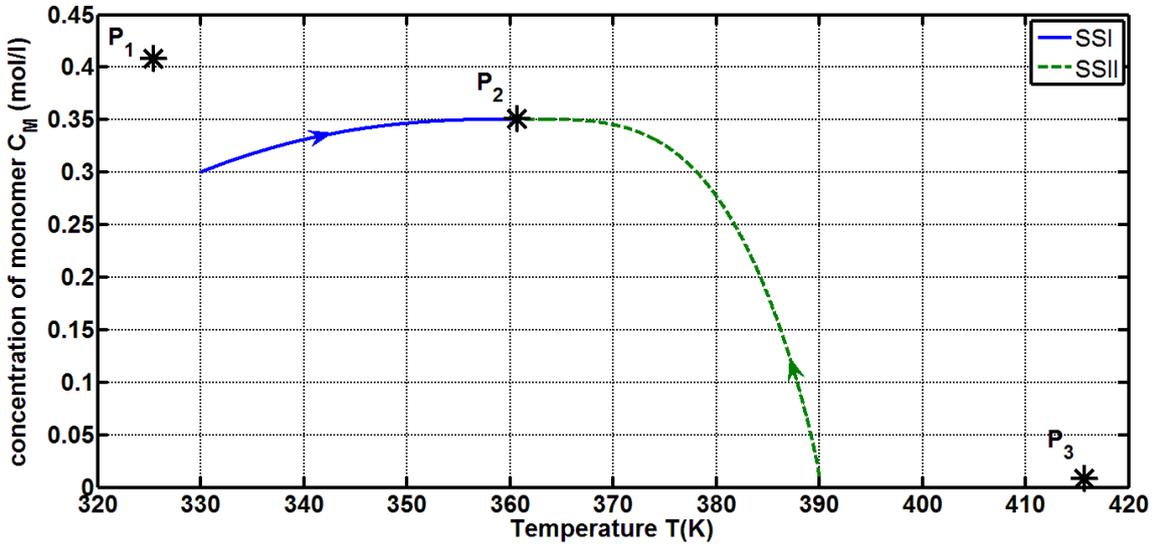
**Table 3.** The Initial Conditions

	$C_I$ (mol/l)	$C_M$ (mol/l)	$T$ (K)
SSI	0.30	2.8	330.0
SSII	0.01	1.3	390.0

**Figure 1** shows that the FRP system (13) has three different equilibrium points  $P^e = (C_M^e, C_I^e, T^e)$  including



**Fig. 1:** Phase plane of the open – loop system



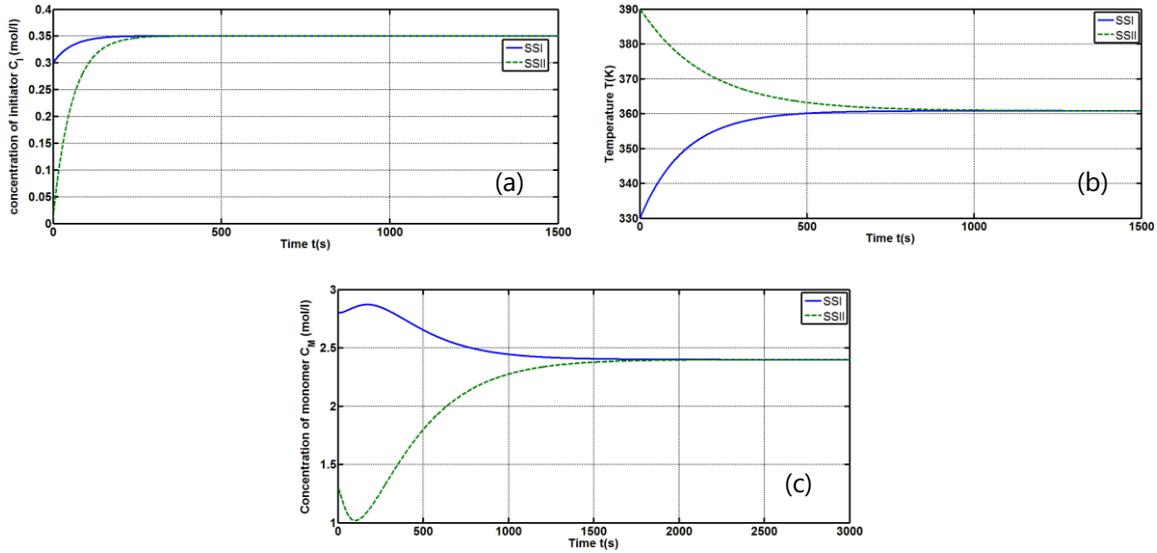
**Fig. 2:** Phase plane of the closed – loop system

$P_1 = (3.295; 0.408; 325.4)$   
 $P_2 = (2.407; 0.351; 360.7)$  and  
 $P_3 = (0.721; 0.0085; 415.7)$  under certain operating conditions (appendix B). Moreover, the steady state point  $P_2$  is unstable-open-loop equilibrium point while  $P_1$  and  $P_3$  are locally stable because the system trajectories originating from SSI and SSII converge to  $P_1$  and  $P_3$ , respectively. In the next subsection, we focus attention on stabilizing exponentially the FRP system

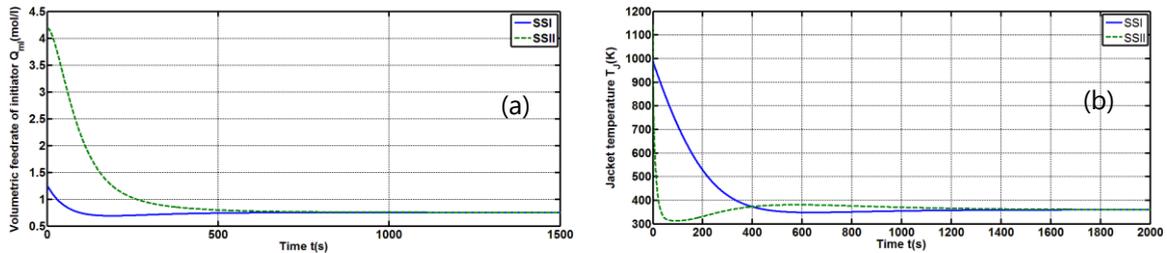
in  $P_2$  because the aforementioned reasons (section 3.2) by using the passivity-based controller (27) and (28).

### Closed – Loop Response

In the case, the passivity-based controller is designed and used for simulations with parameters:  $K_{T1} = 0.018$ ,  $K_{T2} = 0.005$ ,  $R_{d1} = 4$ ,  $R_{d2} = 1$ ,  $R_{d3} = 1$ ,  $\gamma_1 = 0.01$ ,  $\gamma_2 = 0.01$ . **Figure 2** shows that the closed-loop system's responses (regarding to two initial conditions SSI and SSII in **Table 2**)



**Fig. 3:** Closed-loop system's response: (a) concentration of initiator, (b) temperature (c) concentration of monomer



**Fig. 4:** Control input: (a)  $Q_{mI}$ , (b)  $T_J$ . Note also that the dynamics of actual control is input  $Q_2$  can be derived by using (21).

converge asymptotically to  $P_2$ . As a result, the polystyrene production process system in CSTR is stabilized exponentially globally at the desired equilibrium point.

Furthermore, **figure 3** (a), (b) and (c) shows the transient responses of state variables including the concentration of initiator  $C_I$ , the reactor temperature  $T$  and the concentration of monomer  $C_M$  in time domain, respectively. Besides,  $C_I$  and  $T$  (the directly controlled output) reaches the desired steady state after about 500s and 800s, respectively while the response

time of  $C_M$  is around 1500s.

Moreover, the dynamics of two input control variables  $Q_{IF}$  and  $T_J$  are given in **Figure 4 (a)** and **(b)**, respectively. As we can see that the dynamics of  $T_J$  for SSII is faster than that of for SSI in the beginning of reaction course because the heat-generation rate of reactor is greater than heat-removal rate in the case of SSII, so the temperature of coolant of jacket  $T_J$  varies quickly in order to stabilize the system (exponentially) at  $T^e = 360.7$  K.

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## CONCLUSION

In this work, we extended the method of feedback passivation via the natural decomposition of  $f(x)$  together with input coordinate transformations, and then proposed a passivity-based multivariable control via tracking error. Additionally, the new theoretical extensions were applied successfully for the exponential stabilization of the nonlinear chemical process including two inputs and two outputs: the continuous polystyrene production process in CSTR and the Van de Vusse reaction system. In fact, the approach can be totally generalized for the stabilization of a general multivariable chemical process, i.e. the process with  $m$  inputs and  $m$  outputs.

Besides, the numerical simulations shown that globally exponential stabilization of the polymerization system at the desired equilibrium point (including unstable-open-loop steady state) is guaranteed and the behaviors of input control are sufficiently smooth and physically admissible. However, in several cases, these control inputs may vary quickly to in the beginning of reaction course to stabilize the system. So, it poses a theoretical challenge which can be solve by consideration of controller with input saturations (Assala et al., 1997). Finally, the performance of closed-loop system under proposed control is also compared to that of under energy-based control (Hoang, Couenne, Jallut, & Le Gorrec, 2013).

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## APPENDIX A

Symbol	Quantity
$C_M$	: Concentration of monomer (styrene) in CSTR (mol/L)
$C_I$	: Concentration of initiator (AIBN) in CSTR (mol/L)
$C_S$	: Concentration of solvent in CSTR (mol/L)
$T$	: Temperature of CSTR (K)
$\rho$	: Average density of mixture in CSTR (kg/L)
$C_{M_{int}}$	: Initial concentration of monomer (styrene) in CSTR (mol/L)
$C_{I_{int}}$	: Initial concentration of initiator (AIBN) in CSTR (mol/L)
$T_{int}$	: Initial temperature of CSTR (K)

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## APPENDIX B

Symbol	Quantity	Value
$Q_{MF}$	: Flow rate of monomer (styrene) in the feed (1/s)	1.0
$Q_{IF}$	: Flow rate of initiator (AIBN) in the feed (1/s)	0.75
$Q_{SF}$	: Flow rate of solvent in the feed (1/s)	1.0
$C_{MF}$	: Concentration of monomer (styrene) in the feed (mol/L)	9.2
$C_{IF}$	: Concentration of initiator (AIBN) in the feed (mol/L)	1.5
$C_{SF}$	: Concentration of solvent in the feed (mol/L)	4.0
$T_F$	: Inlet temperature of feed (K)	298.15
$T_J$	: Jacket temperature (K)	360
$V$	: Reactor volume (L)	1000
$R$	: Ideal gas law constant J/(mol K)	8.314
$f$	: Efficiency factor of initiator (AIBN)	0.6
$UA$	: The global heat transfer coefficient (W.m <sup>2</sup> /K)	600
$\Delta H$	: Heat of the polymerization reaction (J/mol)	-74400
$c_p$	: Heat capacity of the reacting	1855

mixture in CSTR  
(J.kg/K)

$c_{pF}$	: Heat capacity of the feed (J.kg/K)	1978
$\rho c_p$	: Heat capacity of the feed J/(1.K)	1507.248

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