PASSIVITY-BASED MULTIVARIABLE CONTROL FOR THE STABILIZATION OF CONTINUOUS STYRENE POLYMERIZATION REACTOR

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ABSTRACT

Chemical process systems, and among them free-radical polymerization (FRP) systems, belong to complex nonlinear dynamical systems and usually exhibit highly nonlinear characteristics owing to the reaction kinetics and the constitutive equations caused by transport phenomena, heat and mass transfer. Consequently, this may make the process operated under multiple steady states behavior and therefore fairly difficult to operate and stabilize the systems at the middle steady state with acceptable quality and process performance. In this context, this work proposes an advanced nonlinear control strategy based on the passivity theory and passivity-based control (PBC) (also, briefly speaking, passivity-based approach (PBA)) for the stabilization of a class of FRP processes taking place in a continuous stirred tank reactor (CSTR) at a desired set-point (including open-loop-unstable steady state). More precisely, it is worth noting that the PBA has been recognized as a useful and systematic tool for nonlinear control design due to its potential applications for the stabilization of mechanical and electromechanical systems. Recently, the PBA has been extended and utilized to stabilize a process system. Due to the ubiquity of process systems in biochemical, biotechnology and materials processing industries, an extensive attention has been paid and remains to this kind of systems for the purpose of control design. As a contribution to this active research area, in this work, we adopt the PBA to stabilize FRP systems subject to multiple steady states behavior at a desired equilibrium point (including open-loop-unstable steady state). The polystyrene production process in CSTR is used as an case study to illustrate the theoretical developments in this work.

Essentially, the present work has four main sections as follows. Firstly, the theoretical development of PBA established by the basis of feedback passivation is extended to stabilize exponentially a class of general MIMO nonlinear systems. Secondly, before applying this control design method for the polystyrene production process in a CSTR

which is considered as a case study, the dynamical behaviors of this system are analyzed by using two different approaches where the first one is built by the tools of system theory and the second one is associated with principle of heat balance to determine the desired set-point. Thirdly, once the control problem of the nonlinear chemical process is stated, the PBC is applied to design the feedback laws for the exponential stabilization of the polymerization process at the desired equilibrium point. Finally, the numerical simulations show the effectiveness of this control design method as well as evaluate the effects of the uncertain operating and physical parameters caused by noise and/or disturbance in order to test the robustness of closed-loop system. Additionally, the control performance of closed-loop system under control of the proposed feedback laws is also compared with that under control of a proportional-integral (PI) control in terms of the merit scores of errors including ISE, IAE and ITAE.

ABSTRAK

Sistem proses kimia, seperti sistem pempolimeran polistirena radikal bebas (FRP), tergolong dalam sistem dinamik bukan linear yang kompleks dan biasanya mempamerkan ciri-ciri yang tidak linear kerana kinetik reaksi dan persamaan konstitutif yang disebabkan oleh fenomena pengangkutan, pemindahan haba dan jisim. Akibatnya, ini boleh menjadikan proses itu beroperasi di bawah tingkah laku keadaan berganda dan oleh itu agak sukar untuk mengendalikan dan menstabilkan sistem pada keadaan mantap dengan kualiti dan prestasi proses yang boleh diterima. Dalam konteks ini, penyelidekan ini mencadangkan strategi kawalan linear lanjutan berdasarkan teori pasif dan kawalan berasaskan pasif (PBC) (juga, secara ringkas, pendekatan berasaskan pasif (PBA)) untuk menstabilkan kelas proses FRP yang berlaku dalam reaktor tangki yang berterusan (CSTR) pada titik set yang dikehendaki (termasuk keadaan terbuka yang tidak stabil). Lebih tepat lagi, perlu diperhatikan bahawa PBA telah diiktiraf sebagai alat yang berguna dan sistematik untuk reka bentuk kawalan linear disebabkan oleh aplikasi potensinya untuk penstabilan sistem mekanikal dan elektromekanik. Bagaimanapun baru-baru ini, PBA telah diperluaskan dan digunakan untuk menstabilkan sistem proses kimia saperti biokimia, bioteknologi dan industri pemprosesan bahan. Sebagai sumbangan kepada bidang penyelidikan aktif ini, dalam kerja ini, kami mengguna pakai PBA untuk menstabilkan sistem pempolymeran polistyrena FRP tertakluk kepada tingkah laku keadaan berganda pada titik keseimbangan yang dikehendaki (termasuk keadaan mantap terbuka-tidak mantap) dalam kajian kes ini.

Pada asasnya, kerja penyelidikan ini mempunyai empat bahagian utama seperti berikut. Pertama, perkembangan teori PBA berdasarkan passivation maklum balas diperluaskan dan diperkatakan untuk menstabilkan secara eksponensial kelas sistem nonlinear MIMO. Kedua, sebelum menggunakan kaedah reka bentuk kawalan untuk proses pengeluaran polistiren dalam CSTR yang dianggap sebagai kajian kes, tingkah laku dinamiknya dianalisis dengan menggunakan dua pendekatan yang berbeza di mana yang pertama ditubuhkan oleh alat teori sistem dan yang kedua dikaitkan dengan prinsip keseimbangan haba untuk menentukan keadaan stabil yang diingini. Ketiga, sebaik sahaja masalah kawalan proses kimia bukan linear dicadangkan, PBC digunakan untuk merancang teknik maklum balas untuk penstabilan eksponen proses pempolimeran di titik keseimbangan yang dikehendaki. Akhir sekali, simulasi berangka menunjukkan keberkesanan kaedah reka bentuk kawalan ini serta menganalisis kesan parameter operasi dan fizikal yang tidak menentu yang disebabkan oleh berapa jenis gangguan untuk menguji keteguhan sistem gelung tertutup. Di samping itu, prestasi kawalan undang-undang maklum balas yang dicadangkan juga dibandingkan dengan kawalan yang berkadar proportional-integral (PI) dari segi skor merit bedasar ralat saperti ISE, IAE dan ITAE.

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C_I	:	Concentration of initiator (AIBN) in CSTR.
C_I^e	:	Steady state of concentration of initiator.
C_M	:	Concentration of monomer (styrene) in CSTR.
C_M^e	:	Steady state of concentration of monomer.
C_R	:	Concentration of polymer radical.
C_S	:	Concentration of solvent in CSTR.
C_{IF}	:	Concentration of initiator (AIBN) in the feed.
$C_{I\mathrm{int}}$	:	Initial concentration of initiator (AIBN) in CSTR.
C_{MF}	:	Concentration of monomer (styrene) in the feed.
$C_{M\mathrm{int}}$	:	Initial concentration of monomer (styrene) in CSTR.
P^e	:	Equilibrium point of the system.
Q_g	:	Heat-generation rate.
Q_r	:	Heat-removal rate.
Q_{IF}	:	Volumetric flow rate of initiator (AIBN) in feed.
Q_{MF}	:	Volumetric flow rate of monomer (styrene) in feed.
Q_{SF}	:	Volumetric flow rate of solvent in feed.
R	:	Ideal gas law constant.
T	:	Temperature of reacting mixture in CSTR.
T^e	:	Steady state of reactor temperature.
T_F	:	Inlet temperature of feed in.
T_J	:	Jacket temperature.
T_{int}	:	Initial temperature of reacting mixture in CSTR.
V	:	Reactor volume.
$V(x)$	:	Storage function of passive system.

ΔH	:	Heat of polymerization reaction.
c_p	:	Heat capacity of reacting mixture in CSTR.
c_{pF}	:	Heat capacity of feed.
f	:	Efficient factor of initiator (AIBN).
$s(u, y)$	:	Supply rate of passive system corresponding to input u and ouput y.
u	:	Actual control input.
x	:	State variable of nonlinear system.
x_d	:	State variable of reference trajectory.
$y,\ h(x)$	:	Output of nonlinear system.
$K_1,\ K_2$	:	Turning parameters of reference trajectory.
$\beta_{\max}$	:	The maximum eigenvalue of matrix (R_{di}).
$\gamma_1,\ \gamma_2$	:	Turning parameters of input coordinate transformations.
$\lambda_1,\ \lambda_2,\ \lambda_3$	:	Eigenvalues of the Jacobian matrix of the linearized system near equilibrium point.
$\lambda_{\min}$	:	The minimum eigenvalue of matrix ($R_{di} R_I Rdi$).
ρ	:	Density of reacting mixture.
$\tau_1,\ \tau_2$	:	Turning parameters of integral actions.
υ	:	Internal dynamic control.
$L_{f(x)} V(x)$	:	Lie derivative of the storage function $V(x)$ along the vector-valued function $f(x)$.
AI	:	Artificial intelligent.
AIBN	:	Azobisisobutyronitrile.
ANN	:	Artificial neural networks.
CSTR	:	Continuous stirred tank reactor.

FLC : Fuzzy logic control.

FRP : Free-radical polymerization.

GA : Genetic algorithm.

GMC : Generic model control.

IAE : Integral absolute error.

IDA-PBC : Interconnection and damping assignment Passivity-based control.

IMBC : Inverse model-based control.

ISE : Integral squared error.

ITAE : Integral-time weighted absolute error.

MIMO : Multi input multi output.

MMA : Polymethylmethacrylate.

MPC : Model predictive control.

NAMW : Number average molecular weight.

NMPC : Nonlinear model predictive control.

PBA : Passivity-based approach.

PBC : Passivity-based control.

PCH : Port-controlled Hamiltonian.

PD : Polydispersity.

PI : Proportional integral.

PID : Proportional integral derivative.

PS : Polystyrene.

SISO : Single input single output.

UA : Global heat transfer coefficient.

LIST OF APPENDICES

CHAPTER 1: INTRODUCTION

This chapter aims to give a general background of this work including the overview of the polystyrene production process in CSTR, the recent advanced control strategies to stabilize this system at a desired set-point as well as the applications of passivity-based control (PBC) for nonlinear dynamical systems (Section 1.1). The problem statement that leads the motivation together with the necessity of this work are subsequently emphasized in Section 1.2 while the main objectives of this research work are shown in Section 1.3. Finally, the research scope and the dissertation organization are given in Section 1.4.

1.1 Background

Free-radical polymerization (FRP) processes have been widely operated in industry to synthesize various types of plastic such as polystyrene, polymethylmethacrylate, LDPE and others (Krzysztof Matyjaszewski, 2003; Meyer & Keurentjes, 2005). Together with experimental researches (George & Hayes, 1975; Lederle & Hübner, 2017; Sammaljärvi et al., 2016; Schmidt, Clinch, & Ray, 1984), the theoretical studies on the mathematical modelling, the optimal operation and the process control of FRP processes have also attracted much attention of practitioners as well as researchers recently. This is due to the fact that such process exhibits highly nonlinear characteristics caused by the nonlinearity of reaction kinetics via the Arrhenius laws and the transport phenomena via constitutive equations, etc. Consequently, this can give rise to abnormal dynamical behaviors such as the steady-state multiplicity behavior, the limit cycle and the bifurcation behavior, etc. during the transient phase of the open-loop system dynamics (Freitas Filho, Biscaia, & Pinto, 1994; Jaisinghani & Ray, 1977; Pinto & Ray, 1995; Russo & Bequette, 1998). Furthermore, from the practical viewpoint, FRP reactors are usually operated at the unstable-open-loop equilibrium point because this position can compromise both economic interest and engineering constraints (Bruns & Bailey, 1975). In fact, the conversion of polymerization reaction is indeed quite poor at low-temperature steady state, thereby producing a small amount of polymer although the reactor is asymptotically stable without control. Similarly, even though the high-conversion steady state at high temperature is also locally stable, the polymerization reactor face engineering problem, that is, the catastrophic solidification caused by the high viscosity of reacting mixture despite economic benefit makes difficult to collect the polymer product in the outlet stream. To overcome the theoretical challenge, an appropriate feedback control which is capable of canceling the inherent nonlinearities (possibly together with parameter uncertainty), and enabling us to stabilize asymptotically the polymerization system at the desired steady state is vitally necessary.

Among advanced control strategies, the passivity-based control (PBC) has been considered as a useful design tool of control theory because its design procedure in general has been studied systematically for a class of nonlinear dynamical systems (Bao & Lee, 2007; Brogliato, Lozano, Maschke, & Egeland, 2007; Ortega, Loría, Nicklasson, & Sira-Ramírez, 1998). Moreover, the passivity-based approach has been applied successfully for a broad class of mechanical, electrical and electromechanical systems with satisfactory results (García-Canseco, Astolfi, & Ortega, 2004; Ortega & García-Canseco, 2004b; Ortega, Jiang, & Hill, 1997; Ortega, Van der Schaft, Mareels, & Maschke, 2001). However, applications of PBC in process system, especially chemical processes, have been limited and remain open because the links between the system theory and the energy of reacting systems were poorly understood (Eberard, Maschke, & Van der Schaft, 2007; Favache & Dochain, 2009; Hangos, Bokor, & Szederkényi, 2001; Hoang, Couenne, Jallut, & Le Gorrec, 2012; Hoang, Couenne, Le Gorrec, Chen, & Ydstie, 2013). Therefore, the theoretical developments as well as their applications for process system have become the interesting topic recently, and many attempts have been made to overcome the challenge in this research area (Alonso & Erik Ydstie, 1996; Favache & Dochain, 2010; Favache, Dochain, & Winkin, 2011; Hangos et al., 2001; Hoang, Couenne, Dochain, & Le Gorrec, 2011; Hoang, Couenne, Jallut, & Le Gorrec, 2011; Hoang et al., 2012; Hoang, Couenne, Le Gorrec, et al., 2013; Le Gorrec & Matignon, 2013; Otero-Muras, Szederkényi, Hangos, & Alonso, 2008; Ramírez, Le Gorrec, Maschke, & Couenne, 2016; Ramírez, Sbarbaro, & Ortega, 2009; Ydstie, 2002; Ydstie & Alonso, 1997).

1.2 Problem statement

In this work, the polystyrene production process in CSTR, which is a typical FRP process, is considered as a case study for the stability analysis and the control design in the framework of PBC. The naturally inherent properties of the system dynamics (e.g. the transport phenomena and the reaction kinetics, etc.) pose theoretical challenges related to the highly nonlinear characteristics, which cause the instability of the system trajectory as shown via the observation of unexpected behaviors such as the steady-state multiplicity behavior and bifurcation behavior. On the other hand, the dynamical analysis showed that although the FRP reactor subject to steady-state multiplicity behavior is (locally) stable at the two steady states corresponding to the lowest temperature steady state and the highest one, both of these steady states cannot compromise economic issue (high conversion) and engineering constraint (hight viscosity of product and safe operation in practice). Therefore, from both the theoretical and practical viewpoints, the system requires a control scheme which is capable of stabilizing the system at a desired equilibrium point (including the unstable-open-loop steady state)

In addition, although the passivity theory is clearly recognized as an effective control design tool for the mechanical, electrical systems and single-input single-output (SISO) chemical processes while numerous chemical systems with multivariable dynamics (MIMO systems), especially the FRP processes in CSTR have been limited. Therefore, this research primarily focuses attention on controlling and stabilizing a class of MIMO nonlinear chemical processes, where the FRP process in the CSTR is a case study, at the desired set-point (including the open-loop-unstable steady state) by using the multivariable PBC approach [1]. It worth noting that the polystyrene production process in the CSTR is a representative and typical example of multivariable FRP process and the proposed PBA includes a theoretically extensive version of the control design method published by Sira-Ramírez (1998, 1999) together with provides additional results when a MIMO chemical process is involved in practical operation. Furthermore, since the control performance of closed-loop system can be disturbed by different kinds of noise and/or disturbance in practice, hence, the tests and evaluations of robustness for closed-loop system are vitally necessary.

1.3 Research objectives

This work belongs to the field of process control, particularly advanced control strategies for nonlinear chemical processes and to tackle the theoretical issues stated in the problem statement (Section 1.2), the main objective is the **stabilization of a class of MIMO nonlinear systems, particularly multivariable FRP systems in CSTR at the desired equilibrium point (including unstable steady state) by using passivity-based control** and the line of this research work to obtain the primary objective is given as follow.

1. Analyze the dynamical behavior of the polystyrene production process in a CSTR and determine the desired steady state of the system (the middle-conversion equilibrium point).

2. Design a passivity-based multivariable controller to stabilize the continuous FRP reactor of styrene at the desired steady state. The proposed design procedures are general and can be applied to any kind of systems having same assumptions considered.

[1] Because numerous (bio)chemical processes are multi-input multi-output (MIMO) systems, thus, the considerations of such systems rather than single-input single-output systems for control design are more practical under operation.

3. Evaluate the robustness of closed-loop system under impacts of noise and disturbance.

4. Compare the performance of the closed-loop system under control of the PBC with that under control of a conventional proportional-integral (PI) controller.

1.4 Research scope and organization of dissertation

This research work deals with the design of multivariable PBC for a class of FRP process where the polystyrene production process in CSTR is a case study. Hence, this work belongs to the field of process control and the knowledge used to achieve all the objectives is strongly related to system theory and chemical engineering.

Firstly, the method of feedback passivation design via input coordinate transformations is extended to a class of general MIMO nonlinear systems. More precisely, the system dynamics can be rendered passive through input coordinate transformations under certain conditions. The resulting passive system is subsequently rewritten into a canonical form related to the Port-controlled Hamiltonian (PCH) representation. Additionally, this structure allows showing explicitly the physical meaning of the system including the dissipative, non-dissipative terms and supply rate in terms of the new inputs. A feedback law based on tracking error is then designed for the globally asymptotic stabilization of the polymerization system at the desired reference trajectory passing through the set point.

Secondly, the case study with the polystyrene production process in the CSTR is then studied for the illustrations of the results developed above. The steady-state multiplicity behavior of the system is explained and described by two different ways:

1. Using the Van Heerden diagram and the principle of heat balance in chemical engineering.

2. Using the approximate linearization technique and the stability analysis which is based on the Routh-Hurwitz criterion.

In addition, bifurcation behavior in terms of two bifurcation parameters, including the jacket temperature of CSTR and the volumetric flow rate of initiator (AIBN), are analyzed to predict the multiplicity behavior of the FRP reactor in different operating regions.

Thirdly, after the abnormal behavior of the polymerization process is expressed explicitly to determine the desired set-point through dynamical analyses above, the proposed theoretical developments of PBC are applied to design feedback laws for the asymptotic stabilization of continuous polymerization reactor of styrene. The simulation results including the phase plane, the transient responses of state variables together with the behavior of manipulated variables will then reveal the stability characteristics of closed-loop system. Furthermore, the robustness of the closed-loop system is tested and evaluated by numerical simulations because the chemical processes are usually operated under impacts of noise and/or disturbance.

This dissertation is organized as follows. The complete literature review of the FRP reactor is subsequently presented in Chapter 2. In Chapter 3, Section 3.1 introduces briefly the Lyapunov-based stability analysis including the approximate linearization technique and the Lyapunov theorem whereas Section 3.2 reviews the fundamentals of passivity theory and passive system. In fact, such kind of knowledge which lays the solid foundation of the present research work is vitally important. The theoretical developments of passivity-based control (PBC) through feedback passivation are derived in Section 3.3 and Section 3.4 where the theoretical developments including the feedback passivation design of MIMO system, the canonical form of resulting passive system together with the feedback laws via tracking error are studied and expressed explicitly. Following Chapter 3, Chapter 4 shows the explicit mathematical model of FRP process in CSTR in Section 4.1. Application of linearization technique for the stability analysis of the continuous styrene polymerization reactor is given in Section 4.2. More precisely, the Jacobian matrix of approximately linearized system is computed for the system-theory-based on stability analysis while the mathematical formula of equilibrium points, the heat-generation rate and heat-removal rate are expressed explicitly for the heat-balance-based on stability analysis. The application of PBC to design feedback laws for the asymptotic stabilization of the process is subsequently given in Section 4.3. For the sake of illustration of the theoretical developments, a number of numerical simulations including the open-loop responses and closed-loop ones are carried out in Chapter 5. Finally, the summarized conclusions of this research work together with the prospective future works are given in Chapter 6. The flowchart diagram of this research work is shown in Figure 1.1.

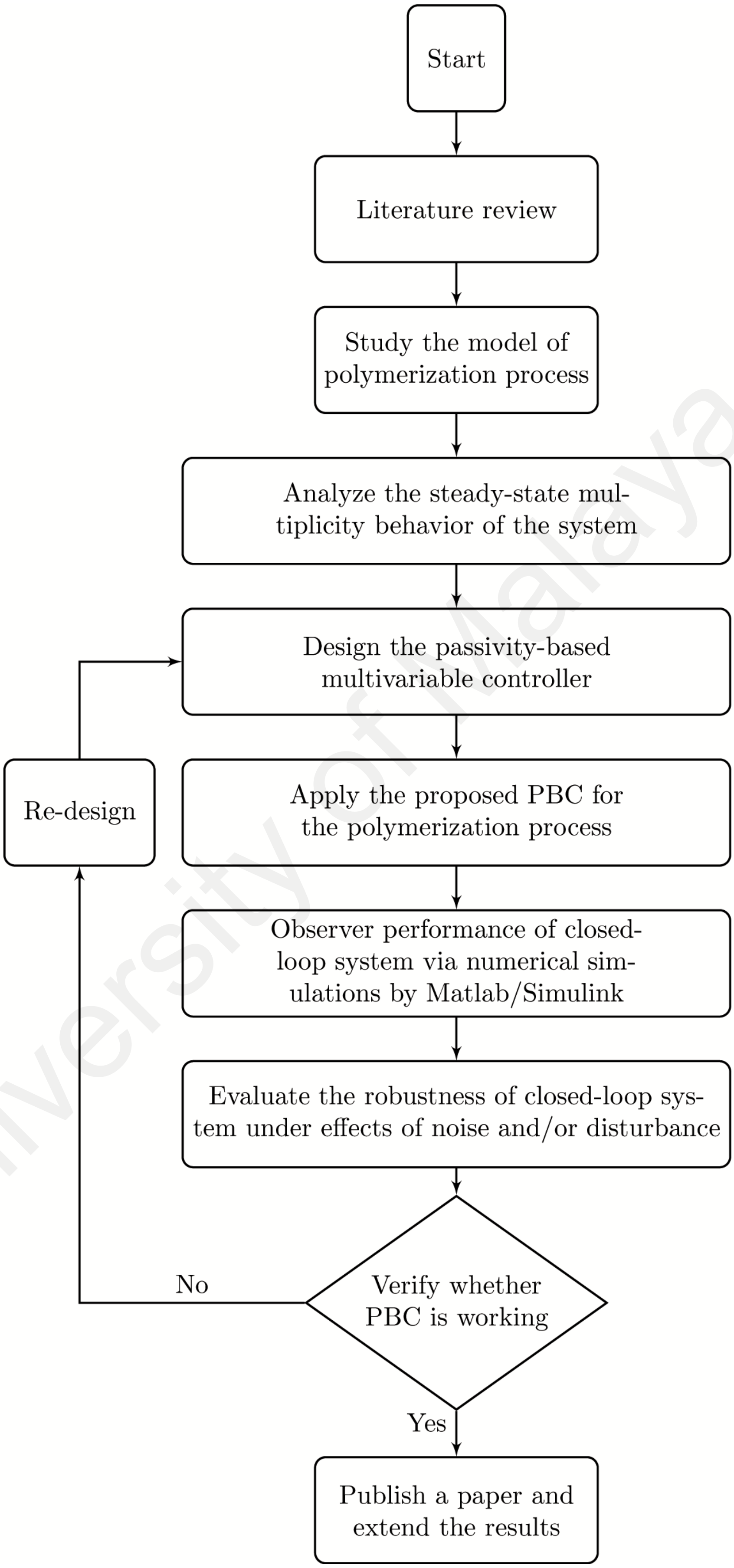


Figure 1.1: Flow chart diagram of this research work

CHAPTER 2: LITERATURE REVIEW

In the first part of the chapter (Section 2.1), the previous researches on the mathematical modeling, the optimal operation and the process control of a class of the free-radical polymerization (FRP) processes taking place in a continuous stirred tank reactor (CSTR) are summarized to emphasize the abnormal dynamical behavior of the system such as the steady-state multiplicity behavior, the limit cycle and the bifurcation behavior. It is shown that these unexpected behaviors caused by the inherent nonlinear properties result in the unstable dynamics. From this challenge, the control design problem to stabilize globally asymptotically the system dynamics at the desired equilibrium point (including middle-conversion steady state) is stated. During the last few decades, a number of advanced control strategies have been proposed and designed to overcome this challenging issue. We shall, therefore, summarize and give subsequently an overview in order to show that the considered control problem is indeed an interesting topic in the control community. Nonetheless, these reviewed approaches depend heavily on the mathematical tools and thus may make their control design procedure more complex.

Among advanced nonlinear control strategies, the passivity theory and passivity-based control (PBC) are recognized clearly as an effective nonlinear control design tool. In the second part of the chapter (Section 2.2), their applications in the mechanical, electrical and electromechanical systems are outlined to illustrate potential advantages for the control design and the stabilization of such systems. Although the applications of passivity-based approach for process control remain open, several attempts are made to overcome the structural restrictions of the system such as relative degree being more than one and unstable zero dynamics; and build connections between the reacting system's energy and system theory. This section, therefore, reviews progress to highlight the previous theoretical developments together with applications of PBC in process control, especially in chemical systems.

2.1 The free-radical polymerization reactor and the polystyrene production process in CSTR

2.1.1 Process description and nonlinear characteristic of continuous FRP process system

Continuous FRP processes have been widely operated and studied for over 40 years but some problems still remain open, for example, the gel effect on the modeling, the optimal operation as well as the process control, which is to obtain a trade-off between economic benefits and engineering restrictions, e.g. the safe operation, the structure of reactors, etc. (Krzysztof Matyjaszewski, 2003; Meyer & Keurentjes, 2005). In practice, the operation of FRP processes can be carried out in either batch reactors or CSTRs under restriction of the free-radical reaction mechanism which is described in Table 2.1 (see also in the literature (Jaisinghani & Ray, 1977; Russo & Bequette, 1998; Van Dootingh, Viel, Rakotopara, Gauthier, & Hobbes, 1992)).

Table 2.1: The free-radical polymerization mechanism

Initiator decomposition	$I \xrightarrow{k_d} 2R^*$
Initiation	$R^* + M \xrightarrow{k_i} P_1^*$
Propagation	$P_n^* + M \xrightarrow{k_p} P_{n+1}^*$
Chain transfer to monomer	$P_n^* + M \xrightarrow{k_{trM}} P_n + P_1^*$
Chain termination by combination	$P_n^* + P_m^* \xrightarrow{k_{tc}} P_{n+m}$
Chain termination by disproportionation	$P_n^* + P_n^* \xrightarrow{k_{td}} P_n + P_m$

In Table 2.1, M and I denote the monomer (styrene) and initiator (AIBN)[1], respectively. Also, R^* is the free-radical specie which is produced by the reaction of initiator decomposition. Additionally, P_n^* and P_m^* represent the growing polymer chain with length n and m, respectively while P_n, P_m and P_{n+m} express the terminated polymer chains with length n, m and $n + m$, respectively.

[1] AIBN stands for Azobisisobutyronitrile.

The practical operation of FRP process is usually accompanied by the unexpected nonlinear dynamical behavior such as multiplicity behaviors, limit cycle or bifurcation behavior caused by the inherent characteristics of the system dynamics, e.g. reaction kinetics and transport phenomena, etc. For instance, the multiplicity behavior displays that a nonlinear system (e.g. a chemical process) can have several different equilibrium points, which are locally stable or unstable. Generally speaking, with a set of specific operating conditions, the dynamical system trajectories can approach to different equilibrium points, depending on the initial conditions of the system trajectory (Bequette, 1998; Levenspiel, 1998; Luyben, 1990; Seborg, Edgar, Mellichamp, & Doyle, 2011). Actually, the locally stable equilibrium point at low temperature has no economic benefit because of bad conversion while the steady state at the high temperature causes engineering problems. For example, the process system may come into unsafe operation or the final product in outlet stream can be affected negatively or spoilt because the process system is stabilized at the high temperature (Aris, 2013; Aris & Amundson, 1958; Subramanian & Mjalli, 2009). Moreover, because the stability property of system dynamics is not global (just local), consequently the product quality is not fixed and clearly affected when the system trajectory starts at different initial conditions, i.e., the steady state of reacting system in the operation is varying according to the initial conditions of state variables. As a result, from the economic and engineering point of view, the equilibrium point with the middle conversion, i.e., unstable-open-loop steady state, is normally chosen as the desired equilibrium point for the purpose of optimal operation, that is, the reaction yield is acceptable and the reactor temperature is sufficiently low.

Furthermore, the bifurcation behavior[2], which also exists in nonlinear system dynamics, is an alteration in periodic orbits or equilibrium points when one or some operating parameters vary. For example, a stable-open-loop equilibrium point becomes an unstable one or vice versa when the operating parameters changes in the wide range. Additionally,

[2]We refer the readers to Govaerts (2000); Khalil (2002) and references cited therein for the rigorous definition of bifurcation behavior and the clarification of different bifurcation diagrams.

the points where the bifurcation behavior occurs are called bifurcation points and usually shown in the bifurcation diagrams.

In practice, the abnormal phenomena such as the steady-state multiplicity behavior and the bifurcation behavior cause the instability of system dynamics in the viewpoint of safe and optimal operation. Furthermore, such abnormal phenomena are verified not only by the simulations studies (Hamer, Akramov, & Ray, 1981; Schmidt & Ray, 1981; Teymour & Ray, 1989) but also the experimental investigations (Schmidt et al., 1984; Teymour & Ray, 1992a, 1992b).

Moreover, the complexity and dependence of these behaviors on the operating parameters have been studied further and obtained by numerous studies in the literature (Freitas Filho et al., 1994; Melo, Biscaia, & Pinto, 2003; Melo, Sampaio, Biscaia Jr, & Pinto, 2001; Russo & Bequette, 1998; Skogestad, Russo, & Bequette, 1997). In these frameworks, the conditions of existence of solutions with respect to the steady-state modeling equations allow predicting the steady-state multiplicity behavior under the different operating conditions through the purely mathematical tools such as the Lyapunov function of system theory and the catastrophic theory. Although the approaches can be applied to analyze the dynamical behavior for a class of nonlinear processes, they rely heavily on the mathematical tools and therefore seem to be complicated and not be applied easily to another process in the light of realization viewpoint.

In this work, the approaches based on the approximate linearization technique and the physics-based principle (also known as the fundamentals of heat balance) are utilized to analyze the dynamical behavior of the nonlinear system near the equilibrium points with applications to the case of polystyrene production process in the CSTR. It is well-known that these methods are not only rather simple as well as systematic but also explore the physical stability of steady state, and although they can be found in some literature with applications for different physical or chemical systems, their adoptions for a certain (nonlinear) process usually play a dispensable role in the exact determination of set point or desirable equilibrium point for control problem. More precisely, the original nonlinear system dynamics is firstly approximated to a linearized model at each equilibrium point, and then the poles of the approximately linearized system will reveal the inherent dynamical properties of the nonlinear system near the corresponding equilibrium point (Khalil, 2002). In fact, the equilibrium point of a nonlinear system can be a stable/unstable node or locus or saddle point if this is also a stable/unstable node or locus or saddle point of the approximately linearized system, respectively (Bequette, 1998; Khalil, 2002). Besides, by using the principle of heat balance (Hoang & Dochain, 2013a; Levenspiel, 1998; Van Heerden, 1953), the Van Heerden diagram representing the curve of heat-generation rate Q_g and the straight line of heat-removal rate Q_r in terms of temperature will not only illustrate the existence of three different equilibrium points of reacting system (the number of intersections between Q_g and Q_r) under certain operating conditions but also give the helpful discussions about the physical meanings of steady-state multiplicity behavior of the reacting system.

Additionally, the analysis of bifurcation behavior has a key role in the prediction of abnormal dynamics such as multiplicity and/or limit cycle in the wide range of operating conditions. Hence, this research work also analyzes the bifurcation behavior of the polystyrene production process in the CSTR in terms of two bifurcation parameters including the jacket temperature and the volumetric flow rate of the initiator to predict the occurrence of steady-state multiplicity behavior with different sets of operating conditions. Based on such analysis, the operating regions where the multiplicity behavior of the continuous polystyrene reactors appears will be obtained.

2.1.2 Application of control strategies for FRP reactors

As mentioned before, the FRP reactor is usually operated at the unstable-open-loop steady state, i.e., the middle-conversion equilibrium point, because this point is able to compromise both economic advantage (i.e. the polymer conversion is reasonable) and engineering constraints (i.e. the safe operation is guaranteed and the viscosity of product is not very high), so the polymer products can be collected easily (Assala, Viel, & Gauthier, 1997; Van Dootingh et al., 1992; Viel, Busvelle, & Gauthier, 1995). As a result, a control scheme, which is capable of stabilizing the system dynamics at the desired equilibrium point (including the unstable-open-loop point), is vitally necessary. In fact, control design methodologies applied to chemical reactors, especially the FRP reactors, have become an attractive topic recently in the process control community. Consequently, a variety of different design strategies based on firm foundations including the Lyapunov theorem (Khalil, 2002), the artificial intelligence (AI) (Nguyen, Prasad, Walker, & Walker, 2002), and model predictive control (MPC) (Grüne & Pannek, 2016) have been proposed recently.

2.1.2.1 AI-based control schemes

Three main design tools including the fuzzy logic, the artificial neural networks (ANN) and the genetic algorithm (GA) (Nguyen et al., 2002) have laid a solid groundwork for the AI-based control schemes. Actually, the main aim of these strategies is to apply the practical knowledge of human beings for the purpose of control design. For example, the process engineers can ask the operators to write down a set of rules associated with the "IF . . . THEN . . . " rules on how to control the process according to their experience. Obviously, such approach which is so-called the fuzzy-logic-based controller emulates the decision-making process of the human; the completely accurate mathematical model of process system seems to be unnecessary, thereby handling the mismatch mathematical model or the uncertain physical and operating parameters of the process. In general, the set of "IF . . . THEN . . . " rules for the control design or the heuristic information can be derived not only from the experience of practitioners and control engineers but also from the development of control algorithms (Passino, Yurkovich, & Reinfrank, 1998). Furthermore, apart from fuzzy logic, the neural networks and the generic algorithm (GA) have been well recognized as useful tools based on the self-learning process of human beings and have been applied successfully not only for the control design but also for the system identification and the optimization (Nguyen et al., 2002).

Actually, the design tools of intelligent control are also combined to create the novel control strategies. For example, ANN and GA have been connected recently with other control schemes such as the predictive control, inverse-model-based control and adaptive method with plenty of excellent applications especially in chemical processes. These combinations have been categorized in the research work of Hussain (1999) and the references cited therein.

As far as the FRP reactors including the batch reactors and CSTRs are concerned, a variety of control strategies established by the design tools of artificial intelligence are proposed in many previous studies. Table 2.2 summarizes the applications of AI-based control schemes for a class of FRP reactors.

However, the global stabilization of closed-loop system under the AI-based control strategies cannot be proved theoretically because such control schemes are designed by using trial-error solutions and the tools of the stability analysis of (nonlinear) system such as the Routh-Hurwitz criterion or Lyapunov theorem are not utilized during the period of control design (Aracil, Heredia, & Ollero, 2000). In fact, the properties of the closed-loop system dynamics are just verified by numerical simulations and experiments in the laboratory. Therefore, the stabilization property of system cannot be actually guaranteed in the wide range of operating conditions.

2.1.2.2 Model predictive control (MPC)

The model predictive control (MPC) schemes have been studied and developed for a few decades to deal with the multivariable constrained control problems (Mayne, 2014; Morari & Lee, 1999). More precisely, the MPC schemes aim to find the optimal control trajectory based on the continuous/discrete process model by solving the constrained finite optimization problem (Mayne, Rawlings, Rao, & Scokaert, 2000) or determine the

Table 2.2: Applications of AI-based control for stabilization of FRP reactors

System	Control strategy	Manipulated variables	Reference
Batch polymerization reactor of PS	Fuzzy logic control with genetic algorithm	Flow rate of coolant water	(Altinten et al., 2006)
Batch polymerization reactor of MMA	PID-fuzzy logic control	Flow rate of coolant water	(Fileti et al., 2007)
Batch polymerization reactor of MMA	• Neural networks-based generic model control (GMC) • Neural networks-based inverse model-based control (IMBC)	Heater power	(Ekpo & Mujtaba, 2008)
Batch polymerization reactor of MMA	Neural networks-based batch-to-batch optimal control strategy	Heater power	(J. Zhang, 2008)
Batch polymerization reactor of PS	Self-tuning PID with genetic algorithm	Flowrate of coolant water	(Altınten et al., 2008)
Batch polymerization reactor of PS	Applied generic model control (GMC)	Heater power	(Özkan et al., 2009)
Batch polymerization reactor of PS	Applied rule-based Takagi - Sugeno fuzzy controller	Reactor cooling water temperature	(Sadoghi Yazdi et al., 2009)
Batch polymerization reactor of PS	• ANN-based MPC • Artificial fuzzy logic control (FLC) • GMC	Heater power	(Hosen et al., 2014)

control input by solving repeatedly online the finite horizon optimal control problem (Raff, Ebenbauer, & Allgöwer, 2007).

In practice, the linear/nonlinear MPC schemes have been applied to design the feedback laws for a variety of process systems such as the paste thickener in the mineral processing (Tan, Bao, & Bickert, 2017; Tan, Setiawan, Bao, & Bickert, 2015), the distillation processes (Balasubramhanya & Doyle III, 2000), the pH neutralization process (Hermansson & Syafiie, 2015), etc. In this section, Table 2.3 gives a shortlist of applications of class of MPC strategies such as NMPC and NNMPC for FRP batch reactors and CSTR.

In some of these applications, MPC schemes alone cannot naturally guarantee the global stabilization of closed-loop system due to finite horizon optimization (Mayne, 2014). Therefore, these control strategies need to be combined with the stability constraints strongly related to the Lyapunov functions.

2.1.2.3 Model-based approach

The model-based control strategies enable us to derive naturally the Lyapunov function, and therefore guarantee the asymptotic stabilization of the closed-loop system because the Lyapunov function candidate to satisfy the Lyapunov theorem (Khalil, 2002) is proposed in the period of control design. In the area of process control of FRP reactors, a class of control strategies was designed to eliminate the high nonlinear characteristics and stabilize asymptotically the system at the desired steady state (including the middle-conversion steady state). For instance, the feedback laws designed by using the input-output linearization technique with/without input constraints were proposed in (Assala et al., 1997; Viel et al., 1995) while the backstepping control (Biswas & Samanta, 2013) and the multivariable feedforward-feedback nonlinear controller (Alvarez & González, 2007; Alvarez, Suárez, & Sánchez, 1990) were derived subsequently. Table 2.4 gives the brief summary

Table 2.3: Applications of model predictive control for stabilization of FRP reactors

System	Control strategy	Manipulated variables	Reference
Polystyrene production in CSTR	NMPC and coordinated control	Flow rate of coolant water and feed rate of monomer	(Hidalgo & Brosilow, 1990)
Batch polymerization reactor of PVC	NNMPC	Jacket temperature	(Nagy & Agachi, 1997)
Polystyrene production in CSTR	NMPC plus a multi-rate extended Kalman filter	Flow rate of coolant water and feed rate of initiator, monomer and solvent	(Prasad et al., 2002)
Batch polymerization reactor of PS	Nonlinear generalized predictive control	Heater power	(Özkan et al., 2006)
Batch polymerization reactor of PS	NMPC	Jacket temperature	(Nagy et al., 2007)
Polystyrene production in CSTR	Explicit moving horizon (model predictive) controller and estimator	Flow rate of coolant water	(Sui et al., 2009)
Batch polymerization reactor of PS	Neural network model predictive control (NNMPC)	Heater power	(Hosen et al., 2011)

of designed control strategies for the typical FRP reactors such as the FRP reactor of polymethylmethacrylate (MMA), FRP reactor of polystyrene (PS).

Although these control methodologies are of great interest, they are computationally expensive in general. In addition, the energy's aspects of the system have not been taken into consideration in the control design.

2.2 The passive system and the passivity-based control

Passivity-based control (PBC) is recognized as a control design of the system theory and is established by the pioneering works of Willems (1972a, 1972b). In this framework,

Table 2.4: Applications of model-based control strategy approach for stabilization of FRP reactors

System	Control strategy	Manipulated variables	Reference
Polymethyl methacrylate production process in CSTR	Nonlinear multivariable feedforward-feedback control	Feed rate of initiator and heat-removal rate	(Alvarez et al., 1990)
Polystyrene production process in CSTR	Input/output linearization technique plus high-gain observer	Jacket temperature and inlet concentration of initiator	(Assala et al., 1997; Viel et al., 1995)
Polystyrene production process in CSTR	Backstepping control	Flow rate of coolant water and inlet concentration of monomer	(Biswas & Samanta, 2013)

the author developed a general passivity theory which defines the dissipative and passive system[3]. Additionally, the important concepts associated with storage function, supply rate and dissipation term of the system are explicitly expressed in the same place. Actually, these concepts indeed allow us to express the energy transformation along the dynamical trajectories of the system from the modeling viewpoint. Furthermore, the pioneering works of Willems (1972a, 1972b) were applied firstly for the stabilization of electrical systems through the following studies (Anderson & Vongpanitlerd, 2006; Guillemin, 1977). More precisely, the passive components of an electric circuit including the inductors, the capacitors and the resistors are generally recognized because they do not produce any energy, and therefore, their networks (electrical circuits) are always stable. Consequently, the first successful applications of passivity theory for the electrical systems laid the solid groundwork for the further theoretical developments together with their potential applications for a broader class of nonlinear system including mechanical and chemical

[3]A passive input-output system is defined on the basis of dissipative property with respect to an appropriate storage function and a supply rate. In other words, a passive system is, of course, dissipative but not in the opposite site.

systems. In fact, several properties of passive system such as zero-state observability and detectability, Kalman – Yacubovich – Popov (KYL) property, equivalence of feedback and passivity of nonlinear system without/with structural uncertainty, and so on are found out subsequently and studied deeply in the literature (Bao & Lee, 2007; Brogliato et al., 2007; Byrnes, Isidori, & Willems, 1991; Lin & Shen, 1999; Sepulchre, Jankovic, & Kokotović, 1997). These properties indeed represent the central features of a nonlinear control design strategy (called PBC as aforementioned), which is applied successfully for the stabilization of a class of mechanical, electrical as well as electromechanical systems such as robot arms, induction motor control and so on (Ortega & García-Canseco, 2004b; Ortega et al., 2001; Petrovic, Ortega, & Stankovic, 2001; Sira-Ramírez, Perez-Moreno, Ortega, & Garcia-Esteban, 1997). The summary of applications of PBC for the different mechanical, electrical and electromechanical systems are given in Table 2.5. In these contributions, the system dynamics is firstly rewritten into the Euler-Lagrange form or (passive) port-Hamiltonian form. The storage function is then strongly related to the (total) energy of the system (including kinetic and potential energy) (Ortega et al., 1997, 1998; Sira-Ramírez et al., 1997; Van der Schaft, 2000b).

Nonetheless, the fact is that it is not easy to transfer the set of (ordinary or partial) differential equations modeling chemical processes into the certain forms such as Euler-Lagrange structure or port controlled Hamiltonian representation because the connections between stability theory and energy of reacting systems have been poorly understood (Eberard et al., 2007; Favache & Dochain, 2009; Hangos et al., 2001; Hoang et al., 2012; Hoang, Couenne, Le Gorrec, et al., 2013). In fact, the challenging issue has become an attractive and interesting research topic recently in the area of process control and some attempts have been made. For instance, in (Batlle, Ortega, Sbarbaro, & Ramíez, 2010; Hoang, Couenne, Le Gorrec, et al., 2013; Ramírez et al., 2009), the authors used the design methodology of interconnection and damping assignment passivity-based control (IDA-

Table 2.5: Applications of PBC in mechanical and electrical engineering system

System	Type of system	Reference
Robot system	SISO	(Berghuis & Nijmeijer, 1993)
Power converter	MIMO	(Perez et al., 2004; Rodriguez et al., 2000; Sira-Ramírez et al., 1997; M. Zhang et al., 2017)
Synchronous generators/electrical motors	MIMO	(Galaz et al., 2003; Manjarekar et al., 2010)
A nonlinear RC circuit	SISO	(Galaz et al., 2003; Manjarekar et al., 2010)
Wheel pendulum	SISO/MIMO	(Delgado & Kotyczka, 2016; Ortega et al., 2008; Shiriaev et al., 1999; Z. Wang & Goldsmith, 2008)
The dynamic positioning of ships	SISO	(Muhammad & Doria-Cerezo, 2012)
The induction machine	SISO	(Batlle et al., 2009)

PBC)[4] to stabilize asymptotically a nonlinear chemical process including m chemical reactants and m reactions occurring in a continuous stirred tank reactor (CSTR). Although the IDA-PBC scheme can be applied for both single-input single-output (SISO) systems and multi-input multi-output (MIMO) systems, the method has limitations, that is, the port controlled Hamiltonian structure of the system dynamics and the solvability of partial-derivative matching equations has to be fulfilled (García-Canseco et al., 2004; Ortega & García-Canseco, 2004a; Ortega et al., 2002; Van der Schaft, 2000a).

[4] We refer the readers to (Dörfler, Johnsen, K, & Allgöwer, 2009; Ortega & García-Canseco, 2004a; Ortega, Van der Schaft, Maschke, & Escobar, 2002) and references cited therein for the full descriptions and further discussion of IDA-PBC.

Table 2.6: Applications of IDA-PBC in process engineering

Process system	Type of system	Reference
Two-tank process	SISO/MIMO	(Johnsen & Allgower, 2007)
Four-tank process	MIMO	(Johnsen & Allgower, 2007; Sbarbaro & Ortega, 2007)
A continuous biochemical process bioreactor	SISO and MIMO	(Bernard et al., 1999; Dieulot & Makkar, 2015; Johnsen & Allgower, 2007)
A continuously stirred tank reactor	SISO	(Hoang, Couenne, Le Gorrec, et al., 2013; Hoang, Juan, & Ydstie, 2013)
The reacting system of synthesis of cyclopentenol from cyclopentadiene in CSTR	MIMO	(Batlle et al., 2010; Ramírez et al., 2009)

In addition, the fundamentals of thermodynamics such as the second law, Clausius-Plank inequality, irreversible entropy production, availability function, etc. are connected to the passivity theory as well as PBC by the pioneering research works of Alonso and Erik Ydstie (1996); Ydstie and Alonso (1997) and Ydstie (2002). In the literature, authors showed that chemical processes could be modeled by the principles of thermodynamics based on supply rate, dissipation of entropy, Helmholtz energy or (general) availability. These connections have become subsequently an active research area of advanced process control. Besides, the thermodynamic approach was also used to build a simple Hamiltonian system models for systems where Kirchhoff convective transport takes place together with transfer and sources of various type (Hangos et al., 2001). In addition, the resulting model can be used for the passivity analysis as well as the nonlinear control design. In (Hoang, Couenne, Dochain, & Le Gorrec, 2011; Hoang, Couenne, Jallut, & Le Gorrec, 2011; Hoang, Dochain, Couenne, & Le Gorrec, 2017; Hoang, Juan, & Ydstie, 2013), the isothermal and non-isothermal CSTRs were transferred to the pseudo Port-Controlled

Hamiltonian (PCH) formulation by using the irreversible thermodynamics viewpoint and then, IDA-PBC was designed to stabilize asymptotically the system at the desired equilibrium point. Furthermore, based on the thermodynamics viewpoint, a number of stability analyses and new passivity properties for a class of chemical reactors were studied in the literature (García-Sandoval, González-Álvarez, & Calderón, 2015; García-Sandoval, Hudon, Dochain, & González-Álvarez, 2016).

Another passivity-based approach for process systems in general and chemical systems in particular can be found in (Sira-Ramírez & Angulo-Núnez, 1997) where the practical applications such as a series of tanks-pipeline system, an exothermic continuously stirred tank reactor system, a bioreactor system and so on are considered. In this study, the authors used an input-coordinate transformation, which is computed by the natural decomposition of $f(x)$, to render a nonlinear system dynamics passive. Then, the resulting passive system is rewritten in the certain canonical form which allows expressing the physical meanings of the system such as the dissipative, non-dissipative terms and the supply rate. From these structural features, a feedback control based on tracking error is designed and proposed for asymptotic stabilization of the system along an arbitrary reference trajectory which takes the set point as a stationary equilibrium point. In fact, this strategy gives a systematic and effective procedure to design PBC schemes and it does not depend on the structure of the set of differential equations which describes system dynamics. Apart from using the natural decomposition of $f(x)$, the original nonlinear system dynamics can achieve the passivation by different ways which depend on the input coordinate transformation,i.e, how to render the nonlinear system passive. In (Fossas, Ros, & Sira-Ramírez, 2004; Sira-Ramírez, 1998), the authors proposed other methods which not only render a nonlinear system passive but also transfer the system dynamics to the well-known port controlled Hamiltonian structure. Moreover, several researches took advantages of feedback passivation design throughout a input coordinate transformation to design the controller for more complicated chemical systems such as the

Table 2.7: Applications of feedback passivation in process engineering

Process system	Type of system	Reference
A series of tank-pipeline system	SISO	(Sira-Ramírez et al., 1997)
The isothermal/non-isothermal reactor	SISO	(Sira-Ramírez et al., 1997)
Bioreactor/biochemical process	SISO	(Fossas et al., 2004)
Continuous fermentation process in CSTR	SISO	(Szederkényi et al., 2002)
The industrial phthalic anhydride fixed-bed reactor	SISO	(Chou & Wu, 2007)
The production of pineapple syrup in a CSTR	SISO	(Riverol, 2001)
The Turbocharged diesel engine	SISO	(Larsen et al., 2000, 2003; Larsen & Kokotović, 1998)

biochemical reactor (Fossas et al., 2004), the continuous fermentation process in CSTR (Szederkényi, Kristensen, Hangos, & Jørgensen, 2002), the production of pineapple syrup in CSTR (Riverol, 2001) and an industrial phthalic anhydride fixed-bed reactor (Chou & Wu, 2007), the turbocharged diesel engine (Larsen, Jankovic, & Kokotović, 2000; Larsen, Janković, & Kokotović, 2003; Larsen & Kokotović, 1998). Nonetheless, the theoretical extensions of the passivity-based approach through input coordinate transformations to design the feedback laws for MIMO systems have not been made yet. Table 2.7 summarized the recent applications of this passivity-based approach.

In that respect, this research work will extend the results of Sira-Ramírez and co-workers in (Sira-Ramírez, 1998; Sira-Ramírez et al., 1997) for the practical implementation when a MIMO chemical process system, namely the polystyrene production process in a CSTR is considered in the unit operation of chemical engineering. The transcription of the SISO control system theory for the stabilization of MIMO chemical processes is not obvious in general due to the complexity of the model equations or the well-posed condition of structural matrices, etc. Note also that a large class of (bio)chemical processes, especially FRP reactors are multivariable, thus the multivariable control approach is vitally essential according to the literature (Dobbie, 1977; Shen, Cai, & Li, 2010; Q.-G. Wang, Ye, Cai, & Hang, 2008). To the best of our knowledge, no further progress of the works of Sira-Ramírez and co-worker in (Sira-Ramírez, 1998; Sira-Ramírez & Angulo-Núnez, 1997) on the control design for MIMO processes has been made yet.

2.3 Summary

Throughout the chapter, a variety of control schemes have been reviewed to emphasize the significance of stabilizing the FRP systems at the desired equilibrium point but their control design procedure may be fairly complicated to apply for class of chemical processes due to their strong reliance on advanced mathematical tools. In addition, the effectiveness of PBC based on the systematic control design procedure and the potential ability to connect system theory and energy of reacting system has not verified for a class of MIMO chemical processes, particularly FRP ones. Consequently, the theoretical developments of PBC and their applications to such systems lead to the research gap of this work.

CHAPTER 3: TRACKING ERROR PASSIVITY-BASED MULTIVARIABLE CONTROL VIA FEEDBACK PASSIVATION

In this chapter, the tracking-error-based multivariable control to stabilize a nonlinear system at the desired trajectory (including the open-loop-unstable equilibrium) is considered as the main contribution of this research work is proposed. In fact, the control approach is developed on the basis of feedback passivation and then applied for the global exponential stabilization of a class of nonlinear systems.

The chapter is coordinated as follows. Firstly, the overview of stability analysis through Lyapunov's indirect method and Lyapunov theorem are given in Section 3.1 while the fundamentals of passivity theory are represented in Section 3.2. Then, the main results of this research work through three propositions which present the feedback passivation technique via the input coordinate transformations, the canonical form of resulting passive system and the multivariable control via tracking error are derived in Section 3.3 and Section 3.4, respectively. Finally, an implementable model of control structure is given in Section 3.5.

3.1 Stability analysis through Lyapunov's indirect method and Lyapunov theorem

3.1.1 The linearization technique and Lyapunov's indirect method

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

$$\dot{x} = f(x) + g(x)u, \quad y = h(x), \tag{3.1}$$

where $x = x(t) \in \mathbb{R}^n$ is the state vector in the operating region $\chi \subset \mathbb{R}^n$; $u = [u_1 \ u_2 \ \ldots \ u_m]^\top$ and $y = [y_1 \ y_2 \ \ldots \ y_m]^\top \in \mathbb{R}^m$ are the control input and the output of the system, respectively. Additionally, the vector-valued (nonlinear) functions $f(x(t)) \in \mathbb{R}^n$, $g(x(t)) \in \mathbb{R}^{n\times m}$ and $h(x(t)) \in \mathbb{R}^m$ are assumed to be smooth with respect to the vector field x in χ. For the sake of clarity, all these functions are expressed as follows

- $f(x(t)) = [f_1(x(t)) \;\; f_2(x(t)) \;\; \ldots \;\; f_n(x(t))]^\top$, with $f_i(x(t)) \in \mathbb{R}^n$, $i = 1, 2, \ldots, n$.
- $g(x(t)) = [g_1(x(t)) \;\; g_2(x(t)) \;\; \ldots \;\; g_m(x(t))]$, with $g_j(x(t)) \in \mathbb{R}^n$, $i = 1, 2, \ldots, m$.
- $h(x(t)) = [h_1(x(t)) \;\; h_2(x(t)) \;\; \ldots \;\; h_m(x(t))]^\top$, with $h_k(x(t)) \in \mathbb{R}$, $i = 1, 2, \ldots, m$.

Definition 3.1 (Jacobian matrix) *(Khalil, 2002). Let $P^e = \left(x_1^e, x_2^e, \ldots, x_n^e\right)$ be an equilibrium point of the nonlinear system* (3.1) *corresponding to the control input u^e and the vector field $f(x)$[1] is continuously differentiable in χ, the matrix A calculated as below*

$$\mathrm{A} = \left.\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}\right|_{P_e} = \left.\frac{\partial f}{\partial x}\right|_{P_e} \tag{3.2}$$

is called the Jacobian matrix at the equilibrium point P^e with respect to the control input u^e.

Obviously, the Jacobian matrix A is a square matrix of the first-order partial derivative of the vector-value functions $f(x)$ with dimension $n \times n$. The following definition gives an explicit expression of the linearized system which is approximated from (3.1) near the equilibrium point P^e.

Definition 3.2 *The nonlinear system* (3.1) *with a steady-state point $P^e = \left(x_1^e, x_2^e, \ldots, x_n^e\right)$ and control input u^e can be approximated to a linear system*

$$\dot{x} = \mathrm{A}x + \mathrm{B}u, \tag{3.3}$$

where A *is the Jacobian matrix of the nonlinear system at P^e* (3.2) *and the matrix B is computed by the formula as follows*

[1]For the sake of simplicity, the notion x can be used instead of $x(t)$.

$$B = \left[\frac{\partial g_1}{\partial u} \quad \frac{\partial g_2}{\partial u} \quad \ldots \quad \frac{\partial g_n}{\partial u} \right]^\top \Bigg|_{(P^e, u^e)} . \tag{3.4}$$

In fact, the approximately linearized system (3.3) is established by the Taylor series expansion with the first-order partial derivative of $f(x)$ and $g(x)$ at a steady-state point $P^e = (x_1^e, x_2^e, \ldots, x_n^e)$ corresponding to the control input u^e. Hence, the nonlinear characteristics of $f(x)$ and $g(x)$ are approximated to the matrix A and matrix B, respectively. Actually, the linearization technique used in this research work is called the approximate linearization technique to distinguish with the feedback linearization technique[2] which is based on a diffeomorphism of the nonlinear system, i.e. the change of state variables can transform exactly the nonlinear system dynamics into a linearized version.

Normally, the stability properties for a nonlinear system can be assessed by finding an appropriate Lyapunov function that fulfills the Lyapunov stability theorem (Khalil, 2002). However, the existence of such function is just the sufficient condition and there is indeed no general procedure to find this function. Consequently, in several cases, the approximately linearized system of nonlinear system (3.3) at the equilibrium points should be used instead of finding a Lyapunov function for the stability analysis. In this section, the two stability criteria are shown as below, which give a procedure to analyze the nonlinear system dynamics without finding the Lyapunov function (Bequette, 1998; Khalil, 2002; Seborg et al., 2011). Note also that two stability criteria here can be applied to a wide class of nonlinear systems and the requirements of finding an appropriate Lyapunov function to satisfy the Lyapunov theorem may be unnecessary.

Stability criteria 1 *The approximately linearized system* (3.3) *is stable at its origin if and only if all of its eigenvalues are located in the left side of the complex plane (or all eigenvalues have the negative real parts).*

[2]We refer the readers to (Isidori, 1995; Khalil, 2002) and references cited therein for full discussions about the feedback linearization technique.

Stability criteria 2 *If the origin of approximately linearized system* (3.3) *is a stable/unstable node or locus, then the corresponding equilibrium point is also a stable/unstable node or locus of the nonlinear system.*

Remark 3.1 *The Stability criteria 1 is also called the classical Routh-Hurwitz stability criterion.*

Remark 3.2 *The Stability criteria 2 can be generalized to the theorem of Lyapunov's indirect method (Khalil, 2002). More precisely, the origin of the nonlinear system*[3] (3.1) *is asymptotically stable if the real part of all eigenvalues of matrix* A *are negative. Also, the origin become unstable if the matrix* A *contains at least one eigenvalue which has a positive real part.*

3.1.2 Lyapunov theorem

Although Stability criteria 1 and Stability criteria 2 based on the approximate linearization technique and Lyapunov's indirect method can be applied to a class of nonlinear systems, these stability assessments are valid in the local region of the equilibrium point. In fact, for some cases, the stability analyses based on the approximately linearized system (3.3) for the nonlinear system (3.1) may give the inappropriate results. Therefore, the stability analysis through the Lyapunov theorem usually plays a central role in the system and control theory, and is then reviewed briefly in this section for the nonlinear system (3.1).

Firstly, let us consider the free system dynamics, which is also called the autonomous system, when the input variable u is identical to zero,

$$\dot{x} = f(x), \tag{3.5}$$

[3]If the origin is not an equilibrium point of the nonlinear system (3.1), the non-zero equilibrium point can be shifted to the origin by the coordinate transformation $x' = x - x^e$ and $u' = u - u^e$ so that the system with state variable x' and control input u' has the equilibrium point at origin

where the components of the n-dimensional vector $f(x)$ are local Lipschitz function of x. i.e., $f(x)$ satisfies the Lipschitz condition as follows:

$$\left\| f(x_1^*) - f(x_2^*) \right\| \leq L \left\| x_1 - x_2 \right\| \tag{3.6}$$

For all x_1^* and x_2^* in a neighborhood of x_0, where L is a positive constant and $\|.\|$ is the Euclidean norm (i.e.,$\|x\| = \sqrt{x^\top x}$). The condition (3.6) insures that (3.5) has a unique solution with the initial condition $x(0) = x_0$. The following definition presents a mathematical explanation of the notion "Stable"

Definition 3.3 *(Khalil, 2002) The equilibrium point* $x = 0$ *of* (3.5) *is*

- *Stable if, for each* $\epsilon > 0$*, there is* $\delta = \delta(\epsilon)$ *such that*

$$\|x(0)\| < \delta \rightarrow \|x(t)\| < \varepsilon, \qquad \forall t \geq 0. \tag{3.7}$$

- *Asymptotically stable if it is stable and* δ *can be chosen such that*

$$\|x(0)\| < \delta \rightarrow \lim_{t\rightarrow\infty} x(t) = 0. \tag{3.8}$$

- *Unstable if it is not stable.*

The Definition 3.3 gives the $\epsilon - \delta$ requirement for the stability analysis. This also means that the origin of the autonomous system (3.5) is stable if any positive neighborhood ϵ is arbitrarily small and there always exists a positive neighborhood such that any system trajectories originating in δ will converge to ϵ. Moreover, in the case, ϵ is equal to zero, the system trajectories approach the origin and the system (3.5) is called asymptotically stable (Khalil, 2002).

However, a nonlinear system may have multiple equilibrium points, which are locally stable or unstable without control actions. Hence, a sufficient condition for the stability of equilibrium point is vitally important and is solved by Theorem 3.1 (also called the Lyapunov stability criterion). The benefit of Theorem 3.1 is that the stability characteristic of equilibrium points can be determined without solving the explicit solutions of (3.5).

Theorem 3.1 *Khalil (2002) Let* $x = 0$ *be an equilibrium point of* (3.5) *and the domain* $D \subset \mathbb{R}^n$ *be a domain containing* $x = 0$*. Let* $\mathrm{V} : D \to \mathbb{R}$ *be a continuously differentiable function such that*

$$\mathrm{V}(0) = 0 \, and \, \mathrm{V}(x) > 0 \quad \forall x \in D/\{0\} \tag{3.9}$$

Then $x = 0$ *is stable. Additionally, if*

$$\dot{\mathrm{V}}(x) < 0 \quad \forall x \in D/\{0\} . \tag{3.10}$$

Then $x = 0$ *is asymptotically stable.*

The continuously differentiable function V satisfying the Theorem 3.1 is called the Lyapunov function and the surface $\mathrm{V}(x) = c$ is called a Lyapunov surface or level surface for some $c > 0$.

Remark 3.3 *If the subset D in Theorem 3.1 is equal to* $\mathbb{R}^n$ *and the Lyapunov function* V *is unbound radically as x goes to infinity, the equilibrium point* $x = 0$ *is globally asymptotically stable.*

Actually, although there is no general procedure to find an appropriate Lyapunov function, in many cases, a class of quadratic functions, i.e. $\mathrm{V}(x) = x^\top Q x$, where Q is a real symmetric matrix, can be used as a Lyapunov candidate functions because the sign definiteness can be easily checked by the signs of eigenvalues or the signs of sub matrices on the main diagonal of matrix Q (Sylvester criterion) (Bellman, 1997). Aside from the quadratic functions, a class of system-energy-based functions can be also considered as a Lyapunov function candidate (Alvarez, Alvarez-Ramírez, Espinosa-Perez, & Schaum, 2011; Khalil, 2002; Ortega et al., 1998). More precisely, for the mechanical systems, the energy functions are usually the sum of potential and kinetic energy (Ortega et al., 2001; Van der Schaft, 2000b) while for the chemical process, the energy function are usually closely related to the thermodynamic functions such as entropy, entropy production, availability, etc (Favache & Dochain, 2010; Hoang, Couenne, Jallut, & Le Gorrec, 2011; Hoang et al., 2012; Hoang, Couenne, Jallut, & Le Gorrec, 2013; Hoang & Dochain, 2013b; Hoang et al., 2017).

The detailed proof of Lyapunov theorem as well as its further discussions can be found in (Bao & Lee, 2007; Khalil, 2002) and references cited therein.

3.2 Fundamentals of passive system

In this subsection, the brief introductions of dissipative and passive systems are given to lay the solid base for the control design of PBC in this research work. Firstly, let us re-consider the nonlinear system Equation (3.1), the following definition expresses the explicit interpretation of dissipative system.

Definition 3.4 *(Bao & Lee, 2007; Willems, 1972a) The nonlinear dynamical system defined by* (3.1) *is said to be dissipative regarding to the supply rate* $s\left(u(t), y(t)\right)$ *if there exists a storage function* $\mathbb{V}(x) : \chi \to \mathbb{R}^+$ *so that the inequality below holds for all* $x \in \chi$ *and* $t_1 > t_0$*,*

$$\mathbb{V}\left(x(t_1)\right) - \mathbb{V}\left(x(t_0)\right) \leq \int_{t_0}^{t_1} s(u(t), y(t))dt. \tag{3.11}$$

The above inequality shows a physical meaning that the increase in the energy of the system from t_0 to t_1 is always smaller than the total amount of energy supplied by an external source at the same time. The value of storage function $\mathbb{V}(x)$ expresses the total energy of the system at any time.

As a consequence of (3.11), if the storage function $\mathbb{V}(x(t))$ is differentiable for all $x \in \chi$, the inequality given by (3.11) is equivalent to

$$\dot{\mathbb{V}}(x(t)) \leq s(u(t), y(t)) . \tag{3.12}$$

It is shown from (3.12) that the rate of increase in $V(x(t))$ is always no greater than the supply rate and also carries a physical interpretation of the energy transformation. In other words, the physical systems in practice usually have dissipation terms which dissipate a part of the system energy because of resistive elements such as resistors and dampers, etc. If the dissipation term is equal to zero, the dissipative system becomes a lossless system, i.e., it conserves all the supplied energy (note also that the supply rate of lossless system here can be any functions between input u and output y) (Brogliato et al., 2007).

Definition 3.5 *(Bao & Lee, 2007) The nonlinear dynamical system* (3.1) *is said to be passive*[4] *if it is dissipative with respect to the supply rate given by* $s(u, y) = u^\top y$.

In general, the supply rate can be any functions of the input u and the output y; once the relationship admits a form defined by an inner product of two vectors (i.e., input vector u and output vector y), the dissipative system becomes a passive system. Therefore, the passive systems belong to a smaller class of the dissipative systems. If strict inequalities given in (3.11) and (3.12) hold with respect to the supply rate $s(u, y) = u^\top y$, the passive system is called a strictly passive system; otherwise when the equalities in (3.11) and (3.12) occur, the passive system becomes the lossless system with the supply rate (3.11) and (3.12) (Bao & Lee, 2007).

[4] We refer the readers to (Hoang et al., 2017; Ortega et al., 2008), and references cited therein, for further information on passive and cyclo-passive concepts.

In fact, the storage functions $\mathbb{V}(x)$ do not always need to carry the explicit physical meaning and any positive (semi)definite functions can actually considered as a storage function $\mathbb{V}(x)$ where the notions of physical energy become the abstract energy, i.e. the implicit energy. For example, Hoang and Dochain (2013a) proposed a storage function based on the combination of the thermal deviation $\frac{1}{2}(T - T_d)^2$ and the inventory-based quadratic form $\frac{1}{2}(x - x_d)^2$, Ramírez et al. (2009) considered the total mass balance while the positive definite quadratic functions, i.e. $\mathbb{V}(x) = x^\top P x$ where P is a positive-definite symmetric (constant) matrix is chosen as a storage function of passive closed-loop system in (Fossas et al., 2004; Sira-Ramírez & Angulo-Núnez, 1997). Moreover, the energy-based storage functions $\mathbb{V}(x)$ such as the total of potential and kinetic energy, entropy, availability and its individual contributions have an important role in the context of stability analysis and control design of passive systems (Hoang et al., 2012).

Additionally, under a zero-state detectability condition (Feng & Lozano, 1999; Ortega et al., 2002) and assume that the storage function $\mathbb{V}(x(t))$ is non-negative (or bounded from below), it follows that an explicit proportional static output feedback law of the form $u = -Ky$, with $K = K^\top$ a so-called damping injection gain, renders the (controlled) passive system dissipative and therefore asymptotically stabilized by means of the Lyapunov approach (Khalil, 2002).

Definition 3.6 *(Bao & Lee, 2007; Khalil, 2002) A passive system is output strictly passive if $s(u, y) = u^\top y - \gamma\varphi(y)$ for some function $\phi(y)$ where γ is a positive scalar. Also, the system is input strictly passive if $s(u, y) = u^\top y - \omega\phi(u)$ for some function $\phi(u)$ where ω is a positive constant.*

Because the passivity can not usually ensure the stability of nonlinear system (3.1), for instance, a passive system has two state $x = [x_1, x_2]^\top$ and the storage function $\mathbb{V}(x) = \dfrac{1}{2}x_1^2$ is positive semidefinite, then the stability of x_2 is not guaranteed by the passivity with

$\mathbb{V}(x)$. Therefore, an additional conditions on zero-state observability and detectability are given.

Definition 3.7 *(Bao & Lee, 2007) A system as given in* (3.1) *is* zero-state observable (ZSO) *if for any* $x \in \chi$

$$y(t) = h\big(x(t, t_0, x, 0)\big) = 0 \quad \forall t \geq t_0 \geq 0 \quad \textit{implies} \quad x = 0, \tag{3.13}$$

and the system is locally ZSO if there exists a neighborhood χ_n *of 0, such that for all* $x \in \chi_n$*,* (3.13) *holds. The system is* zero-state detectable (ZOD) *if for any* $x \in \chi$*,*

$$y(t) = h\big(x(t, t_0, x, 0)\big) = 0 \quad \forall t \geq t_0 \geq 0 \quad \textit{implies} \quad \lim_{x \to 0} x(t, t_0, x_0, 0) = 0, \tag{3.14}$$

and the system is locally ZSD if there exists a neighborhood χ_n *of 0, such that for all* $x \in \chi_n$*,* (3.14) *holds.*

3.3 The feedback passivation design through input coordinate transformations

A systematic approach to passivate a nonlinear SISO system via an input coordinate transformation was firstly proposed in (Sira-Ramírez & Angulo-Núnez, 1997). This approach was also applied for the control design of several physical and chemical processes (Chou & Wu, 2007; Riverol, 2001) but limited to the SISO system. In this section, the passivation approach is generalized and applied to render a MIMO system passive for the purpose of stabilization via tracking-error passivity-based multivariable control. The core ideas of the methodology are:

1. Firstly, the system dynamics, which may not be passive initially, is passivated using an appropriate input coordinate transformation (also called feedback passivation), i.e., from the input u to a novel input υ. The dynamics is therefore passive with

respect to the supply rate s defined on the basic of the novel input υ and the output y

2. Secondly, the resulting passive system is then expressed in a canonical form that allows us to show the physical meanings of the system dynamics structure.

3. Finally, the tracking-error-based multivariable controller is then designed for the purpose of stabilization by considering the canonical form derived.

The aim of the feedback passivation is to render a nonlinear dynamical system passive using a novel input υ instead of the actual input u (Bao & Lee, 2007; Sepulchre et al., 1997). In the framework of the approach adopted, the passivation design is achieved based on the (natural) decomposition property of the function $f(x)$ regarding to a storage function $\mathbb{V}(x)$[5]. More precisely, the function is assumed to be expressed as a sum of three different elements[6]

$$f(x) = f_I(x) + f_d(x) + f_{nd}(x), \tag{3.15}$$

such that

- $L_{f_I(x)}\mathbb{V}(x) = 0;\ \forall x \in \chi,$
- $L_{f_{nd}(x)}\mathbb{V}(x)$ is either non-negative or sign-undefined in χ,
- $L_{f_d(x)}\mathbb{V}(x) \leq 0;\ \forall x \in \chi,$

where the functions $f_I(x) \in \mathbb{R}^n, f_d(x) \in \mathbb{R}^n$ and $f_{nd}(x) \in \mathbb{R}^n$ are considered as the invariant, dissipative and non-dissipative components of $f(x)$, respectively. The notation

[5]Discussions on the (strict) separability condition can be found in (Favache et al., 2011; Hoang et al., 2017)

[6]Such decomposition is made arbitrarily as long as the requirements are met. Note also that in (Guay & Hudon, 2016; Hudon, Hoang, Gacía-Sandoval, & Dochain, 2015), the authors proposed a geometric decomposition technique, based on the Hodge decomposition theorem, to re-express a given vector field $f(x)$ into a potential-driven form. More precisely, this allows us to encode the divergence of the given vector field into its exact and anti-exact components, and into its co-exact and anti-co-exact components.

of $L_{f(x)}\mathbb{V}(x)$ is the Lie derivative of the storage function $\mathbb{V}(x)$ along the vector-valued function $f(x)$ (Khalil, 2002), i.e.,

$$L_{f(x)}\mathbb{V}(x) = \frac{\partial \mathbb{V}(x)}{\partial x}^{\top} f(x) \in \mathbb{R}. \tag{3.16}$$

The following assumptions are considered.

Assumption 3.1 *The non-dissipative term $f_{nd}(x) \in \mathbb{R}^n$ can be expressed to be a sum of m different non-dissipative terms $f_{nd,i}(x) \in \mathbb{R}^n$ such that* [7]

$$f_{nd}(x) = \sum_{i=1}^{m} f_{nd,\,i}(x). \tag{3.17}$$

Assumption 3.2 *The transversality condition defined by,*

$$L_{g_i(x)}\mathbb{V}(x) \neq 0, \quad \forall x \in \chi \quad and \quad i = 1, 2, \ldots, m \tag{3.18}$$

holds.

From a mathematical point of view, the transversality condition expresses the meaning that vector fields $g_i(x)$, $i = 1, 2, \ldots, m$ are not orthogonal to the gradient of $\mathbb{V}(x)$ with respect to x in χ. In other words, the vector fields $g_i(x)$, $i = 1, 2, \ldots, m$ are not tangential to the tangent space of the surface defined by $\mathbb{V}(x)$ = constant (Sira-Ramírez, 1998, 1999). Even if Assumption 3.2 seems strong, this is feasible and valid in some instances (see e.g., (Chou & Wu, 2007; Fossas et al., 2004; Riverol, 2001; Sira-Ramírez & Angulo-Núnez, 1997; Szederkényi et al., 2002) for a large class of physico-chemical process systems including the isothermal/non-isothermal CSTRs, the bioreactor system, the

[7] Even if it is difficult to identify sufficiently m components of $f_{nd}(x)$, we can arbitrarily choose k elements with $1 \leq k < m$ such that $f_{nd}(x) = \sum_{i=1}^{k} f_{nd,\,i}(x)$ while other components (i.e., $(m-k)$ components) are equal to zero.

phthalic anhydride fixed-bed reactor and the non-isothermal tank used in the production of pineapple syrup in CSTR). In this work, this assumption holds for the FRP reactors.

The following proposition provides the generalizations of the output feedback passivation under Assumption 3.1 and Assumption 3.2.

Proposition 3.1 *The nonlinear multivariable system described by* (3.1) *is transferred to an output strictly passive system with respect to a storage function* $\mathbb{V}(x)$ *if* m *input coordination transformations* $u_i = 1, 2, \ldots, m$ *are expressed by*

$$u_i = \frac{h_i(x)}{L_{g_i(x)}\mathbb{V}(x)}\upsilon_i - \gamma_i \frac{h_i^2(x)}{L_{g_i(x)}\mathbb{V}(x)} - \frac{L_{f_{nd,\ i}(x)}\mathbb{V}(x)}{L_{g_i(x)}\mathbb{V}(x)}, \tag{3.19}$$

where $\upsilon_i,\ i = 1, 2, \ldots, m$ *are the new inputs and the positive scalars* $\gamma_i,\ i = 1, 2, \ldots, m$ *are arbitrary.*

Proof. Consider the nonlinear multivariable system (3.1), the time derivative of the storage function $\mathbb{V}(x)$ is given by

$$\begin{aligned} \dot{\mathbb{V}} &= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top \frac{dx}{dt} \\ &= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top g(x)u \\ &= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top \sum_{i=1}^{m} g_i(x)u_i. \end{aligned} \tag{3.20}$$

By using the natural decomposition defined in (3.15), we obtain

$$\dot{\mathbb{V}} = \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f_I(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f_d(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f_{nd}(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top \sum_{i=1}^{m} g_i(x)u_i. \tag{3.21}$$

Equation (3.21) is then rewritten by using (3.17) as follow

$$\begin{aligned}\dot{\mathbb{V}} &= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f_I(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top f_d(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top \sum_{i=1}^{m} f_{nd,\, i}(x) + \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top \sum_{i=1}^{m} g_i(x)u_i \\ &= L_{f_I(x)}\mathbb{V}(x) + L_{f_d(x)}\mathbb{V}(x) + \sum_{i=1}^{m} L_{f_{nd,\, i}(x)}\mathbb{V}(x) + \sum_{i=1}^{m} \left[L_{g_i(x)}\mathbb{V}(x)\right] u_i. \end{aligned} \tag{3.22}$$

Substituting (3.19) into (3.22) for $i = 1, 2, \ldots, m$, (3.22) is rewritten as below

$$\dot{\mathbb{V}} \ = L_{f_d(x)}\mathbb{V}(x) + \sum_{i=1}^{m} \left[h_i(x)\upsilon_i - \gamma_i h_i^2(x)\right]. \tag{3.23}$$

Due to the condition $L_{f_d(x)}\mathbb{V}(x) \leq 0$, we obtain

$$\dot{\mathbb{V}} \ \leq \upsilon^\top y - y^\top R_\gamma y, \tag{3.24}$$

where $R_\gamma = \operatorname{diag}(\gamma_1, \gamma_2, \ldots, \gamma_m)$ and the new input $\upsilon = [\upsilon_1 \ \upsilon_2 \ \ldots \ \upsilon_m]^\top$. Hence, the nonlinear system (3.1) is (strictly) passive with respect to the new input υ and output y. The latter completes the proof. □

Remark 3.4 *the positive scalar γ in Definition 3.6 becomes the square matrix which contains the γ_i in the main diagonal. Additionally, γ_i corresponds with the internal input υ_i and output y_i of resulting passive system.*

Remark 3.5 *An original nonlinear system can also achieve passivation by several different ways which depend on input coordinate transformations. In (Fossas et al., 2004; Sira-Ramírez, 1998), authors proposed other methods but all of them are just valid if the transversality condition (Assumption 3.2) holds.*

Remark 3.6 *If the components in the natural decomposition given by* (3.15) *of function* $f(x)$*, namely* $f_I(x)$ *and* $f_d(x)$*, cannot be found easily, then the whole function* $f(x)$ *can be assumed to be the non-dissipative component* $f_{nd}(x)$*.*

Remark 3.7 *For the non-square system (the number of input is not equal to that of output), if the number of inputs are more than that of output, we can pick up the appropriate manipulated inputs and fix others. However, the chosen control inputs and outputs must satisfy the necessary and sufficient conditions of feedback passivation design. On the other hand, if there are more outputs than inputs, the outputs satisfying the necessary and sufficient conditions of feedback passivation are selected while others converge to the corresponding equilibrium points once the chosen outputs are stabilized*

3.4 General canonical form of passive system and feedback control design

A passive system shows that the energy stored in the system is always no greater than the energy supplied to the system from an external source. Based on this (main) feature of passive system, we shall propose a systematic procedure for the control design via the use of physical meaning of the dissipative term. Before the control strategy is described, let us give a canonical form of the passive system obtained from Proposition 3.1 so that we can see the nature of the dissipative term.

Proposition 3.2 *A passive system with respect to a storage function* $\mathbb{V}(x)$ *with the input* $\upsilon = [\upsilon_1\ \upsilon_2\ \dots\ \upsilon_m]^\top$ *and the output* $y = h(x)$ *of Proposition 3.1 is represented by the canonical form defined as follow*

$$\dot{x} = -R(x)\frac{\partial \mathbb{V}}{\partial x} + J(x)\frac{\partial \mathbb{V}}{\partial x} + M(x)\upsilon, \tag{3.25}$$

where $R(x)$ *and* $J(x)$ *are the positive semidefinite symmetric and skew-symmetric matrices, respectively,*

$$f_d(x) - \sum_{i=i}^{m} g_i(x)\gamma_i \frac{h_i^2(x)}{L_{g_i(x)}\mathbb{V}(x)} = -R(x)\frac{\partial \mathbb{V}}{\partial x}, \tag{3.26}$$

$$f_I(x) + f_{nd}(x) - \sum_{i=1}^{m} g_i(x) \frac{L_{f_{nd,\ i}(x)} \mathbb{V}(x)}{L_{g_i(x)} \mathbb{V}(x)} = J(x) \frac{\partial \mathbb{V}}{\partial x}, \tag{3.27}$$

and the matrix $M(x)$ is defined as follows

$$M(x) = \left[g_1(x) \frac{h_1(x)}{L_{g_1(x)} \mathbb{V}} \quad g_2(x) \frac{h_2(x)}{L_{g_2(x)} \mathbb{V}} \quad \ldots \quad g_m(x) \frac{h_m(x)}{L_{g_m(x)} \mathbb{V}} \right]. \tag{3.28}$$

Proof. Using the natural decomposition of the vector function $f(x)$ given by (3.15) and substituting m input coordinate transformations given defined by (3.19) into the nonlinear system (3.1), we obtain

$$\dot{x} = f_d(x) + f_{nd}(x) + f_I(x) + \sum_{i=i}^{m} g_i(x) \left[\frac{h_i(x)}{L_{g_i(x)} \mathbb{V}(x)} \upsilon_i - \gamma_i \frac{h_i^2(x)}{L_{g_i(x)} \mathbb{V}(x)} - \frac{L_{f_{nd,\ i}(x)} \mathbb{V}(x)}{L_{g_i(x)} \mathbb{V}(x)} \right]. \tag{3.29}$$

Then, (3.29) is rewritten as follows

$$\dot{x} = \left(f_d(x) - \sum_{i=i}^{m} g_i(x) \gamma_i \frac{h_i^2(x)}{L_{g_i(x)} \mathbb{V}(x)} \right) + \left(f_I(x) + f_{nd}(x) - \sum_{i=i}^{m} g_i(x) \frac{L_{f_{nd,i}(x)} \mathbb{V}(x)}{L_{g_i(x)} \mathbb{V}(x)} \right) + \sum_{i=1}^{m} g_i(x) \frac{h_i(x)}{L_{g_i(x)} \mathbb{V}(x)} \upsilon_i. \tag{3.30}$$

Firstly, it is straightforward to show that

$$\left(\frac{\partial \mathbb{V}}{\partial x} \right)^{\top} \left[f_d(x) - \sum_{i=1}^{m} g_i(x) \gamma_i \frac{h_i^2(x)}{L_{g_i(x)} \mathbb{V}(x)} \right] \leq 0. \tag{3.31}$$

Hence, there exists a positive semidefinite symmetric matrix $R(x)$ to satisfy the property $-\left(\frac{\partial \mathbb{V}}{\partial x} \right)^{\top} R(x) \frac{\partial \mathbb{V}}{\partial x} \leq 0$ such that (3.26) is met.

Secondly, it is clearly to see that

$$f_I(x) + f_{nd}(x) \ - \sum_{i=1}^{m} g_i(x) \frac{L_{f_{nd,\ i}(x)} \mathbb{V}(x)}{L_{g_i(x)} \mathbb{V}(x)} = f_I(x) + \sum_{i=1}^{m} \left[I - g_i(x) \frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top}}{L_{g_i(x)} \mathbb{V}(x)} \right] f_{nd,\ i}(x). \tag{3.32}$$

Since $L_{f_I(x)} \mathbb{V}(x) = 0$ and

$$\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} \left[I - g_i(x) \frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top}}{L_{g_i(x)} \mathbb{V}(x)} \right] = \left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} - \left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} g_i(x) \frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top}}{L_{g_i(x)} \mathbb{V}(x)} \equiv 0, i = 1, 2, \ldots, m,$$

therefore, from (3.32) we have $\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} \left[f_I(x) + f_{nd}(x) \ - \sum_{i=1}^{m} g_i(x) \frac{L_{f_{nd,\ i}(x)} \mathbb{V}(x)}{L_{g_i(x)} \mathbb{V}(x)} \right] = 0$. So, there exists a skew-symmetric matrix $J(x)$ to satisfy the property $\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} J(x) \frac{\partial \mathbb{V}}{\partial x} = 0$ such that (3.27) holds.

Finally, the dynamics of passive system (3.29) is represented as (3.25) where the matrix $M(x)$ is given by (3.28). The latter concludes the proof. □

Remark 3.8 *The canonical form* (3.25) *of the passive system defined by Proposition 3.2 is equivalent to the well-known port-Hamiltonian structure.*

Remark 3.9 *The physical meanings of system are described by three components in* (3.30)*. More precisely,*

- *The first element, including $f_d(x)$ and $\sum_{i=i}^{m} g_i(x) \gamma_i \frac{h_i^2(x)}{L_{g_i(x)} \mathbb{V}(x)}$, expresses the natural dissipation of the system and the artificial dissipative component with respect to new input υ, respectively.*
- *The second element $f_I(x) + f_{nd}(x) - \sum_{i=i}^{m} g_i(x) \frac{L_{f_{nd,\ i}(x)} \mathbb{V}(x)}{L_{g_i(x)} \mathbb{V}(x)}$ is the interconnection element which is invariant or workless in terms of the new input υ.*

- *The third element* $\sum_{i=1}^{m} g_i(x)\frac{h_i(x)}{L_{g_i(x)}\mathbb{V}(x)}\upsilon_i$ *is the power supply of the system with respect to the new input* υ.

Remark 3.10 *The matrix defined by*

$$N_i(x) = \left[I - g_i(x)\frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top}{L_{g_i(x)}\mathbb{V}(x)} \right], \quad i = 1, 2, \ldots, m \tag{3.33}$$

can be considered as a projection operator onto the tangent space to the level surface $\mathbb{V}(x)$ = *constant, along the distribution span* $(g_i(x))$ *with respect to the new input* υ. *This projection operator satisfies the properties (see, e.g., (Sira-Ramírez, 1998; Sira-Ramírez & Angulo-Núnez, 1997) for the proof of a simple SISO case):*

$$\begin{cases} N_i(x)g_i(x) = 0, \\ \left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top N_i(x) = 0, \quad \forall x \in \chi. \\ {N_i}^2(x) = N_i(x), \end{cases} \tag{3.34}$$

In this work, the brief proof can be given as follows. Firstly, the property $N(x)g(x) = 0$ is established by the fact that

$$\begin{aligned} N_i(x)g_i(x) &= \left[I - g_i(x)\frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top}{L_{g_i(x)}\mathbb{V}(x)} \right] g_i(x) \\ &= g_i(x) - g_i(x)\frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^\top}{L_{g_i(x)}\mathbb{V}(x)} g_i(x) \\ &= g_i(x) - g_i(x)\frac{L_{g_i(x)}\mathbb{V}(x)}{L_{g_i(x)}\mathbb{V}(x)} \\ &= 0. \end{aligned} \tag{3.35}$$

Similarly, the second property is led from the fact that

$$
\begin{aligned}
\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} N_i(x) &= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} \left[I - g_i(x) \frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top}}{L_{g_i(x)} V(x)} \right] \\
&= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} - \left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} g_i(x) \frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top}}{L_{g_i(x)} \mathbb{V}(x)} \\
&= \left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top} - L_{g_i(x)} \mathbb{V}(x) \frac{\left(\frac{\partial \mathbb{V}}{\partial x}\right)^{\top}}{L_{g_i(x)} \mathbb{V}(x)} \qquad (3.36) \\
&= 0.
\end{aligned}
$$

Based on the first property, we obtain $N_i(x) g_i(x) \frac{\partial \mathbb{V}}{\partial x_j} = 0, \quad j = 1, 2, \ldots, n.$ Therefore, $N_i(x)\left[I - N_i(x)\right] = 0.$ Finally, the properties (3.34) are proved completely.

It can be shown that each projection operator permits to eliminate the unexpected nonlinear characteristics of m non-dissipative terms $f_{nd,\, i}(x),\ i = 1, 2, \ldots, m$ in (3.32). In other words, any unstable behaviours arising from $f_{nd,\, i}(x),\ i = 1, 2, \ldots, m$ can neither increase nor decrease the value of the storage function $\mathbb{V}(x)$ along the system trajectory described by the canonical form (3.25).

From Propositions 3.1 and 3.2, it is shown that the method of using an input coordinate transformation (also known as the output feedback passivation design[8]) to passivate a nonlinear dynamical system is extended for a multivariable nonlinear system. In addition, the generalized canonical form (3.25) is expressed for any storage functions which satisfy Assumption 3.2. These extensions are one of the primary contributions of this research work.

Next, the following proposition proposes a feedback controller via tracking-error method. More precisely, the reference trajectory x_d is chosen such that its time evolution

[8] We refer the readers to (Byrnes et al., 1991; Larsen et al., 2003; Lin & Shen, 1999; Sepulchre et al., 1997) for more details on the necessary and sufficient condition (including the relative degree equal to one and weakly minimum phase behavior of the system) of output feedback passivation.

converges globally asymptotically or exponentially to the desired equilibrium point (i.e., the set-point) while the system trajectory x tracks the reference trajectory x_d exponentially when time goes to infinity.

Proposition 3.3 *If the storage energy function $\mathbb{V}(x)$ of the passive system obtained from Propositions 3.1 and 3.2 is a quadratic function, i.e., $\mathbb{V}(x) = \frac{1}{2}x^\top R_{di}x$ where R_{di} is positive definite symmetric (constant) matrix then the system trajectory x converges globally exponentially to the reference trajectory x_d governed by*

$$\dot{x}_d = -R(x)\frac{\partial \mathbb{V}(x_d)}{\partial x_d} + J(x)\frac{\partial \mathbb{V}(x_d)}{\partial x_d} + R_I\frac{\partial \mathbb{H}(e)}{\partial e} + M(x)\upsilon, \tag{3.37}$$

where $e = x - x_d$ is the error state vector, $\mathbb{H}(e) = \frac{1}{2}e^\top R_{di}e$ and R_I is an arbitrarily chosen positive definite symmetric (constant) matrix. The matrices $R(x)$, $J(x)$ and $M(x)$ are derived using (3.26),(3.27) *and* (3.28)*, respectively.*

Proof. First of all, it can be checked easily that [9]

$$\frac{\partial \mathbb{V}(x)}{\partial x} - \frac{\partial \mathbb{V}(x_d)}{\partial x_d} = \frac{\partial \mathbb{H}(e)}{\partial e}. \tag{3.38}$$

On the other hand, the time derivative of storage function $\mathbb{H}(e)$ along the error state vector e is given as follows

$$\dot{\mathbb{H}}(e) = \left[\frac{\partial \mathbb{H}(e)}{\partial e}\right]^\top \dot{e}. \tag{3.39}$$

Using equations (3.25), (3.37) and (3.38), it gives[10]

$$\dot{e} = \{J(x) - [R(x) + R_I]\}\frac{\partial \mathbb{H}(e)}{\partial e}. \tag{3.40}$$

[9]Note also that $\mathbb{H}(e) = \mathbb{H}(x - x_d)$ and thus, $\mathbb{H}(e) = \frac{1}{2}\left[\frac{\partial \mathbb{H}(e)}{\partial x} - \frac{\partial \mathbb{H}(e)}{\partial x_d}\right]$.

[10]The dynamics of the error state vector e is naturally formatted in a port-Hamiltonian structure.

From the equality (3.40), (3.39) becomes

$$\begin{aligned}\dot{\mathbb{H}}(e) &= \left[\frac{\partial \mathbb{H}(e)}{\partial e}\right]^\top \{J(x) - [R(x) + R_I]\} \frac{\partial \mathbb{H}(e)}{\partial e} \\ &= -\left[\frac{\partial \mathbb{H}(e)}{\partial e}\right]^\top [R(x) + R_I] \frac{\partial \mathbb{H}(e)}{\partial e} < 0. \end{aligned} \tag{3.41}$$

The exponential convergence property of the system trajectory to the reference trajectory (i.e., the error e exponentially converges to zero) is straightforward. Indeed, from (3.41), we derive

$$\dot{\mathbb{H}}(e) < -e^\top R_{di} R_I R_{di} e. \tag{3.42}$$

Hence,

$$\dot{\mathbb{H}}(e) < -\lambda_{\min} e^\top e, \tag{3.43}$$

where $\lambda_{\min} = \min \operatorname{eig}(R_{di} R_I R_{di})$. Based on the definition $\mathbb{H}(e)$, the inequality $e^\top e > \frac{2}{\beta_{\max}} \mathbb{H}(e)$ holds where $\beta_{\max} = \max \operatorname{eig}(R_{di})$, (3.43) therefore becomes

$$\dot{\mathbb{H}}(e) < -2\frac{\lambda_{\min}}{\beta_{\max}} \mathbb{H}(e). \tag{3.44}$$

Since $\dot{\mathbb{H}(e)}(e)$ is (strictly) negative and bounded above by itself, it follows that $\mathbb{H}(e) \to 0$ as $t \to \infty$ with an exponential decay, i.e., $x(t)$ exponentially tracks $x_d(t)$. The latter concludes the proof. □

Remark 3.11 *Once the reference trajectory x_d is assigned, the internal dynamic controller $\upsilon = [\upsilon_1\ \upsilon_2\ \ldots\ \upsilon_m]^\top$ is derived immediately by substituting the reference trajectory x_d to* (3.37)*. However, let us note that just m components of x_d can be chosen to assign (Sira-Ramírez & Angulo-Núnez, 1997) due to the constraint imposed by the degree of freedom of the system* (3.37) *and the solvability (i.e., the corresponding $m \times m$ submatrix* *of $M(x)$ is of full rank). The actual control $u = [u_1\ u_2\ \dots\ u_m]^\top$ is then computed by considering m input coordinate transformations given by* (3.19).

Remark 3.12 *In this work, the developed reference trajectory* (3.37) *is totally different compared to the reference trajectory given in (Fossas et al., 2004). Indeed, the reference trajectory* (3.37) *allows us to show explicitly the physical meanings of the auxiliary system associated with the vector field x_d (i.e., the interconnection and damping injection terms). On the other hand, this simplifies the complexity of the controller design in case of MIMO systems in general.*

Remark 3.13 *Although Proposition 3.3 shows the exponentially global stabilization of internal system from input υ to output y, the actual control inputs u are computed explicitly from υ by the input coordinate transformations. Therefore, the global stability of closed-loop system from input u to output y is stil guaranteed*

3.5 The proposed PBC scheme

In practice, the PBC is implemented as a feedback controller which calculates the control inputs via feedback signals from sensors, set points together with mathematical algorithms. In this research, we assume that all output signals are measured possibly with sufficiently fast speed. Otherwise, the estimators as well as the observers should be studied and included in the control scheme (Ali, Hoang, Hussain, & Dochain, 2015). Finally, Figure 3.1 shows the PBC scheme.

In Figure 3.1, $\alpha(x)$ and $\beta(x)$ are column vectors expressed explicitly as follow.

- $\alpha(x) = [\alpha_1, \alpha_2, \dots, \alpha_m]$ where $\alpha_i = -\gamma_i \frac{h_i^2(x)}{L_{g_i(x)}\mathbb{V}(x)} - \frac{L_{f_{nd,\ i}(x)}\mathbb{V}(x)}{L_{g_i(x)}\mathbb{V}(x)}$
- $\beta(x) = [\beta_1, \beta_2, \dots, \beta_m]$ where $\beta_i = \frac{h_i(x)}{L_{g_i(x)}\mathbb{V}(x)}$

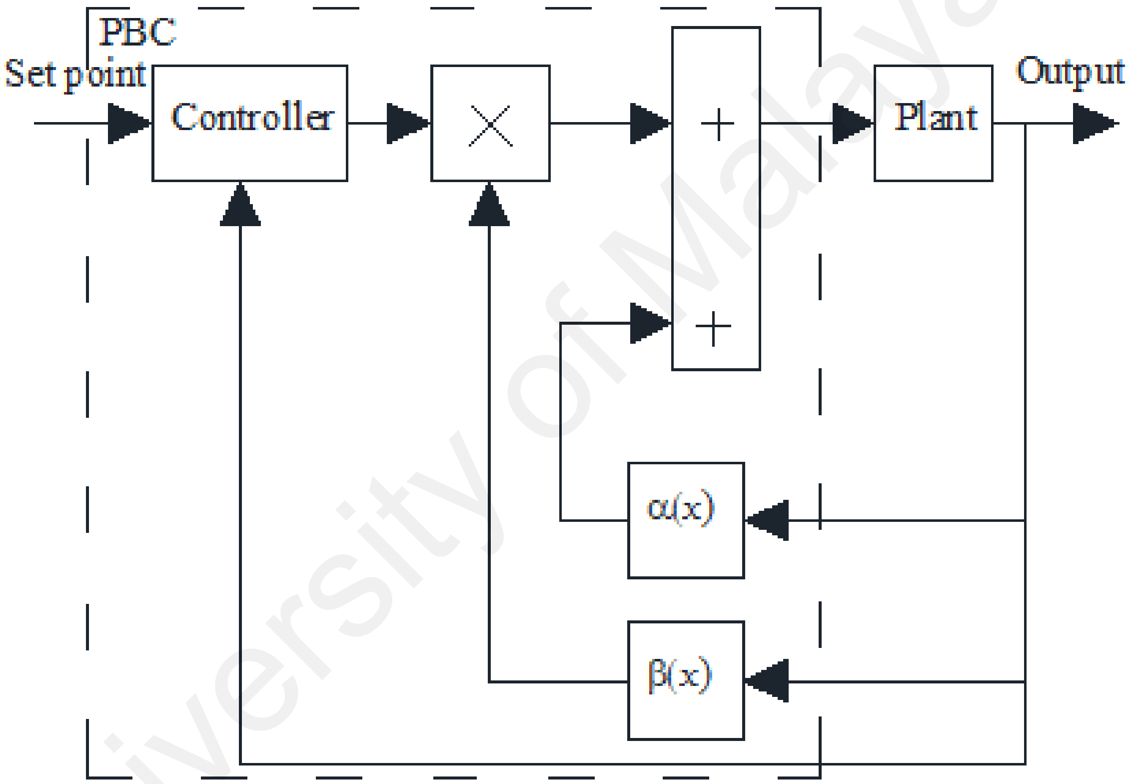


Figure 3.1: The block diagram of proposed passivity-based control

CHAPTER 4: APPLICATION TO THE CONTROL DESIGN FOR THE STABILIZATION OF POLYSTYRENE PRODUCTION IN CSTR

This chapter, firstly, describes the mathematical model of the continuous polystyrene production process in the CSTR (Section 4.1). Although the model was introduced shortly in Section 2.1, it will be really convenient for the readers if the model of the FRP process of styrene in CSTR is reminded with more detailed descriptions about the practical operation and the physical parameters. Then, in Section 4.2, the approximate linearization technique presented in Section 3.1 is applied to analyze the stability property of the polymerization system near equilibrium points. In the same vein, the mathematical formulas of heat-removal rate and heat-generation rate are also expressed explicitly and they will be used to draw the Van Heerden diagram in Chapter 5. By using the diagram, the stability property of the system is concluded according to the principle of heat balance.

As far as the control problem is concerned, the middle-conversion steady state is determined as the desired equilibrium point and then the control design methodology which is proposed in Sections 3.3 and 3.4 is applied to calculate the mathematical formulas of multivariable controller for the stabilization of the continuous polystyrene production process in the CSTR in Section 4.3.

4.1 The mathematical model of continuous polystyrene production in CSTR

The free-radical solution polymerization reactions taking place in the CSTR play a vital role in the petrochemical industry to produce polystyrene (PS) or polymethyl-methacrylate (MMA), etc. (Krzysztof Matyjaszewski, 2003; Meyer & Keurentjes, 2005).

In fact, monomer styrene is fed into the CSTR and the reaction system is initiated by initiator (AIBN) which is also fed to the reactor (see Figure 4.1) and the growth of monomer molecules into polymer occurs under constraints of free-radical mechanism. Additionally, its reaction kinetics' constants can be seen in Table 4.1 (Russo & Bequette,

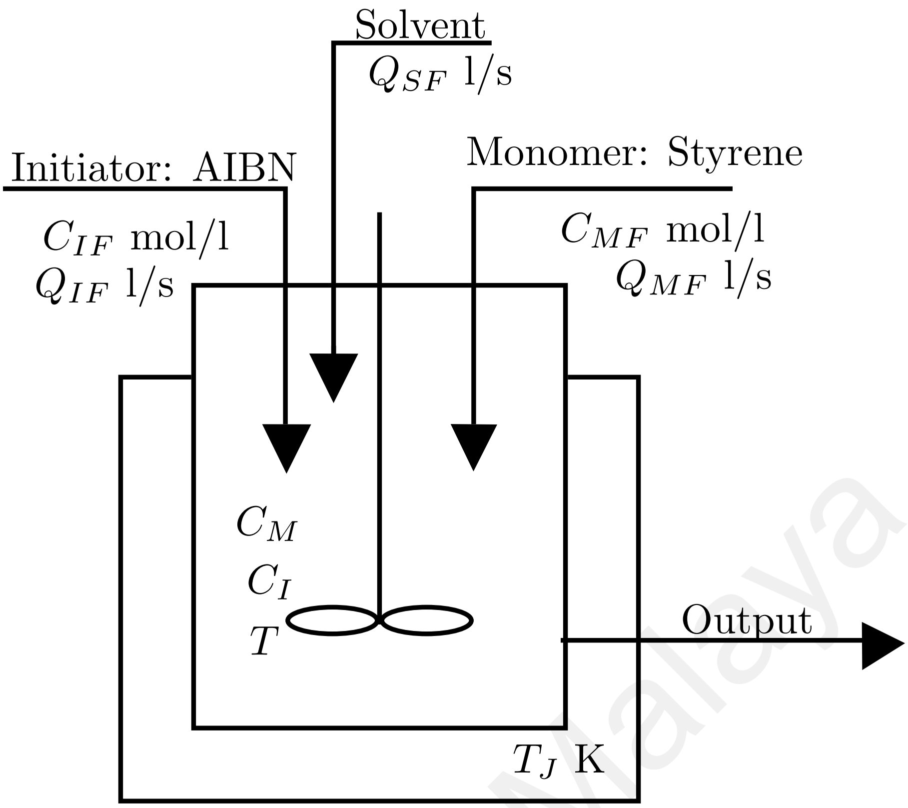


Figure 4.1: The FRP reactor for the production of polystyrene

1998; Van Dootingh et al., 1992). As far as the mathematical modelling is concerned, some following assumptions are considered.

- All reactions are irreversible and elementary.
- The polymer radical species do not exist for a long time compared to the other system time constants so that the quasi-steady-state approximation holds.
- The polymer propagation rate is represented by a single rate formula.
- The exchange of kinetic and potential energy, which is produced the shaft work of the agitator, between inlet and outlet streams is negligible.
- The CSTR is mixed perfectly.
- The heat capacity of the system, the density of reacting mixture and overall heat transfer coefficient are constant consistently.

Based on the material and energy balance equations, the mathematical model of the polystyrene production process in the CSTR can then be written as below (Biswas & Samanta, 2013; Hidalgo & Brosilow, 1990; Russo & Bequette, 1998):

$$\begin{cases} \frac{dC_M}{dt} = \frac{Q_{MF}}{V} C_{MF} - \frac{Q_{MF}+Q_{IF}+Q_{SF}}{V} C_M - \left(k_p + k_{ttM}\right) C_M C_R - 2 f k_d C_I \\ \frac{dC_I}{dt} = \frac{Q_{IF}}{V} C_{IF} - \frac{Q_{MF}+Q_{IF}+Q_{SF}}{V} C_I - k_d C_I \\ \frac{dC_S}{dt} = \frac{Q_{SF}}{V} C_{SF} - \frac{Q_{MF}+Q_{IF}+Q_{SF}}{V} C_S \\ \frac{dT}{dt} = \frac{Q_{MF}+Q_{IF}+Q_{SF}}{V} \left(\frac{c_{pF}}{c_p} T_F - T\right) - \frac{k_p C_M \Delta H C_R}{\rho c_p} + \frac{UA}{\rho V c_p} \left(T_J - T\right), \end{cases} \tag{4.1}$$

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_{ttM} are reaction rates in the free-radical mechanism and given by the Arrhenius law in Table 4.1. In this model, the variable C_R denotes the concentration of polymer radical which is defined by

$$C_R = \sqrt{\frac{2 f k_d C_I}{k_{tc} + k_{td}}}. \tag{4.2}$$

Table 4.1: Styrene polymerization reaction's physical parameters

Reaction rate	**Units**
$k_d = 1.58 \times 10^{15} \exp\left(\frac{-1.28\times10^5}{RT}\right)$	s^{-1}
$k_i = 2.184 \times 10^3 \exp\left(\frac{-1.15\times10^5}{RT}\right)$	$\mathrm{l.mol^{-2}.s^{-1}}$
$k_p = 1.051 \times 10^7 \exp\left(\frac{-2.954\times10^4}{RT}\right)$	$\mathrm{l.mol^{-1}.s^{-1}}$
$k_{tc} = 6.275 \times 10^8 \exp\left(\frac{-7.026\times10^3}{RT}\right)$	$\mathrm{l.mol^{-1}.s^{-1}}$
$k_{td} = 0$	$\mathrm{l.mol^{-1}.s^{-1}}$
$k_{ttM} = 2.31 \times 10^6 \exp\left(\frac{-5.3\times10^4}{RT}\right)$	$\mathrm{l.mol^{-1}.s^{-1}}$

Once the product properties of free-radical polymer including the number average molecular weight (NAMW) and polydispersity (PD) are taken into considerations, the method of moment (Ray, 1972) is used to characterize the polymer property distribution. This is due to the fact that, the NAWM and PD are fairly well defined by the first leading moments and the molecular weights of monomer (Prasad et al., 2002; Van Dootingh et al., 1992; Viel et al., 1995). However, the dynamics of polymerization system (4.1) do not rely on the dynamics of the first leading moments; therefore, the dynamical analysis and the control design can be considered independently (Van Dootingh et al., 1992; Viel et al., 1995).

4.2 Application of approximate linearization technique for the stability analysis of the continuous polystyrene production in CSTR

4.2.1 Equilibrium points of the polymerization system

The equilibrium points of system are also called stationary operating points or steady states. At these points, the time derivatives of state variables, i.e. the time derivative of concentration and temperature of system are equal to zero. The following proposition shows that the equilibrium points of the polymerization system (4.1) can be expressed explicitly through the physical and operating parameters.

Proposition 4.1 *The equilibrium point $P^e = \left(C_M^e, C_I^e, T^e\right)$ of the system is calculated by the formulas as follows*

$$C_I^e = \frac{\frac{Q_{IF}}{V} C_{IF}}{\frac{Q_{MF}+Q_{SF}+Q_{IF}}{V} + k_d\left(T^e\right)}, \tag{4.3}$$

$$C_M^e = \frac{\frac{Q_{MF}}{V} C_{MF} - 2f\, k_d\left(T^e\right) C_I^e}{\frac{Q_{MF}+Q_{SF}+Q_{IF}}{V} - \left[k_p\left(T^e\right) + k_{ttM}\left(T^e\right)\right] C_R\left(C_I^e, T^e\right)}, \tag{4.4}$$

where T^e is a root of the nonlinear equation below

$$\frac{Q_{MF}+Q_{SF}+Q_{IF}}{V}\left(\frac{c_{pF}}{c_p} T_F - T^e\right) + \frac{UA}{\rho V c_p}\left(T_J - T^e\right) = \frac{k_p C_M \Delta H}{\rho c_p} C_R. \tag{4.5}$$

Proof. The equilibrium point $P^e = \left(C_M^e, C_I^e, T^e\right)$ is identified by setting the time derivative of state variables (4.1) to be zero, or $\frac{d}{dt}\Big|_{\left(C_M^e, C_I^e, T^e\right)} = 0$, we obtain

$$\begin{aligned}
&\frac{Q_{MF}}{V}C_{MF} - \frac{Q_{MF}+Q_{SF}+Q_{IF}}{V}C_M^e - \left[k_p\left(T^e\right) + k_{ttM}\left(T^e\right)\right]C_M^e C_R\left(C_I^e, T^e\right) \\
&\hspace{20em} - 2f\,k_d\left(T^e\right)C_I^e = 0, \\
&\frac{Q_{IF}}{V}C_{IF} - \frac{Q_{MF}+Q_{SF}+Q_{IF}}{V}C_I^e - k_d\left(T^e\right)C_I^e = 0, \\
&\frac{Q_{MF}+Q_{SF}+Q_{IF}}{V}\left(\frac{c_{pF}}{c_p}T_F - T^e\right) + \frac{UA}{\rho V c_p}\left(T_J - T^e\right) - \frac{k_p\left(T^e\right)C_M^e \Delta H}{\rho c_p}C_R\left(C_I^e, T^e\right) = 0.
\end{aligned} \tag{4.6}$$

Obviously, the first and second equations of (4.6) have two solutions which are calculated by (4.3) and (4.4), respectively. Finally, by substituting (4.3) and (4.4) into the third equation of (4.6), (4.5) is achieved immediately. □

By following Proposition 4.1, the equilibrium points of the system (4.1) under certain operating conditions are computed and then presented in the phase plane. In addition, the system trajectories drawn from different initial conditions reveal the characteristic of system dynamics. Together with the phase portrait, the Van Heerden diagram is also used to predict the multiplicity behavior, i.e. the occurrence of this abnormal phenomenon when the jacket temperature changes and the volumetric flow rate of initiator is fixed. In the Van Heerden diagram, besides of the equilibrium points $P^e = \left(C_M^e, C_I^e, T^e\right)$, the curve of heat-generation rate Q_g and the straight line of heat-removal rate Q_r are also drawn and the number of intersections between Q_g and Q_r is identical to the number of the equilibrium points of the polymerization system (4.1). The following proposition expresses explicitly the mathematical formulas of Q_g and Q_r.

Proposition 4.2 *Heat-generation rate Q_g and heat-removal rate Q_r of the FRP process of styrene in CSTR* (4.1) *are calculated by*

$$Q_g = -\frac{k_p(T)\Delta H}{\rho c_p} \frac{\frac{Q_{MF}}{V} C_{MF} - 2 f k_d (T) C_I}{\frac{Q_{MF}+Q_{SF}+Q_{IF}}{V} - \left[k_p (T) + k_{ttM} (T)\right] C_R (C_I, T)} C_R (C_I, T) \tag{4.7}$$

where C_R is mentioned in (4.2) *and*

$$Q_r = -\frac{Q_{MF} + Q_{SF} + Q_{IF}}{V} \left(\frac{c_{pF}}{c_p} T_F - T\right) - \frac{UA}{\rho V c_p} (T_J - T) . \tag{4.8}$$

Proof. The third equation of (4.1) is separated into two different parts as follows

$$\frac{dT}{dt} = -Q_r + Q_g \tag{4.9}$$

where Q_r and Q_g are calculated by (4.8) and (4.7), respectively.

It is clearly to notice that the first part of the right hand-side (4.9) presents the amount of heat Q_r (4.8) which is given out by the coolant flow in the jacket of reactor while the second part expresses the amount of heat Q_g (4.8) which is released by the exothermic FRP reaction system. The latter completes the proof. □

Remark 4.1 *Clearly, Q_r and Q_g is a straight line and a nonlinear curve in terms of T, respectively.*

4.2.2 The Jacobian matrix of linearized system

In this section, the linearization technique and the stability criteria in the Section 3.1 are applied to evaluate the stability of system (4.1) near equilibrium point $P^e = \left(C_M^e, C_I^e, T^e\right)$ with $u^e = T_J$. Firstly, the Jacobian matrix A are computed as follows

$$A = \left.\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\right|_{P^e}, \tag{4.10}$$

where

$$a_{11} = \frac{\partial f_1}{\partial x_1} = \frac{Q_{MF} + Q_{IF} + Q_{SF}}{V} - \left(k_p(T^e) + k_{ttM}(T^e)\right) C_R(C_I^e, T^e),$$

$$a_{12} = \frac{\partial f_1}{\partial x_2} = -\left(k_p(T^e) + k_{ttM}(T^e)\right) C_M^e \frac{1}{2}\sqrt{\frac{f\, k_d(T^e)}{C_I^e\,(k_{tc}(T^e) + k_{td}(T^e))}} - 2f k_d(T^e),$$

$$\begin{aligned} a_{13} = \frac{\partial f_1}{\partial x_3} =& \frac{C_M^e C_R\left(C_I^e, T^e\right)}{RT^{e2}}\left[E_p k_p\left(T^e\right) + E_{ttM} k_{ttM}\left(T^e\right)\right] \\ &- \frac{-E_d(k_{tc} + k_{td})^2 + E_{tc}k_{tc} + E_{td}k_{td}}{2RT^{e\,2}\,(k_{tc} + k_{td})} C_M^e C_R\left(C_I^e, T^e\right)\left(k_p(T^e) + k_{ttM}(T^e)\right) \\ &+ \frac{2f E_d k_d\left(T^e\right) C_I^e}{RT^{e2}}, \end{aligned}$$

$$a_{22} = \frac{\partial f_2}{\partial x_2} = -\frac{Q_{MF} + Q_{IF} + Q_{SF}}{V} - k_d(T^e), \quad a_{23} = \frac{\partial f_2}{\partial x_3} = -\frac{E_d}{RT^{e2}} k_d(T^e) C_I^e,$$

$$a_{31} = \frac{\partial f_3}{\partial x_1} = -\frac{k_p(T^e)\Delta H}{\rho c_p} C_R\left(C_I^e, T^e\right),$$

$$a_{32} = \frac{\partial f_3}{\partial x_2} = -\frac{k_p(T^e) C_M^e \Delta H}{\rho c_p}\sqrt{\frac{f\, k_d(T^e)}{C_I^e\,(k_{tc}(T^e) + k_{td}(T^e))}},$$

$$a_{33} = \frac{\partial f_3}{\partial x_3} = -\frac{Q_{mF} + Q_{mI}}{V} - \frac{UA}{\rho V c_p} + \frac{k_p\left(T^e\right) C_M^e \Delta H}{\rho c_p R T^{e2}} C_R\left(C_I^e, T^e\right)\left[E_p - \frac{-E_d\left(k_{tc} + k_{td}\right) + E_{tc}k_{tc} + E_{td}k_{td}}{k_{tc} + k_{td}}\right].$$

Then, the eigenvalues of the Jacobian matrix are calculated with the corresponding numerical values of equilibrium points and the operating parameters. We can derive subsequently the conclusion of stability property of the polystyrene production process in CSTR around equilibrium points according to two stability criteria mentioned in Section 3.1.

4.3 The control design

4.3.1 Control problem statement

As far as the control scheme is concerned, the jacket temperature T_J and the volumetric feed rate of initiator Q_{IF} are chosen as manipulated inputs. Also, the reactor temperature T and the concentration of initiator C_{IF} are selected as the controlled outputs. Note also that the monomer conversion can also be directly controlled via the concentration of initiator.

In this section, the control strategy developed in Section 3.3 and Section 3.4 is applied to stabilize the desired output variables (T and C_I) of the polystyrene production process in CSTR at the desired steady state (including open-loop unstable point).

4.3.2 The passivation of system via input coordinate transformations

As mentioned before, T_J and Q_{IF} are chosen as manipulated variables. However, for the sake of convenience, let us denote

$$Q_2 = \frac{Q_{IF}}{V} \tag{4.11}$$

and Q_2 is then used instead of Q_{IF} for the control design with no confusion.

Since the concentration of solvent does not have impact on the dynamics of the system (i.e., the reaction invariant dynamics) (Biswas & Samanta, 2013; Dochain, Perrier, & Ydstie, 1992; Hoang, Couenne, Le Gorrec, et al., 2013; Rodrigues, Srinivasan, Billeter,

& Bonvin, 2015; Waller & Makila, 1981), the state vector is reduced to $x = (C_M, C_I, T)^\top$. From the dynamics (4.1), the reduced dynamics of the system is rewritten as (3.1), with $f(x) = \begin{bmatrix} Q_1 x_{1F} - Qx_1 - \left(k_p + k_{ttM}\right) x_1 C_R - 2f k_d x_2 \\ -Qx_2 - k_d x_2 \\ Q\left(x_{3F} - x_3\right) - Ax_3 - CC_R x_1 k_p \end{bmatrix}$, $h(x) = [x_2 \; x_3]^\top$, $g(x) = \begin{bmatrix} 0 & 0 \\ x_2 & 0 \\ 0 & A \end{bmatrix}$ and $u = [Q_2 \; T_J]^\top$ where $A = \frac{UA}{\rho V c_p}$, $Q_1 = \frac{Q_{MF}}{V}$, $C = \frac{\Delta H}{\rho c_p}$, $Q = \frac{Q_{MF}+Q_{SF}}{V}$ and $x_F = (x_{1F} \; x_{2F} \; x_{3F})^\top = (C_{MF} \; C_{IF} \; \frac{c_{pF}}{c_p} T_F)^\top$.

Remark 4.2 *Note that the operating region $\chi = \{x \,| x_i > 0, i = 1, 2, 3\}$ 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; Assala et al., 1997; Hoang, Couenne, Le Gorrec, et al., 2013).*

Let us choose $R_{di} = \mathrm{diag}(1, 1, 1)$ (see Proposition 3.3), the storage function becomes $\mathbb{V}(x) = \frac{1}{2}\sum_{1}^{3} x_i^2$. In this case, Assumption 3.2, including $L_{g_1}V(x) = x_2 x_{2F} \neq 0$ and $L_{g_2}\mathbb{V}(x) = Ax_3 \neq 0$, holds in the operating region χ. Therefore, the system dynamics (3.1) can be passivated by two input coordinate transformations which are calculated from Proposition 3.1.

Firstly, a natural decomposition of $f(x)$ is given by

$$f_d(x) = \begin{bmatrix} -Qx_1 - \left(k_p + k_{ttM}\right) x_1 C_R - 2f k_d x_2 \\ -Qx_2 - k_d x_2 \\ -Qx_3 - Ax_3 \end{bmatrix}, \tag{4.12}$$

$$f_{nd,\,1} = 0 \text{ and } f_{nd,\,2}(x) = \begin{bmatrix} Q_1 x_{1F} \\ 0 \\ Qx_{3F} - k_p x_1 CC_R \end{bmatrix}, \tag{4.13}$$

The function $f_I(x)$ is not available because no function $f_I(x)$ can be found to satisfy the property $L_{f_I(x)}V(x) = 0;\ \forall x \in \chi$.

From (3.19), two explicit input coordinate transformations are derived as follows,

$$u_1 = \frac{1}{x_{2F}}\upsilon_1 - \frac{\gamma_1 x_2}{x_{2F}}, \tag{4.14}$$

$$u_2 = \frac{1}{A}\upsilon_2 - \frac{\gamma_2 x_3}{A} - \frac{Q_1 x_{1F} x_1 + \left(Q x_{3F} - k_p x_1 C C_R\right) x_3}{A x_3}. \tag{4.15}$$

These two explicit forms (4.14) and (4.15) allow us to obtain the actual control inputs directly. This is an interesting and important feature of the control design. Note also that new additional inputs υ_1 and υ_2 may have no physical interpretation.

4.3.3 The general canonical form of passive system

The system (4.1) after passivated by (4.14) and (4.15) is rewritten by the canonical form as follows (Proposition 3.2)

$$\dot{x} = -R(x)\frac{\partial V}{\partial x} + J(x)\frac{\partial V}{\partial x} + M(x)\upsilon, \tag{4.16}$$

where

$$R = \begin{bmatrix} Q + \left(k_p + k_{ttM}\right) C_R + 2f\, k_d \frac{x_2}{x_1} & 0 & 0 \\ 0 & Q + k_d + \gamma_1 & 0 \\ 0 & 0 & Q + A + \gamma_2 \end{bmatrix}, \tag{4.17}$$

$$J(x) = \begin{bmatrix} 0 & \frac{Q_1 x_{1F}}{x_2} & 0 \\ -\frac{Q_1 x_{1F}}{x_2} & 0 & \frac{Q_1 x_{1F} x_1}{x_2 x_3} \\ 0 & -\frac{Q_1 x_{1F} x_1}{x_2 x_3} & 0 \end{bmatrix} \tag{4.18}$$

and

$$M(x) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{4.19}$$

4.3.4 The PBC via tracking error

Let $x_d = (x_{1d}, x_{2d}, x_{3d})$ be a reference trajectory of the system (4.16). Based on Proposition 3.3, the vector field x_d is represented as below

$$\dot{x}_{1d} = -R_1 x_{1d} + \frac{Q_1 x_{1F}}{x_2} x_{d1} + R_{d1}(x_1 - x_{1d}), \tag{4.20a}$$

$$\dot{x}_{2d} = -R_2 x_{2d} - \frac{Q_1 x_{1F}}{x_2} x_{1d} + \frac{Q_1 x_1 x_{1F}}{x_2 x_3} x_{3d} + R_{d2}(x_2 - x_{2d}) + \upsilon_1, \tag{4.20b}$$

$$\dot{x}_{3d} = -R_3 x_{3d} - \frac{Q_1 x_1 x_{1F}}{x_2 x_3} x_{2d} + R_{d3}(x_3 - x_{3d},) + \upsilon_2, \tag{4.20c}$$

where $R_1 > 0$, $R_2 > 0$ and $R_3 > 0$ are the elements of matrix $R(x) = \text{diag}(R_1, R_2, R_3)$ while $R_{d1} > 0$, $R_{d2} > 0$ and $R_{d3} > 0$ are the arbitrary elements of positive definite matrix.

The desired reference trajectory $x_d = (x_{1d}\ x_{2d}\ x_{3d})^\top$ is selected in such a way that its dynamics converges to the set point $x^e = \left(x_1^e\ x_2^e\ x_3^e\right)^\top$ (possibly coincident with the unstable steady state B in Figure 5.1). From Remark 3.11 and the expression of the matrix $M(x)$ (4.19), only two components of x_d, that is, x_{1d} and x_{2d}, are chosen to assign as $\dot{x}_{2d} = K_1\left(x_2^e - x_{2d}\right)$ and $\dot{x}_{3d} = K_2\left(x_3^e - x_{3d}\right)$ where K_1 and K_2 are gains of the controller. Consequently, it is straightforward to check that $x_{2d}(t)$ and $x_{3d}(t)$ converge exponentially to x_2^e and x_3^e, respectively, when time goes to infinity.

From (4.20b) and (4.20c), the internal dynamic controller can be obtained as below

$$\upsilon_1 = R_2 x_{2d} + \frac{Q_1 x_{1F}}{x_2} x_{1d} - \frac{Q_1 x_1 x_{1F}}{x_2 x_3} x_{3d} - R_{d2}(x_2 - x_{2d}) + K_1\left(x_2^e - x_{2d}\right), \tag{4.21}$$

$$\upsilon_2 = R_3 x_{3d} + \frac{Q_1 x_1 x_{1F}}{x_2 x_3} x_{2d} - R_{d3}(x_3 - x_{3d}) + K_2\left(x_3^e - x_{3d}\right). \tag{4.22}$$

As a consequence, the actual control input $u = [u_1\ u_2]^\top = [Q_2\ T_J]^\top$ is derived using (4.14), (4.15), (4.21) and (4.22).

Remark 4.3 *In cases where the presence of noise and/or disturbance is taken into account, to make sure that the closed-loop system has zero steady-state error to arbitrary step commands, the integral actions, which can be added to the previous controller u_1 and u_2 (as suggested the authors in (Chou & Wu, 2007; Donaire & Junco, 2009), are given as follows*

$$u_{I1} = \tau_1 \int_0^t (x_{d2}(\sigma) - x_2(\sigma))\, d\sigma, \tag{4.23}$$

$$u_{I2} = \tau_2 \int_0^t (x_{d3}(\sigma) - x_3(\sigma))\, d\sigma. \tag{4.24}$$

where τ_1 and τ_2 are the tuning parameters.

Consequently, the actual control input is expressed as follows,

$$\begin{aligned} u_1 = \frac{1}{x_{2F}} \left[R_2 x_{2d} + \frac{Q_1 x_{1F}}{x_2} x_{1d} - \frac{Q_1 x_1 x_{1F}}{x_2 x_3} x_{3d} - R_{d2}\left(x_2 - x_{2d}\right) + K_1\left(x_2^e - x_{2d}\right) \right] \\ - \frac{\gamma_1 x_2}{x_{2F}} + \tau_I \int_0^t (x_{d2}(\sigma) - x_2(\sigma))\, d\sigma, \end{aligned} \tag{4.25}$$

$$\begin{aligned} u_2 = \frac{1}{A} \left[R_3 x_{3d} + \frac{Q_1 x_1 x_{1F}}{x_2 x_3} x_{2d} - R_{d3}\left(x_3 - x_{3d}\right) + K_2\left(x_3^e - x_{3d}\right) \right] - \frac{\gamma_2 x_3}{A} \\ - \frac{Q_1 x_{1F} x_1 + \left(Q x_{3F} - k_p x_1 C C_R\right) x_3}{A x_3} + \tau_2 \int_0^t (x_{d3}(\sigma) - x_3(\sigma))\, d\sigma. \end{aligned} \tag{4.26}$$

It is worth noting that the resulting passive system (formatted in a canonical form (4.16)) can also be stabilized with PID passivity-based control at a constant equilibrium (via negative feedback interconnection) (Donaire & Junco, 2009; Montoya, 2016). However, the control strategy proposed in this work is based on tracking-error where the desired reference trajectory dynamics passing through the set point is not constant and appropriately assigned.

CHAPTER 5: RESULTS AND DISCUSSIONS

In Chapter 4, the linearization technique and the theoretical developments of feedback passivation method through input coordinate transformations have been already applied to design the tracking-error plus passivity-based multivariable control for the continuous polystyrene production process in the CSTR. These extensions indeed considered as the main contributions of this research work are illustrated by the simulations studies (the numerical values of physical, operating parameters and initial conditions are given in Appendices A and B) in Chapter 5. More precisely, in Section 5.1, the open loop responses of the polymerization system are presented by the Van Heerden diagram, the phase plane and the bifurcation diagrams. Based on these representations, the stability properties of open-loop system dynamics under certain operating conditions are explained in detail. Additionally, the desired equilibrium point which compromises both the economic benefits and engineering constraints is determined for the purpose of global stabilization of the polymerization system. In fact, such stability analyses lay a solid foundation for the control problem statement which is to design the feedback laws to stabilize and optimize the practical operation of the polystyrene production process in CSTR.

In Section 5.2, the closed-loop responses of the system under the proposed controller without effects of noise and/or disturbance are conducted as follow. The phase plane of closed-loop system representing the convergence of system strategies starting at the different initial conditions to the desired equilibrium point is derived. The transient responses of state variables and the behaviors of manipulated inputs in the time domain are represented subsequently to derive the helpful discussions of dynamics of closed-loop system under the normal conditions (no noise and/or disturbance).

Actually, the continuous styrene polymerization system is disturbed by different types of noise and disturbance in practice. Therefore, Section 5.3 aims to evaluate the robustness of dynamics of the closed-loop system under impacts of noise and disturbance.

From this assessment, the practitioners and researchers can see the effects of noise and/or disturbance in the dynamics of closed-loop system as well as the convergence capability of the proposed PBC in the practical implementation.

Finally, the control performance of closed-loop system under the proposed PBC scheme is compared with that of under the conventional proportional integral (PI) control in terms of the merit scores such as ISE and ITAE in Section 5.4. Based on this comparison, the advantages of the proposed PBC are given.

5.1 The open loop response of the system

5.1.1 The Van Heerden diagram and the phase plane of open-loop system

Firstly, the equilibrium points $P^e = \left(C_M^e, C_I^e, T^e\right)$ are computed by following Proposition 4.1 with operating conditions as well as physical parameters which are listed in Appendix A and Table 4.1. The numerical values are given by $P_1 = (3.295; 0.408; 325.4)$, $P_2 = (2.407; 0.351; 360.7)$ and $P_3 = (0.721; 0.0085; 415.7)$.

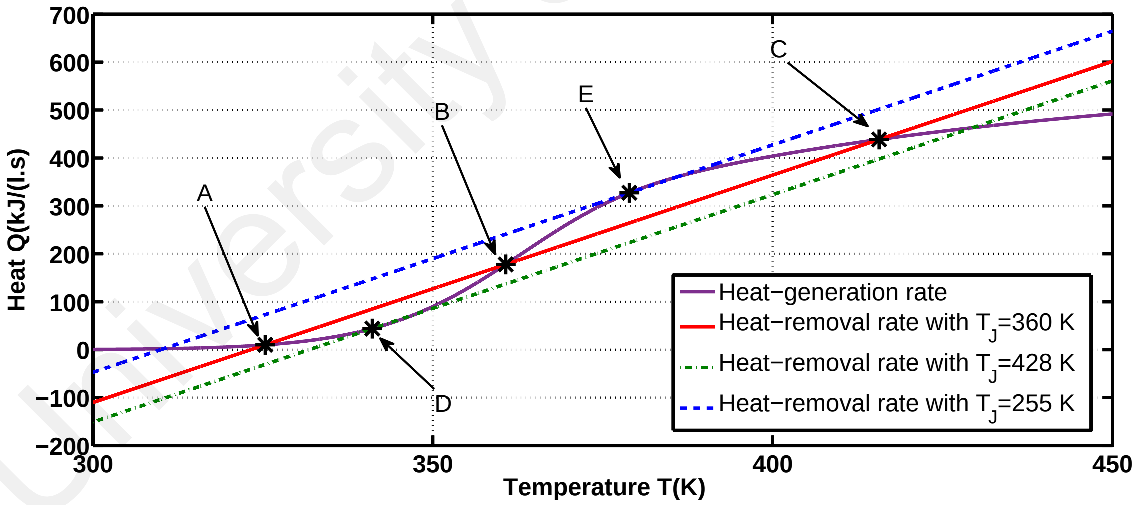


Figure 5.1: The Van Heerden diagram

The Figure 5.1 shows the Van Heerden diagram where points A, B and C correspond the steady states P_1, P_2 and P_3 respectively. As we can see, the heat-removal rate Q_r is a straight line in terms of T while the heat-generation rate Q_g is a nonlinear curve with an inflection point in terms of T. Additionally, the straight line of Q_r intersects the curve of

Table 5.1: The eigenvalues corresponding to the equilibrium points

Eigenvalue	The equilibrium point P^e		
	P_1	P_2	P_3
λ_1	-0.0026	0.0051	-0.0041
λ_2	-0.0026	-0.0025	-0.0055
λ_2	-0.0028	-0.0029	-0.1186

Q_g with $T_J = 360$K into three different points including points A, B and C. That means the polystyrene production process in the CSTR (4.1) has three different equilibrium points. Also, for any $T_J \in (255, 428)$ K, the styrene FRP system always has three different steady state points.

We assume that the input $u^e = T_J$ can be changed in some cases to meet the operating requirements. It is clear to see that the straight lines of Q_r corresponding to $T_J = 255$ K or $T_J = 428$ K are tangential to the nonlinear curve of Q_g at $T^e = 378.9$ K (point E) or $T^e = 341.1$ K (point D), respectively (Figure 5.1). Consequently, the FRP system just has two steady states. Finally, in the case T_J is out of the region $\beta = (255, 428)$ K, the styrene FRP system has only one equilibrium point.

To evaluate the stability of polystyrene production process in the CSTR (4.1), all eigenvalues corresponding to the equilibrium points P_1, P_2 and P_3 at $T_J = 360$ K are tabulated in Table 5.1. In fact, the equilibrium point P_2 regarding to the medium-conversion steady state is an unstable-open-loop point because one of its eigenvalues $\lambda_1 = 0.0025$ has the positive real part (Stability criteria 1) while the system is locally asymptotically stable at other equilibrium points (the low-conversion steady state P_1 and high-conversion steady state P_3) because the real parts of all their eigenvalues are negative.

On the other hand, the stability property of these steady states is also determined from the viewpoint of principle of heat balance. For instance, at point A corresponding to P_1, if the reactor temperature increases from 325.4 K, Q_r will be larger than Q_g; it means the reactor will be cooled down, then reactor temperature will decrease to 325.4 K and consequently the styrene FRP system will be remained at the point A. While if the reactor temperature decreases from 325.4 K, the system will be heated up because Q_r will be smaller than Q_g, the temperature will increase subsequently again to 325.4 K and so the styrene FRP system will be still remained at the point A. Similarly, the system is locally asymptotically stable at any neighborhoods of point C corresponding to P_3.

However, at point B corresponding to P_2, if the reactor temperature T suddenly increases or decreases, i.e. moving out of B due to any perturbations, Q_g will be greater or smaller than Q_r, respectively. Hence, the temperature reactor T will continue to go up or go down to approach another equilibrium points, respectively. For example, in the case that the system is cooled down, i.e. the reactor temperature T decreases from 360.7 K, consequently, the system approaches point A. Vice versa, the steady state of reactor reaches point C if the reactor temperature T increases from 360.7 K.

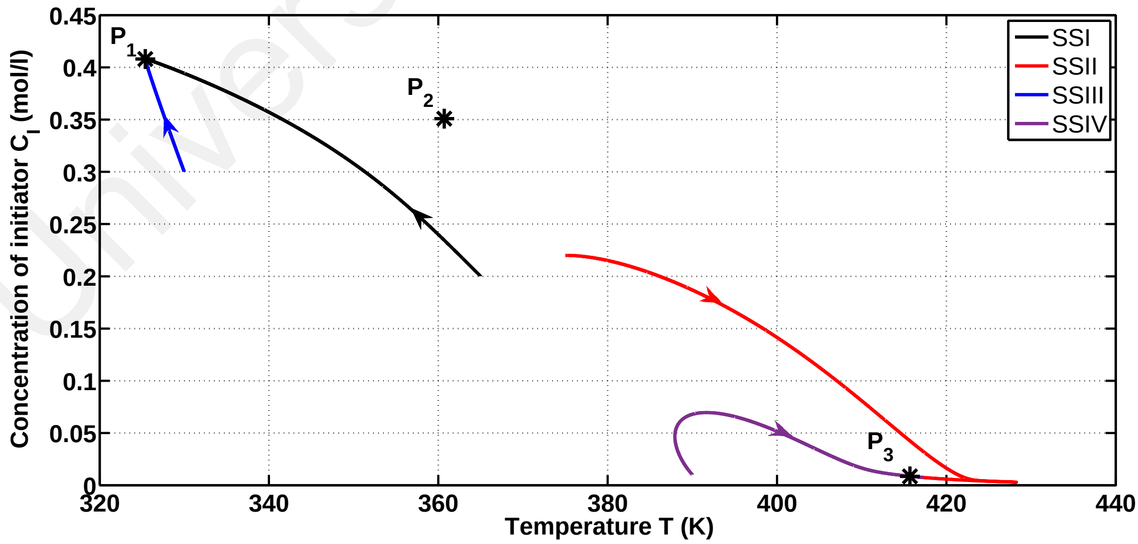


Figure 5.2: Representation of the open-loop phase plane

The open-loop phase plane is shown in Figure 5.2. Clearly, all of trajectories of the system, which originates from six different initial conditions including SSI, SSII, SSIII and SSIV (the numerical values are listed in Appendix B), just approach P_1 or P_3. In fact, the convergence of these trajectories depends on their initial conditions. For example, the system trajectories originating from SSI and SSIII converge to P_1 while the other trajectories originating from SSII and SSIV converge to P_3. Furthermore, by using the Stability criteria 2 and Remark 3.2, both points A and C are the asymptotically stable nodes of approximately linearized system at the equilibrium point P_1 and P_3, and the nonlinear system.

Remark 5.1 *When the system just has two equilibrium points, it means that the straight line of Q_g is tangential to the curve of Q_r at a point and intersects this curve at another point. Moreover, the system is asymptotically stable at the intersection point and the tangential point is an unstable-open-loop equilibrium point (for example, points E and D in Figure 5.1).*

Remark 5.2 *If the jacket temperature T_J is out of the region $\beta = (255, 428)$ K, the system has only one equilibrium point and so this point is definitely a stable-open-loop equilibrium point.*

Remark 5.3 *The system trajectories approach to the steady-state point directly without oscillations because all eigenvalues of the Jacobian matrix of the linearized model at the corresponding equilibrium points (see in Table 5.1) have no imaginary part (Khalil, 2002).*

5.1.2 The bifurcation diagrams

As we can see in the previous section, the multiplicity behavior does not exist when jacket temperature T_J is out of the region $\beta = (255, 428)$ K. That means the stability property of the system can change in terms of jacket temperature T_J which is called a bifurcation parameter. In this section, this abnormal phenomenon is carried out when the volumetric flow rate of initiator (AIBN) Q_{IF} is considered as a second bifurcation parameter together with the first bifurcation parameter T_J. More precisely, the amplitudes of equilibrium points versus jacket temperature are drawn [1] with different volumetric flow rates of initiator (AIBN) Q_{IF}.

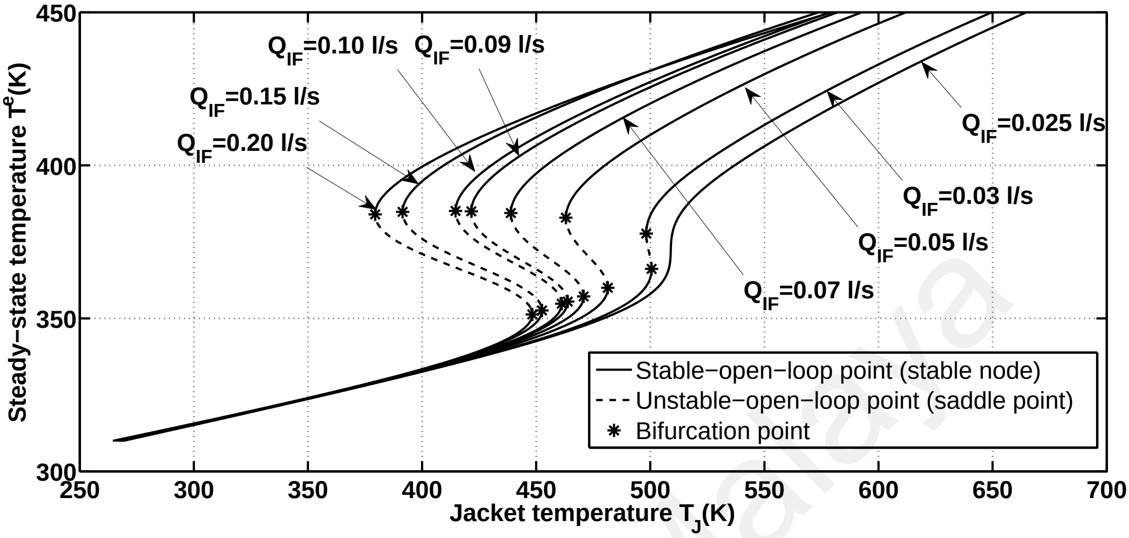


Figure 5.3: Effect of flowrate of initiator on the bifurcation diagram of FRP system ($Q_{IF} \in [0.025; 0.2]$) ℓ/s

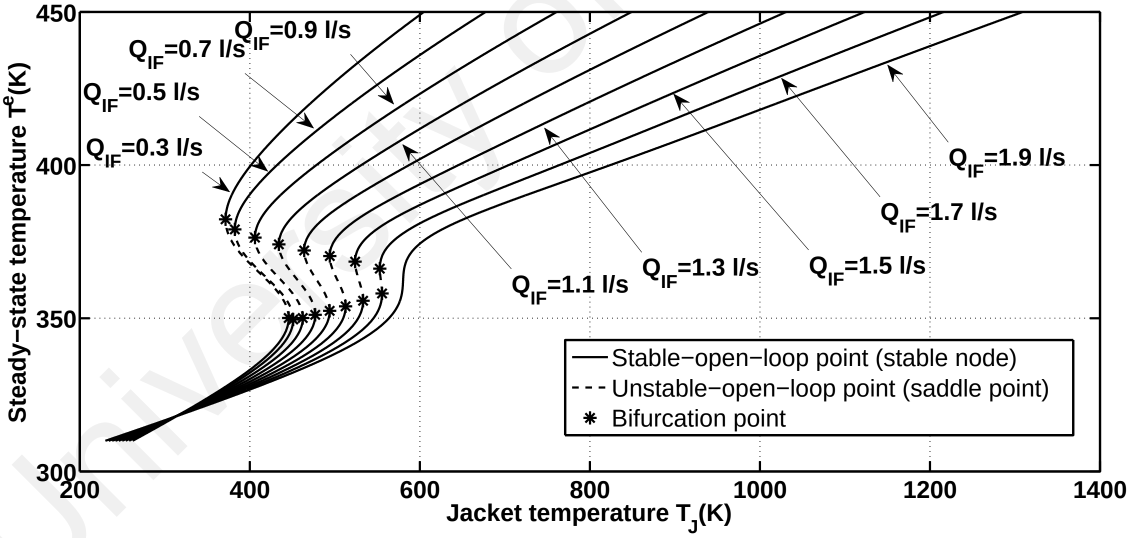


Figure 5.4: Effect of flowrate of initiator on the bifurcation diagram of FRP system ($Q_{IF} \in [0.3; 1.9]$) ℓ/s

The Figure 5.3 and Figure 5.4 show the bifurcation diagram of the polystyrene production process in the CSTR with $Q_{IF} \in [0.025; 0.2], \ell$/s and $Q_{IF} \in [0.3; 1.9]$ ℓ/s, respectively, together with different jacket temperatures T_J. It can be clearly seen that if the bifurcation parameter Q_{IF} goes down to 0.025 ℓ/s or goes up to 1.9 ℓ/s, the domain of

[1] The sketch is called a bifurcation diagram.

the unstable-open-loop equilibrium points will diminish gradually to zero. Additionally, if Q_{IF} is smaller than 0.025 ℓ/s or greater than 1.9 ℓ/s, this region will disappear, i.e. the steady-state multiplicity behavior of reactor will disappear because the system has only one stable-open-loop equilibrium point.

Based on the appearance of the bifurcation diagrams in Figure 5.3 and Figure 5.4, the bifurcation behavior represented here is called the saddle-node bifurcation with two saddle-node bifurcation points which are the starting point and the ending point of each dashed line in Figure 5.3 and Figure 5.4.

5.2 Closed loop response without effects of noise and/or disturbance

In the first case, the numerical simulations are run with normal condition (the impacts of noise and/or disturbance on its dynamical behaviour are not included). After tuning, the control parameters of PBC are $K_1 = 0.018$, $K_2 = 0.005$, $R_{d1} = 4$, $R_{d2} = 1$, $R_{d3} = 1$, $\gamma_1 = \gamma_2 = 0.01$, $\tau_1 = 0.5$ and $\tau_2 = 1$. Figure 5.5 shows the transient responses of closed-loop system in phase plane. All of system trajectories that start from four different initial conditions converge exponentially to the desired equilibrium point $x^e \equiv P_2$ when using the proposed controller (4.25) and (4.26).

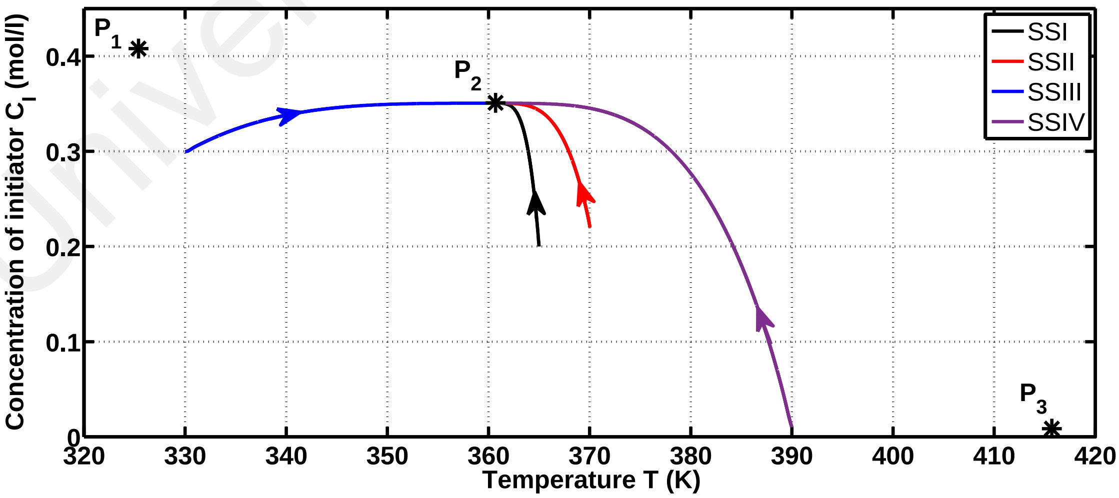


Figure 5.5: Representation of the closed-loop phase plane

Moreover, Figures 5.6a to 5.6c shows the transient responses of the output variables including the reactor temperature T, the concentration of initiator C_I and the concentration of styrene C_M in the time domain. As shown, T and C_I (the directly controlled variables) reach the desired steady states value after about 800s and 500s, respectively, while the response time of C_M is about 1800s. Furthermore, the dynamics of two manipulated variables, Q_{IF} and T_J, are given in Figures 5.7a and 5.7b (note also that the dynamics of the (alternative) actual control input Q_2 can be derived using (4.11)). As we can see that the dynamics of T_J for SSI, SSII and SSIV is faster than that of T_J for SSIII in the beginning of reaction course. In the case of SSI, SSII and SSIV, because the heat-generation rate is larger than the heat-removal rate at $t = 0$ (see Figure 5.1), T_J varies quickly in order to stabilize the system (exponentially) at $T^e = 360.7$ K.

The trajectories of temperature and concentration of monomer and initiator in simulation studies are compared with the temperature profile and experimental results in literature (Prasad et al., 2002). This show that our simulations fit the same pattern as experimental results (range of real data ($T \in [300, 400]$K, $C_I \in [0.05, 0.4]$ mol/l and $C_M \in [0, 8]$ mol/l)) therefore, they are acceptable.

5.3 Closed loop response with effects of noise and/or disturbance

5.3.1 Effects of disturbance in inlet temperature

Figure 5.8a shows that the uncertain changes of the initial inlet temperature T_F caused by the internal disturbance while the representations of the state variables T, C_I and C_M are given in Figures 5.8b to 5.8d, respectively. Besides, the dynamics of manipulated variables Q_{IF} and T_J are shown in Figures 5.9a and 5.9b, respectively.

In Figure 5.8a, T_F is assumed to remain at 298 K in the beginning, then it increases to 308 K at 500 s and keeps unchanged until the operating time is 1000 s. Additionally, the external disturbance in T_F continues to affect the system at 1500s and 2500 s, more precisely, T_F reaches 313 K and then goes down to 283 K, respectively. Moreover, as seen in Figures 5.8b to 5.8d, the transient responses of the output variables are very similar to these in the case without impacts of the disturbance in T_F. Furthermore, Figure 5.9b shows that the dynamics of T_J has step changes at 500 s, 1500 s and 2500 s while the step changes do not appear in the dynamics of Q_{IF} as seen in Figure 5.9a. This is due to the fact that the changes of T_F cause the direct changes of the non-dissipative term $f_{nd}(x)$ (4.13), but the nonlinearity of $f_{nd}(x)$ is canceled totally by the projection operators (3.33). Hence although T_F is affected by the external disturbance, the performance of output variables can still be guaranteed. In other words, the proposed PBC algorithm adjusts Q_{IF} and T_J to bring the system back to the desired reference trajectory x_d. Based on the results, the polymerization system is robust at the desired steady state point P_2.

5.3.2 Effects of disturbance in inlet concentration of initiator

In this case, the disturbance in inlet concentration of initiator C_{IF} is a series of step changes as expressed in Figure 5.10a. More precisely, C_{IF} goes up to 1.6 and 1.8; and goes down to 1.35 when the system is affected by the external disturbance at 500s, 1500s and 2500s, respectively. In addition, the transient responses of the state variables T, C_I and C_M are shown in Figures 5.10b to 5.10d, respectively while Figures 5.11a and 5.11b provide the dynamics of the manipulated variables, Q_{IF} and T_J, respectively.

As shown, the system trajectory converges to the desired equilibrium point under the impacts of disturbance in C_{IF}. The manipulated variables Q_{IF} and T_J show the step changes at 500s, 1500s and 2500s, respectively, in order to compensate and eliminate the effects of disturbance shown in Figure 5.10a. Thus, we can conclude that the polymerization reactor subject to the feedback law (4.25) and (4.26) is robust under the external disturbance in C_{IF}.

5.3.3 Effects of uncertain heat transfer coefficient

In practice, the heat transfer coefficient UA is sensitive during the operation because the heat transfer tubes regularly get stuck due to fouling, thereby reducing the heat transfer coefficient. Also, the adhesion of dirt on the layer of the vessel also makes the heat transfer coefficient decrease (Biswas & Samanta, 2013). In this case, we assume that a series of gradual change is imparted in the UA. More precisely, UA goes up gradually to 630 and 660 W/m^2.K; and goes down steadily to 510 at 500s, 1500s and 2500s, respectively Figure 5.12a.

The transient responses of output variables (T, C_I and C_M) in the case of the uncertain heat transfer coefficient UA are given in Figures 5.12b to 5.12d, respectively, while Figures 5.13a and 5.13b provide the behavior of manipulated variables (Q_{IF} and T_J), respectively. Obviously, the output variables still approach to the desired values in spite of the uncertainty of UA because the proposed PBC can handle this situation. More precisely, the convergence capability of the system trajectory x along the reference trajectory is guaranteed by the positive definiteness of $R_D = R(x) + R_I$ (Proposition 3.3) while the UA is covered in the damping matrix (4.17). Hence, once the reference trajectory x_d is stabilized globally, the system trajectory is also stabilized globally despite the uncertainty of UA.

Therefore, the polymerization reactor (4.1) under the proposed control (4.25) and (4.26) are robust for this case study.

5.3.4 Effects of random noise in the volumetric feed rate of monomer

As far as the influence of random noise is concerned, a series of random fluctuations in the feed rate of monomer Q_{MF} is observed at 2000s, i.e. Q_{MF} fluctuates between 0.8 to 1.25 mol/ℓ in Figure 5.14a.

As we can see clearly that, although there are continuous oscillations in Q_{MF}, the output variables (T, C_I and C_M) given in Figures 5.14b to 5.14d, respectively, approach the desired steady states while the behavior of control variables (Q_{IF} and T_J) appear the continuous fluctuations to stabilize the system in Figures 5.15a and 5.15b, respectively. This is due to the fact that $Q_1 x_{1F} = \frac{Q_{MF}}{V} x_{1F}$ is one of elements of the non-dissipative term $f_{nd}(x)$ (4.13), so its unstable behaviors caused by the random noise is removed by the proposed PBC (as discussed in Section 3.4). Hence, the convergence of system trajectory x to the reference trajectory x_d is governed by the positive-definite matrix $R_I = \text{diag}\,[R_{d1}, R_{d2}, R_{d3}]$ (Section 3.4), if reference trajectory x_d has no fluctuation, the system trajectory x also has no fluctuation. Additionally, once the matrix R_I is chosen appropriately, the control algorithm also adjusts T_J and Q_{IF} appropriately to stabilize the system. Hence, the continuous oscillations of manipulated variables are observed.

Therefore, it is straightforward to conclude that the PBC (4.25) and (4.26) depicts a high level of convergence capabilities and stability according to these results.

5.4 Comparison of control performance between the proposed PBC and the conventional PI control

In this section, the control performance of proposed PBC scheme is compared to that of the decentralized conventional proportional integral (PI) control actions governed by,

$$T_J(t) = T_{J0} + K_{PT}\,[x_3{}^e - T(t)] + K_{IT}\int_0^t [x_3{}^e - T(t)]\,dt \tag{5.1}$$

$$Q_{IF}(t) = Q_{IF0} + K_{PQ}\left[x_2^e - x_2(t)\right] + K_{IQ}\int_0^t \left[x_2^e - x_2(t)\right]dt \tag{5.2}$$

where K_{PT}, K_{PQ}, K_{IT} and K_{IQ} are the tuning parameters of PI controllers (5.1) and (5.2). Additionally, for the purpose of comparison, the closed-loop system under the PI control is stabilized at the steady state P_2, hence, $T_{J0},\ Q_{IF0},\ x_2^e$ and x_3^e are chosen to be 360, 0.75; 0.351 and 360.7, respectively.

Firstly, the transfer function matrix of linearized system is given as follow

$$G = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} \tag{5.3}$$

where

$$G_{11}(s) = \frac{2.87\times 10^5 s^2 + 1.51\times 10^3 s^3 + 1.99}{2.5\times 10^8 s^3 + 2\times 10^6 s^2 + 5.34\times 10^3 s + 4.76}$$

$$G_{12}(s) = -\frac{0.0026(s + 0.0028)}{2.5 \times 10^8 s^3 + 2 \times 10^6 s^2 + 5.34 \times 10^3 s + 4.76}$$

$$G_{21}(s) = -\frac{1.86 \times 10^6 + 9.75 \times 10^3 + 12.76}{2.5 \times 10^8 s^3 + 2 \times 10^6 s^2 + 5.34 \times 10^3 s + 4.76}$$

$$G_{22}(s) = \frac{24.875 \times 10^{-4}(s + 2.75 \times 10^{-3})(s + 2.8 \times 10^{-3})}{2.5 \times 10^8 s^3 + 2 \times 10^6 s^2 + 5.34 \times 10^3 s + 4.76}$$

The transfer functions $G_{11}(s)$ and $G_{22}(s)$ correspond to pairs of input and output $(u, y) = (Q_2, C_{IF})$ and $(u, y) = (T_J, T)$, respectively while $G_{12}(s)$ and $G_{21}(s)$ express the interaction effects among loops.

Secondly, we can assume the interaction effects among loops can be ignored for sake of simplicity in case they do not deteriorate the control performance of close-loop system (Seborg et al., 2011). In this research, the Cohen-coon tuning method is applied for tuning individual loops $G_{11}(s)$ and $G_{22}(s)$ where the time when half and 0.632 of output in step response occurs (κ_1 and κ_2, respectively) for each transfer function on the main diagonal of (5.3) are determined by simulations. Next, the control parameters are evaluated by following Table 5.2.

Table 5.2: The cohen-coon tuning rules

	K_P	K_I
P	$\frac{1}{Kr}(1 + \frac{r}{3})$	
PI	$\frac{1}{Kr}(0.9 + \frac{r}{12})$	$\frac{K_P(9 + 20r)}{\tau_{del}(30 + 3r)}$

where $\tau_{del} = \frac{\kappa_1 - \ln(2)\kappa_2}{1 - \ln(2)}$, $K = \frac{\text{output}}{\text{input}}$ and $r = \frac{\tau_{del}}{\kappa_2 - \tau_{del}}$.

For the linearized system (5.3), Figure 5.16a and Figure 5.16b show the step response of $G_{11}(s)$ and $G_{22}(s)$ in time domain, as a consequence, κ_1, κ_2, τ_{del}, K and r of the Cohen-coon are computed and displayed in Table 5.3. Control parameters of PI controller are subsequently calculated by following Table 5.3.

Table 5.3: Tuning parameter in the Cohen-coon rules

	κ_1	κ_2	τ_{del}	K	r
$G_{11}(s)$	254	363	7.78	0.42	0.02
$G_{22}(s)$	272	385	16.07	1.05	0.043

Table 5.4: Parameters of PI controller

Controller	K_p	K_I
$G_{11}(s)$	98.47	3.97
$G_{22}(s)$	19.8	0.40

The parameters in Section 5.4 are then adjusted to allow the closed-loop system to have less oscillations and achieve the set point quicker. Finally, K_{PT}, K_{PQ}, K_{IT} and K_{IQ} are selected to be 21.5, 98, 4 and 0.1, respectively.

For sake of illustration, the system trajectory is assumed to start at the initial condition SSI (see Appendix B). The transient responses of the output variables (T, C_I and C_M) given in Figures 5.17a to 5.17c demonstrate that the settling time of the reactor temperature and the concentration of initiator under the proposed PBC are shorter than those under the decentralized PI control (5.2) and (5.1), thus the settling time of concentration monomer of the former system is also shorter than that of latter one.

Moreover, the control quality of the proposed PBC scheme is also evaluated by the merit scores of errors including the integral squared error (ISE) and the integral-time weighted absolute error (ITAE). The mathematical formulas of these merit scores of errors are expressed as follows (Seborg et al., 2011; Q.-G. Wang et al., 2008).

$$\text{ISE} = \int_0^\infty \left[\left(C_B(t) - C_B^e \right)^2 + (T(t) - T^e)^2 \right] dt, \tag{5.4a}$$

$$\text{IAE} = \int_0^\infty \left[\left| C_B(t) - C_B^e \right| + \left| T(t) - T^e \right| \right] dt, \tag{5.4b}$$

$$\text{ITAE} = \int_0^\infty t \left[\left| C_B(t) - C_B^e \right| + \left| T(t) - T^e \right| \right] dt. \tag{5.4c}$$

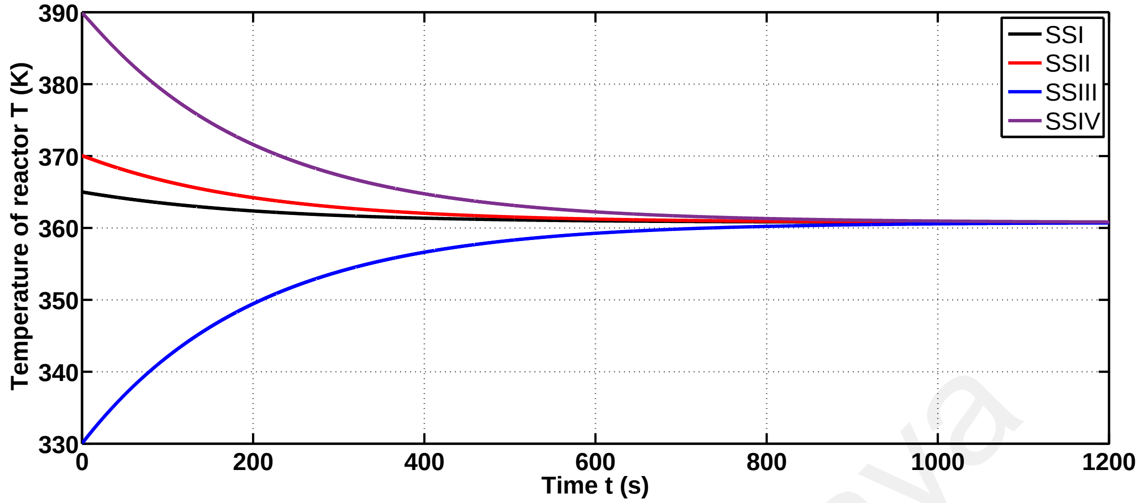
In fact, IAE (5.4b) considers all errors in a uniform manner and does not add any weights to the errors in system's responses while ISE (5.4a) tends to penalize the large errors which usually appear in the beginning of process more than small ones which usually appear in the end of process. The reason is that if large errors are greater than one, their squares are significantly bigger than these of small errors and when a error is less than one, its effect can be negligible. On the other hand, ITAE weights the errors existing after long time heavier than these at the beginning of process by using (5.4c) and the ITAE turning can enable the closed-loop system to avoid the sustained oscillation. Furthermore, the system with smaller IAE has less oscillation and while the transient responses of system dynamics can reach the set point faster if the ISE of system is smaller (Seborg et al., 2011).

The calculated merit scores of errors including IAE, ISE and ITAE are computed by the simulation time $t = 3000s$ and are tabulated in Table 5.5. Obviously, the closed-loop system under the proposed PBC strategy obtains the better control performance than that under the conventional PI strategy (5.1) and (5.2) since all the considered merit scores of the former system are significantly lower than those of latter one. This is due to the fact that transient behaviors of close-loop system under the PBC have less oscillation and reach the set point faster than those under the proposed PI control.

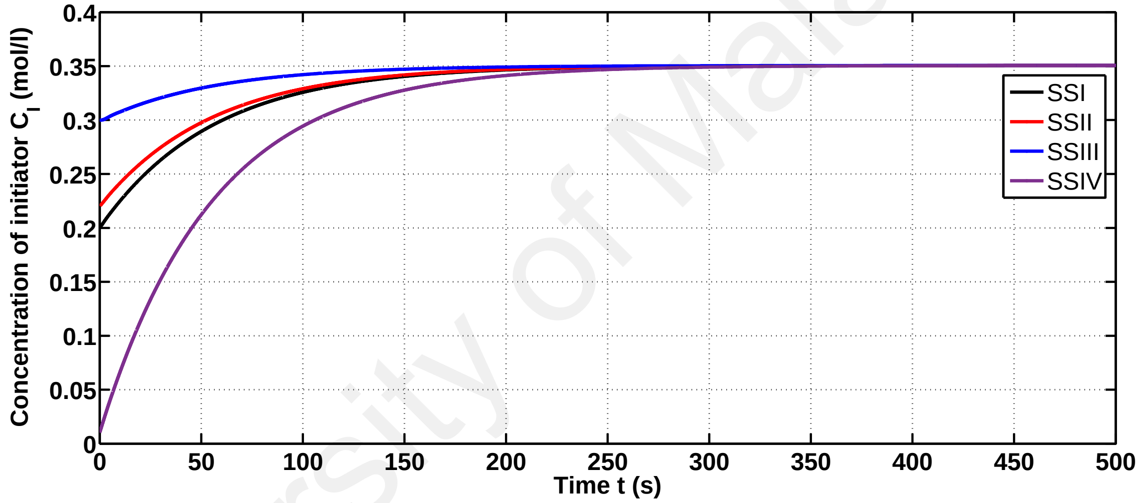
Table 5.5: The merit score for the proposed PBC and PI control

		The merit score		
Controller		ISE	IAE	ITAE
	PBC	1038	2016	3.681×10^5
	PI	2043	4125	1.164×10^6

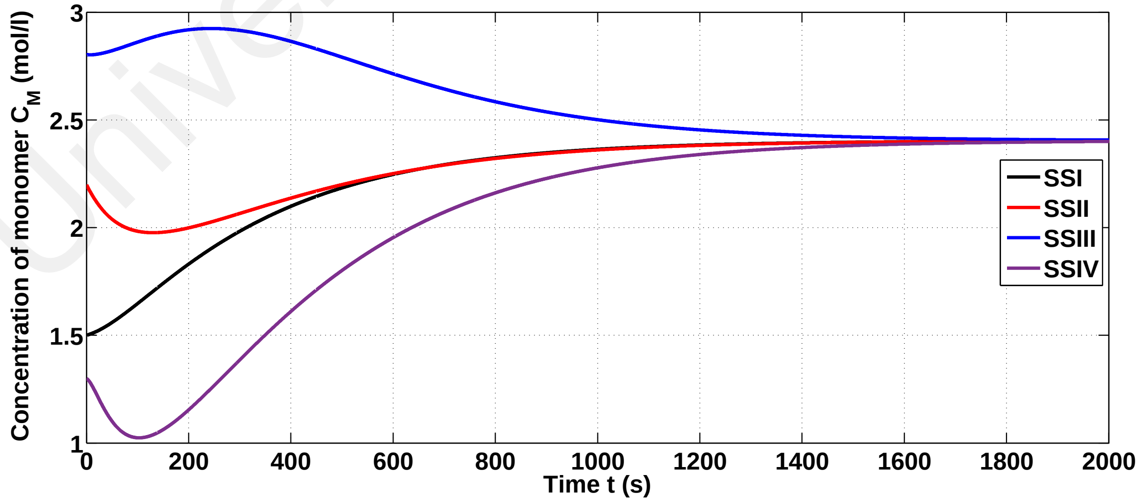
Furthermore, the performance of closed-loop FRP system disturbed by disturbance in T_F is assessed for the purpose of comparison. The Figures 5.18b to 5.18d aim to compare the control performance of the proposed PBC scheme with the conventional PI control when the system dynamics is affected by the external disturbance in T_F (see Figure 5.18a). In general, both controllers are able to stabilize the closed-loop system at the set point P_2, but the closed-loop system of proposed PBC have less oscillation than that of its counterpart and the system trajectory under the proposed PBC also achieve the set point faster.



(a) Reactor temperature.

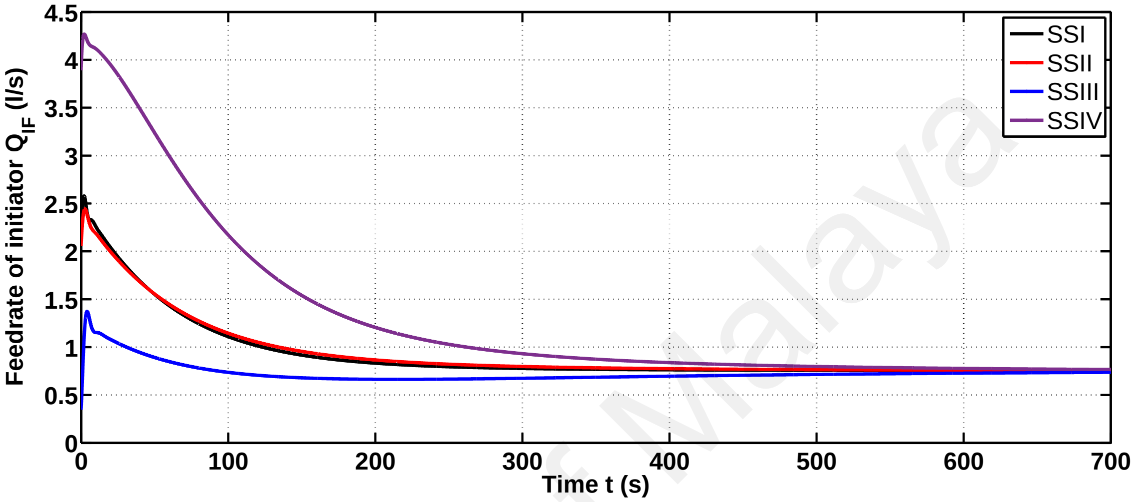


(b) The concentration of initiator.

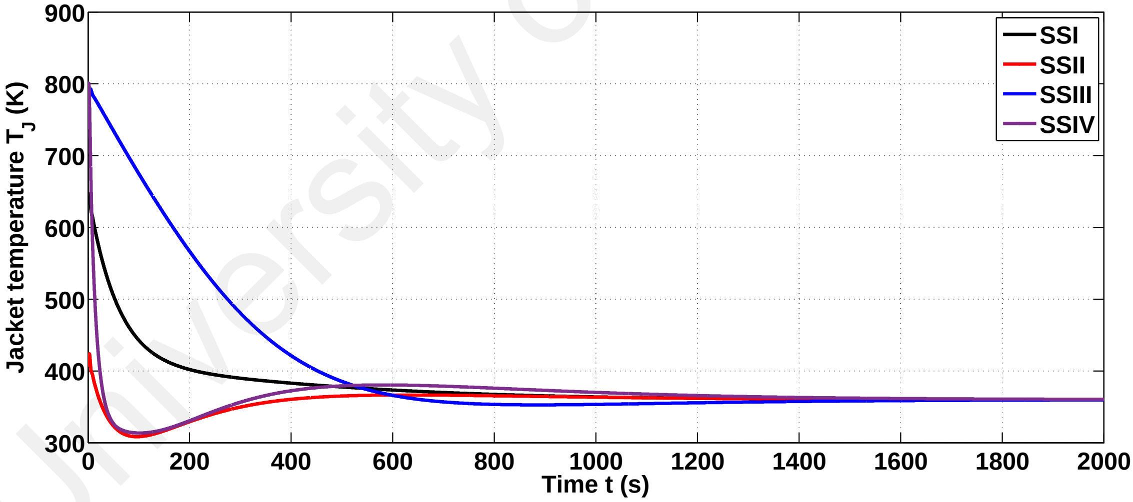


(c) The concentration of monomer.

Figure 5.6: Closed-loop system's response

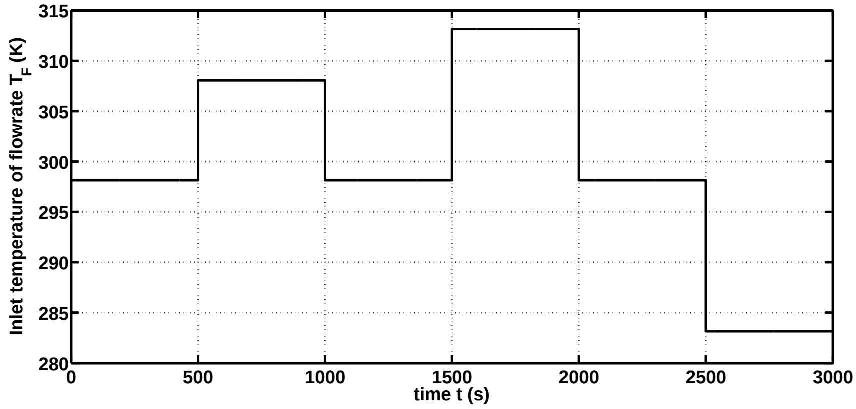


(a) Volumetric flowrate of initiator.

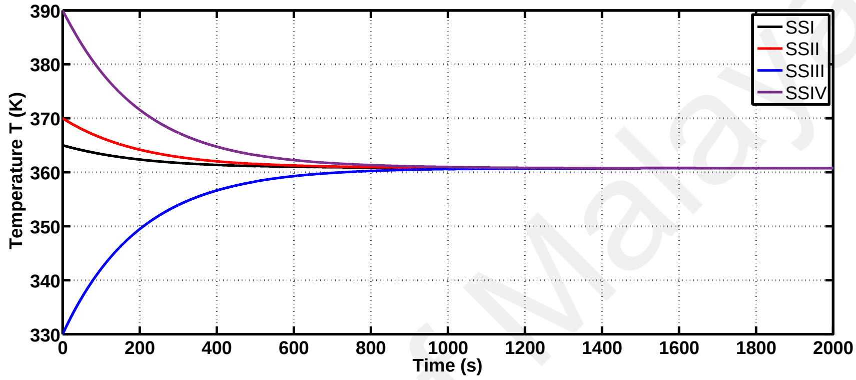


(b) Jacket temperature.

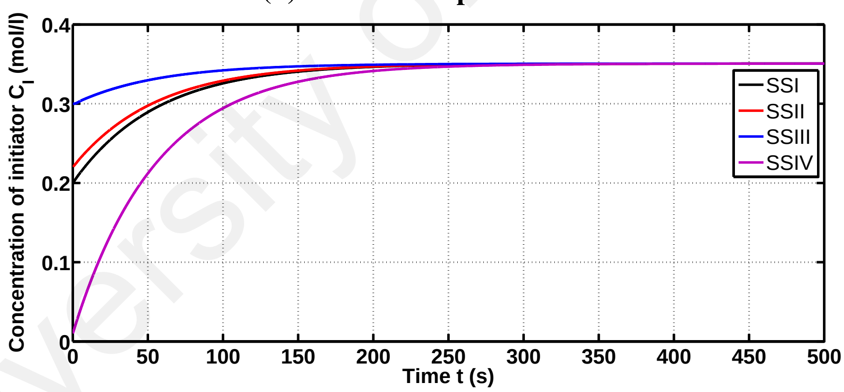
Figure 5.7: The control input



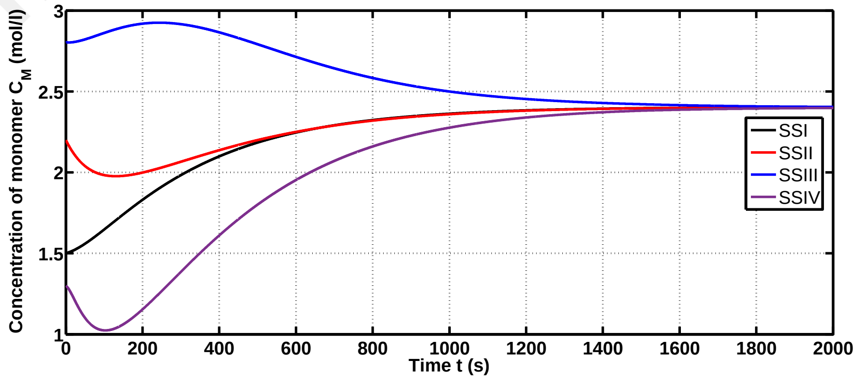
(a) the disturbance in inlet temperature.



(b) Reactor temperature.

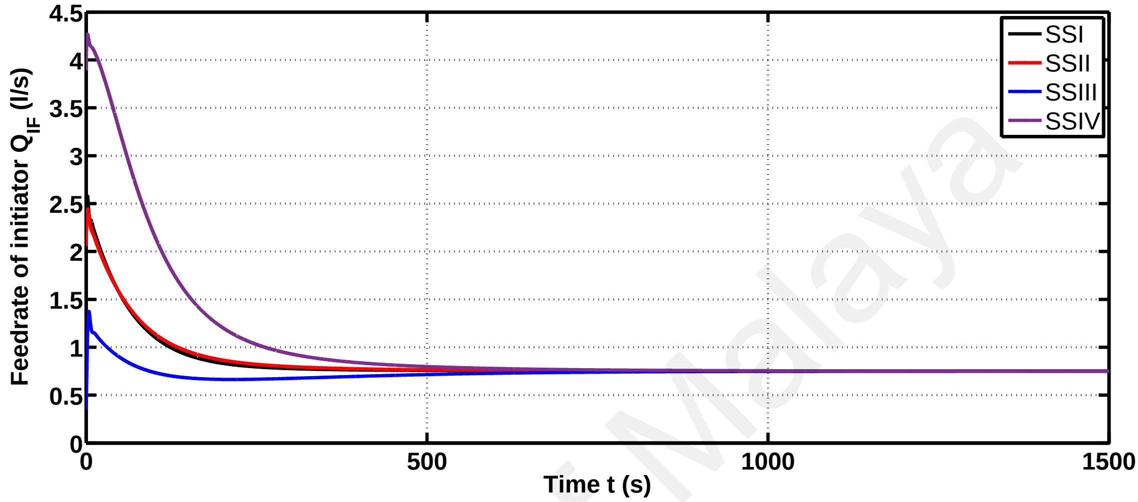


(c) The concentration of initiator.

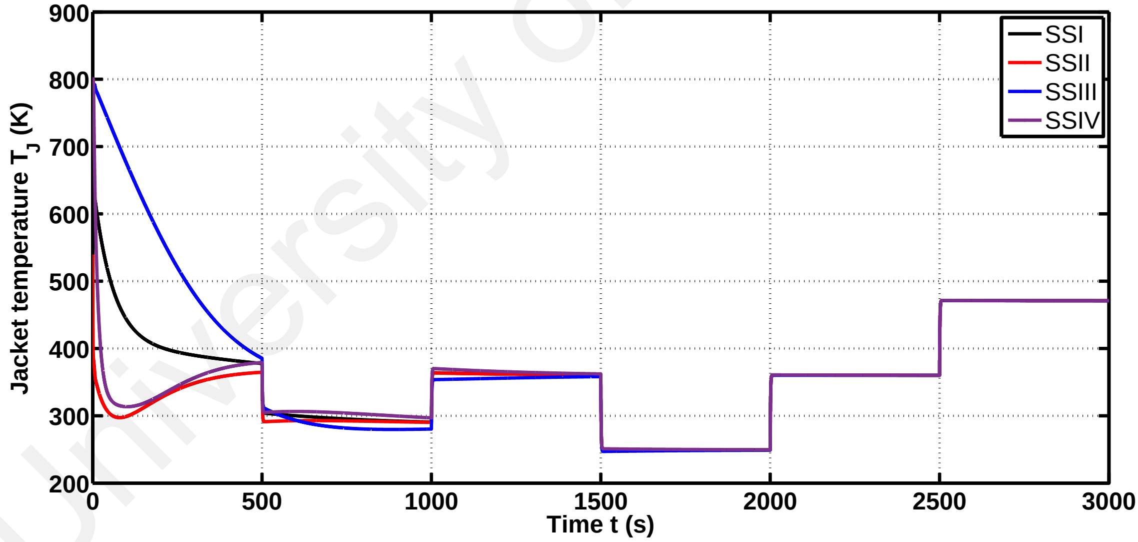


(d) The concentration of monomer.

Figure 5.8: The transient responses of state variables when the system is affected by the disturbance in T_F

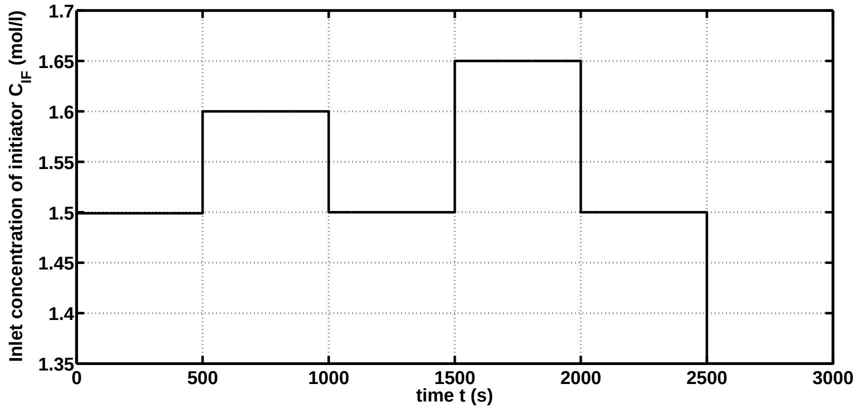


(a) Volumetric flowrate of initiator.

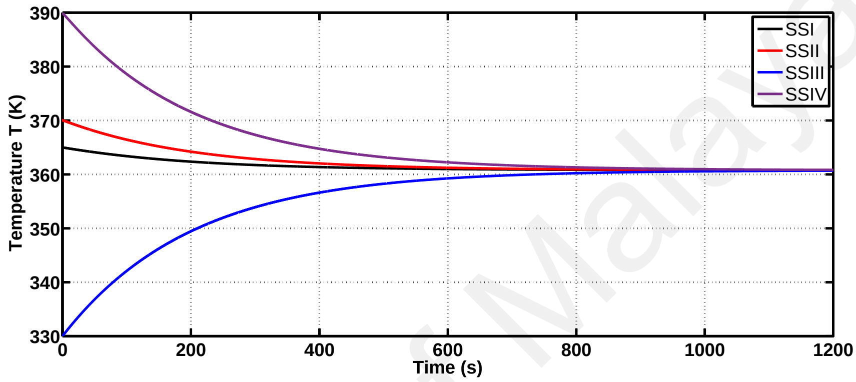


(b) Jacket temperature.

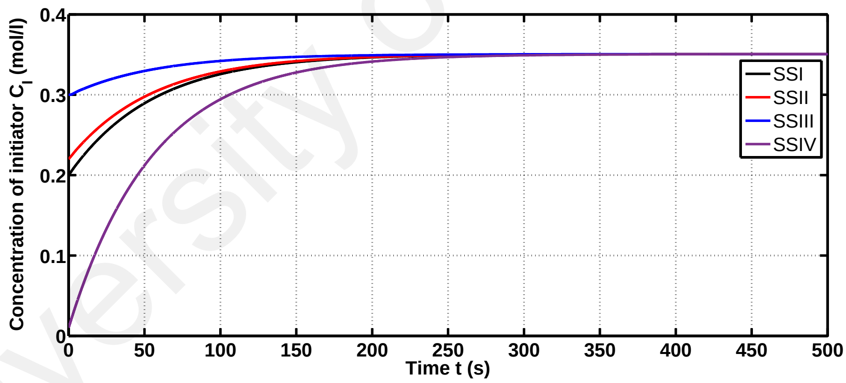
Figure 5.9: The control input when the system is affected by disturbance in T_F



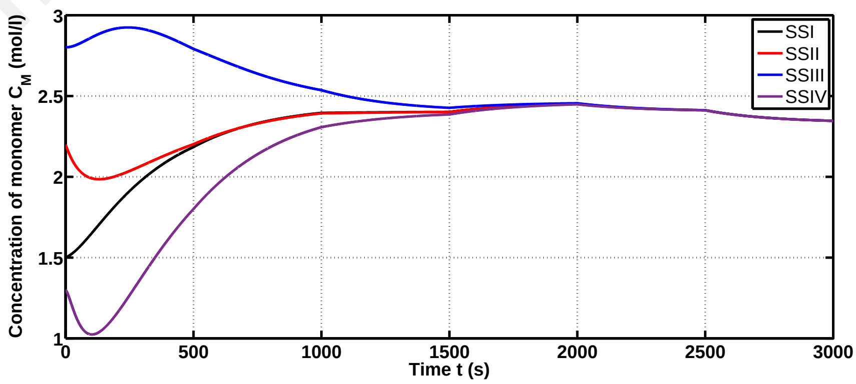
(a) the disturbance in inlet concentration of initiator.



(b) Reactor temperature.

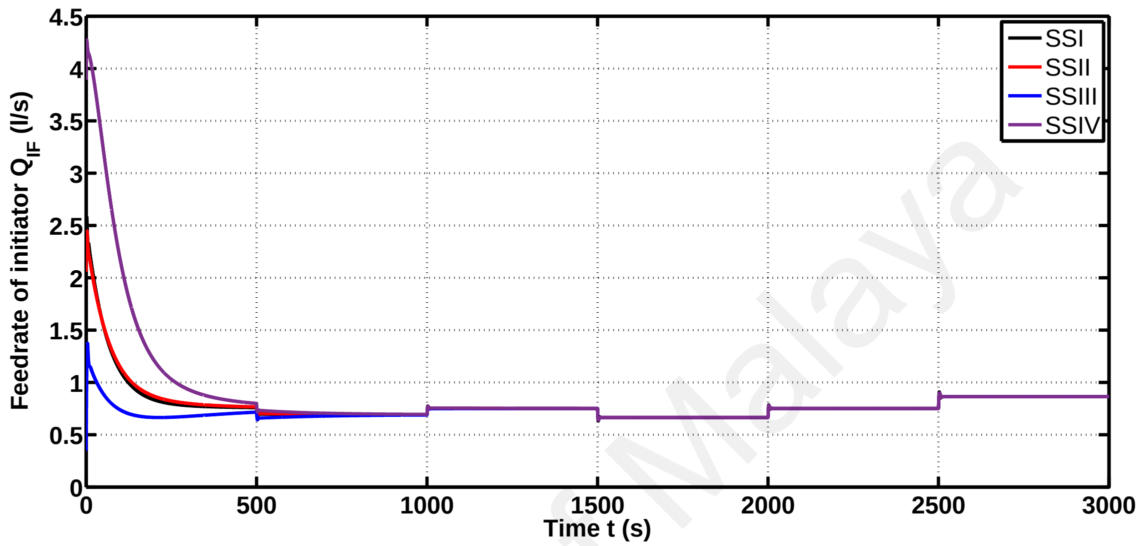


(c) The concentration of initiator.

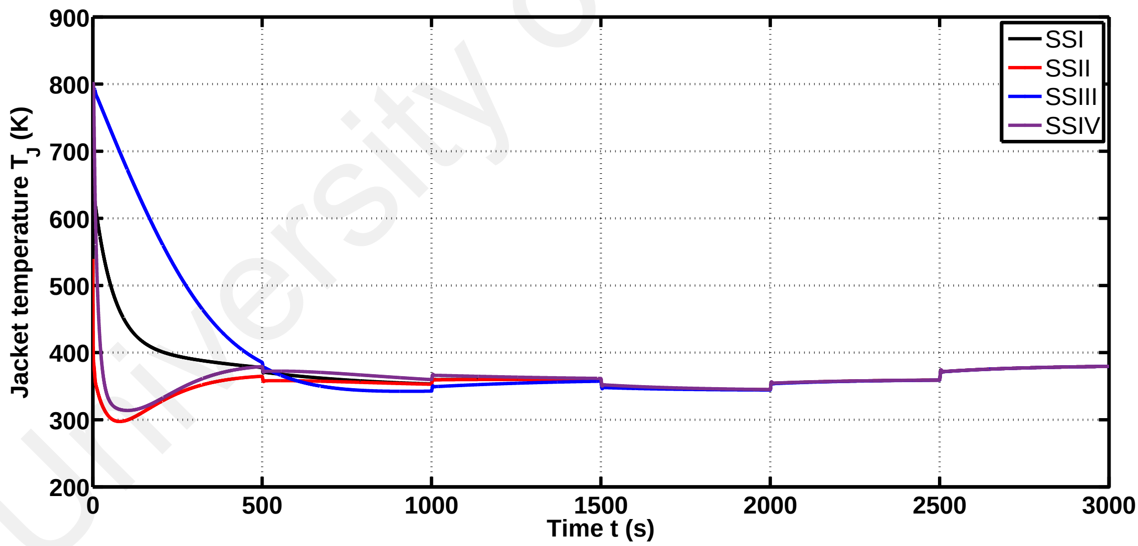


(d) The concentration of monomer.

Figure 5.10: The transient responses of state variables when the system is affected by the disturbance in C_{IF}

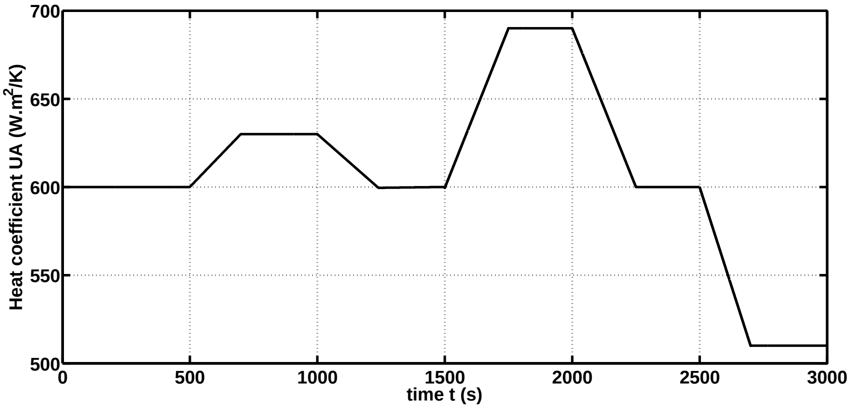


(a) Volumetric flowrate of initiator.

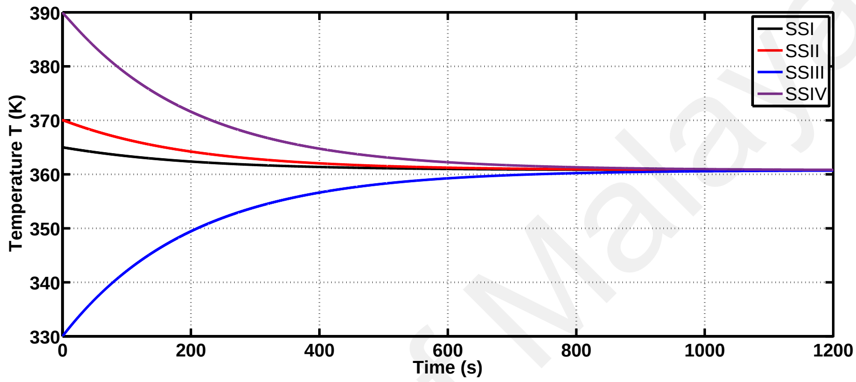


(b) Jacket temperature.

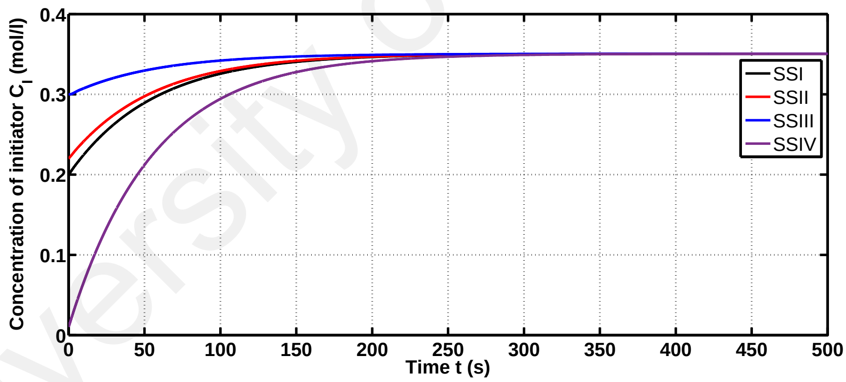
Figure 5.11: The control input when the system is affected by disturbance in C_{IF}



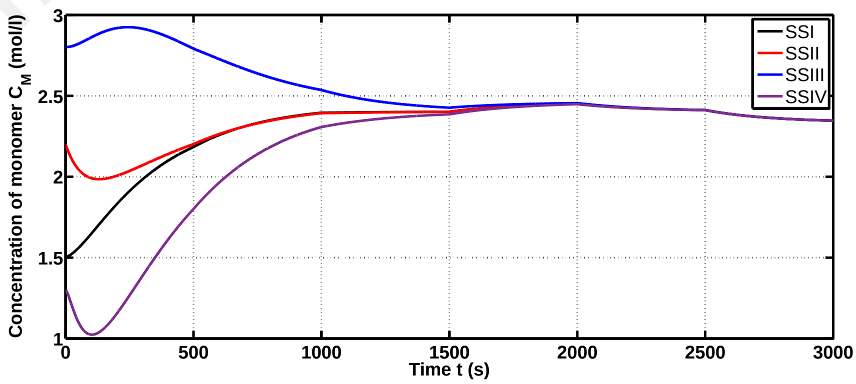
(a) The uncertainty of heat transfer coefficient UA.



(b) Reactor temperature.

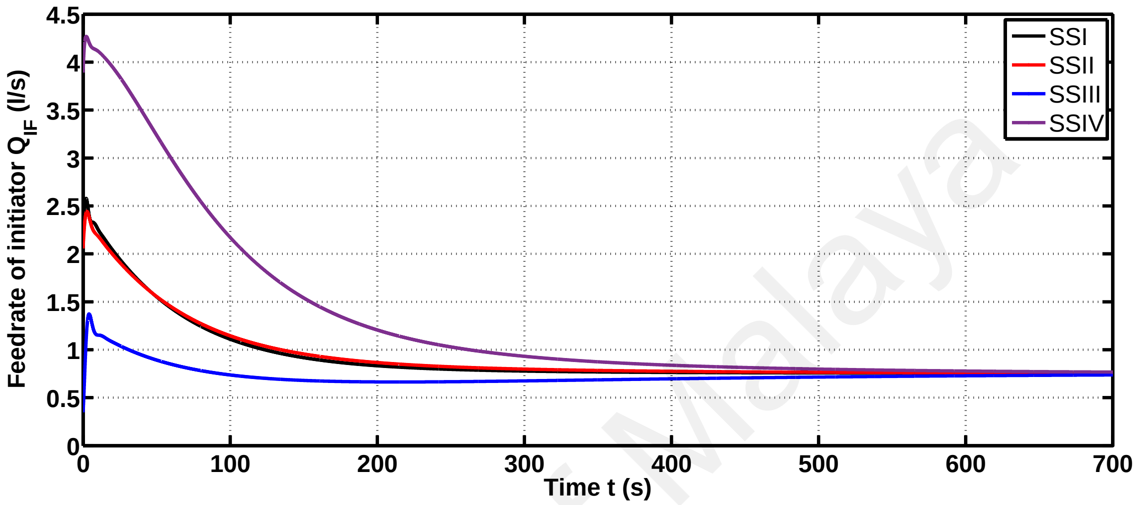


(c) The concentration of initiator.

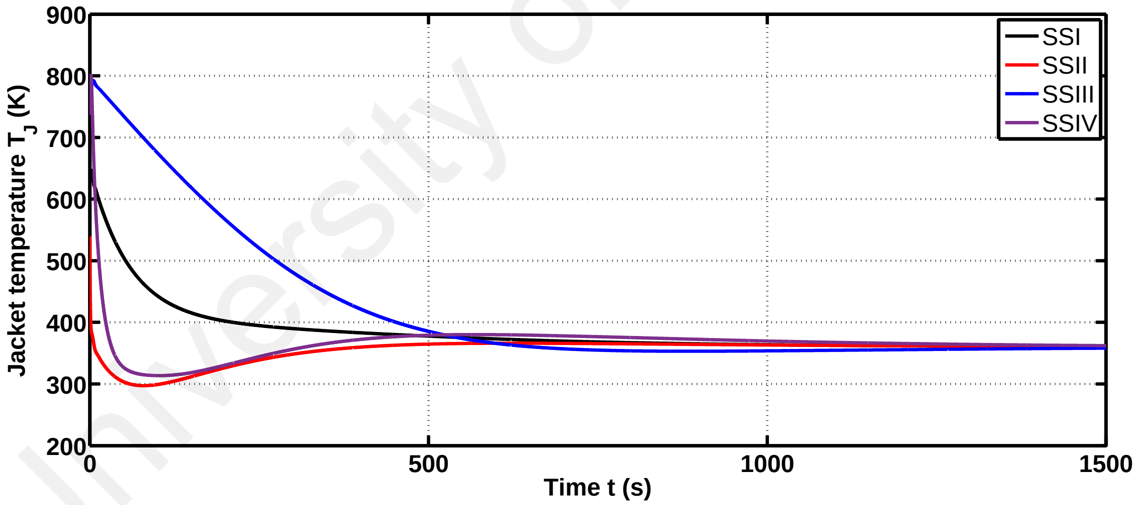


(d) The concentration of monomer.

Figure 5.12: The transient responses of state variables when the system is affected by uncertain heat transfer coefficient UA

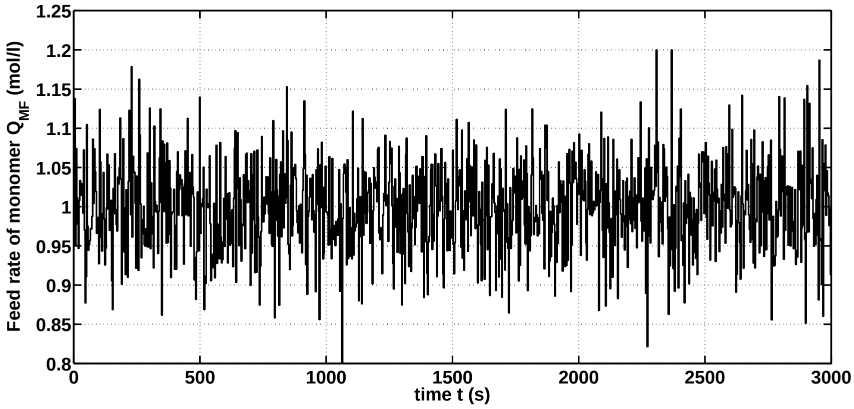


(a) Volumetric flowrate of initiator.

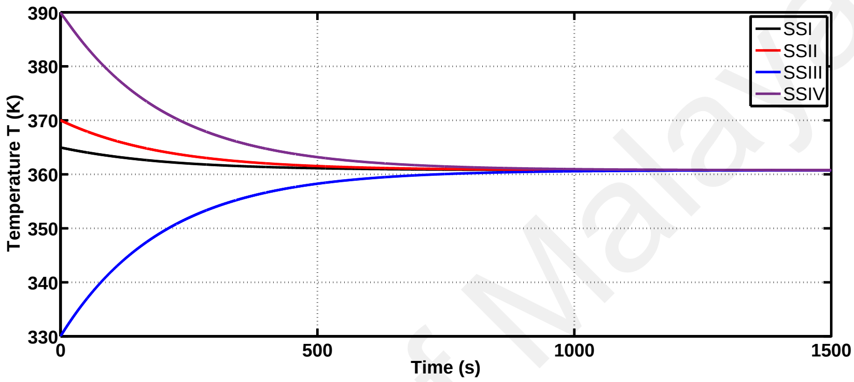


(b) Jacket temperature.

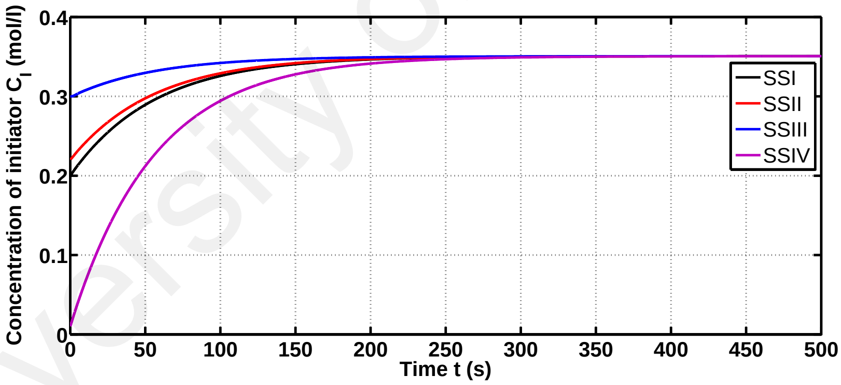
Figure 5.13: The control input when the system is affected by uncertain heat transfer coefficient UA



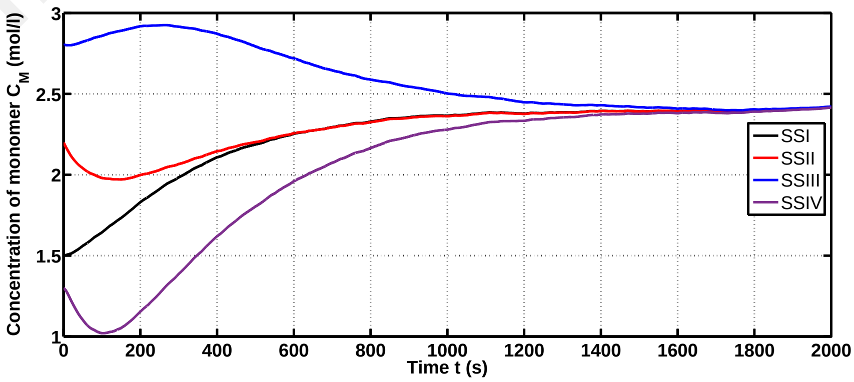
(a) Random noise in volumetric feedrate of monomer.



(b) Reactor temperature.

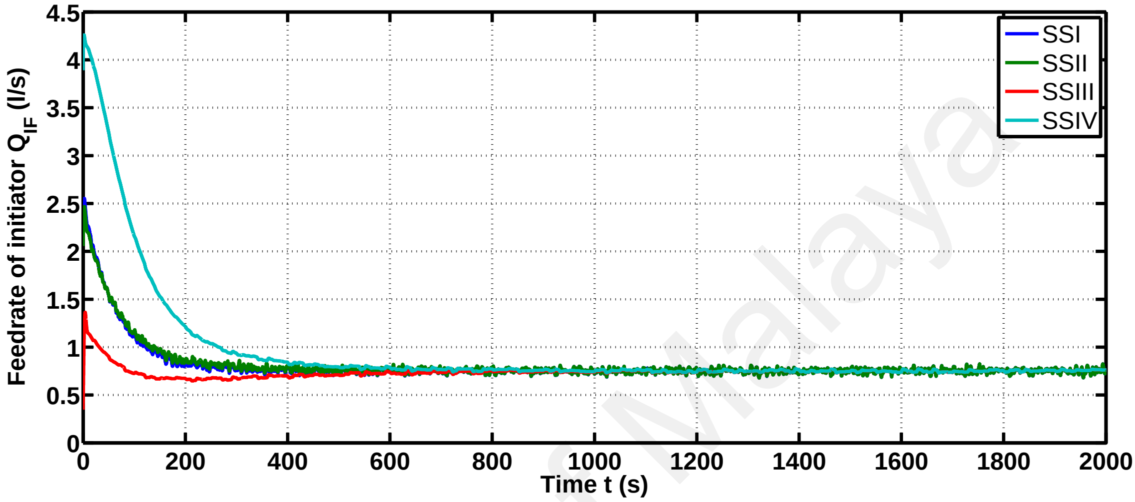


(c) The concentration of initiator.

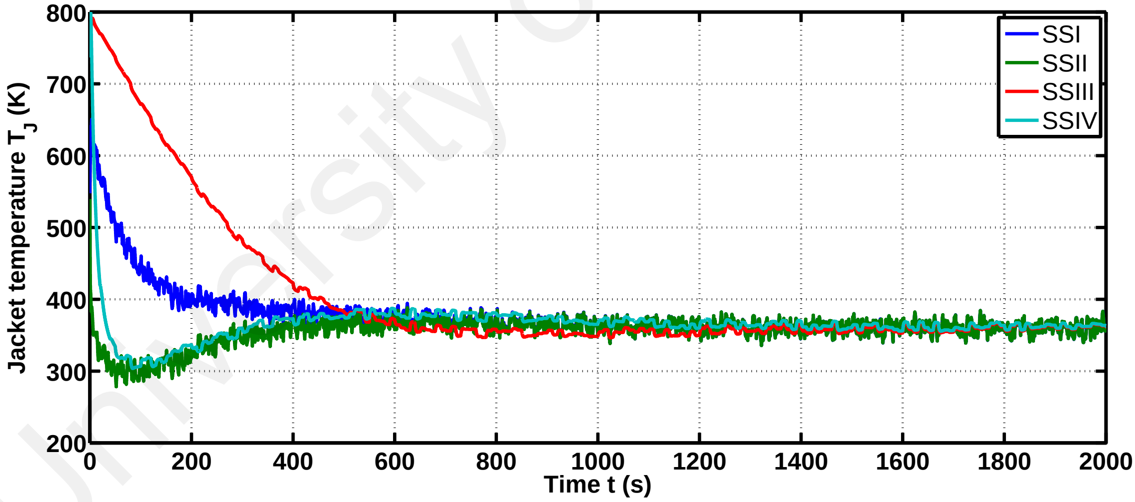


(d) The concentration of monomer.

Figure 5.14: The transient responses of state variables when the system is affected by random noise of Q_{MF}

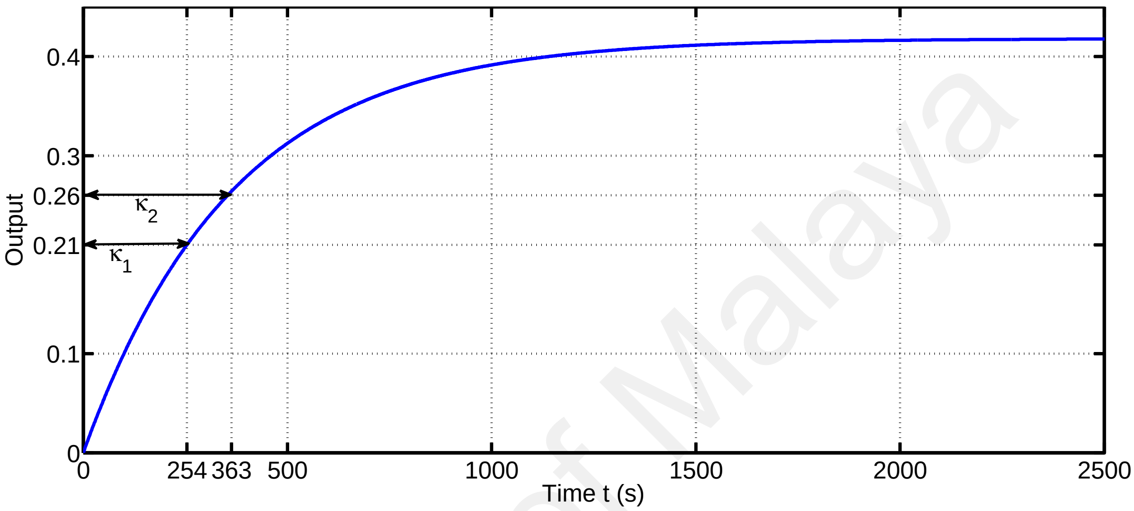


(a) Volumetric flowrate of initiator.

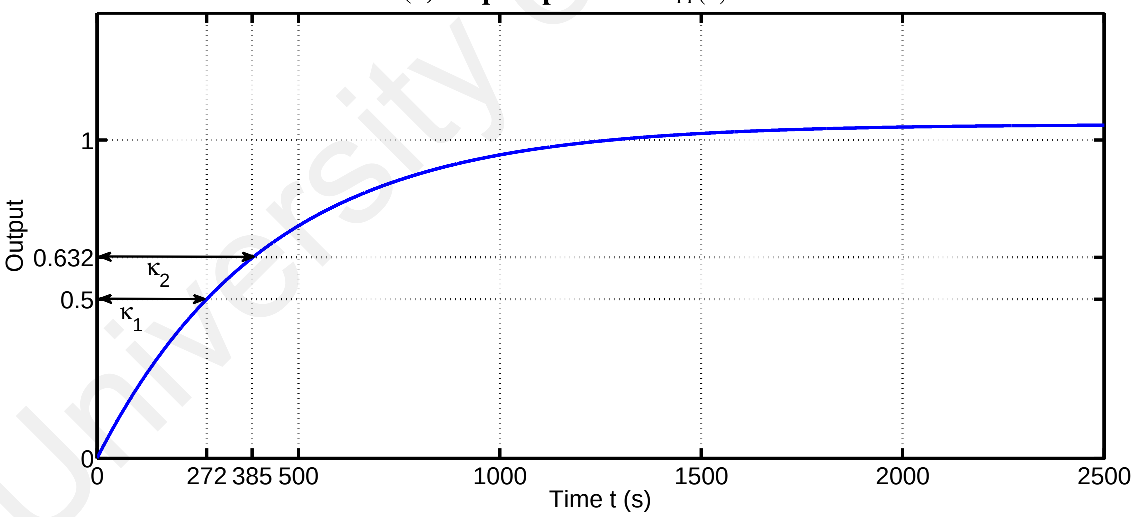


(b) Jacket temperature.

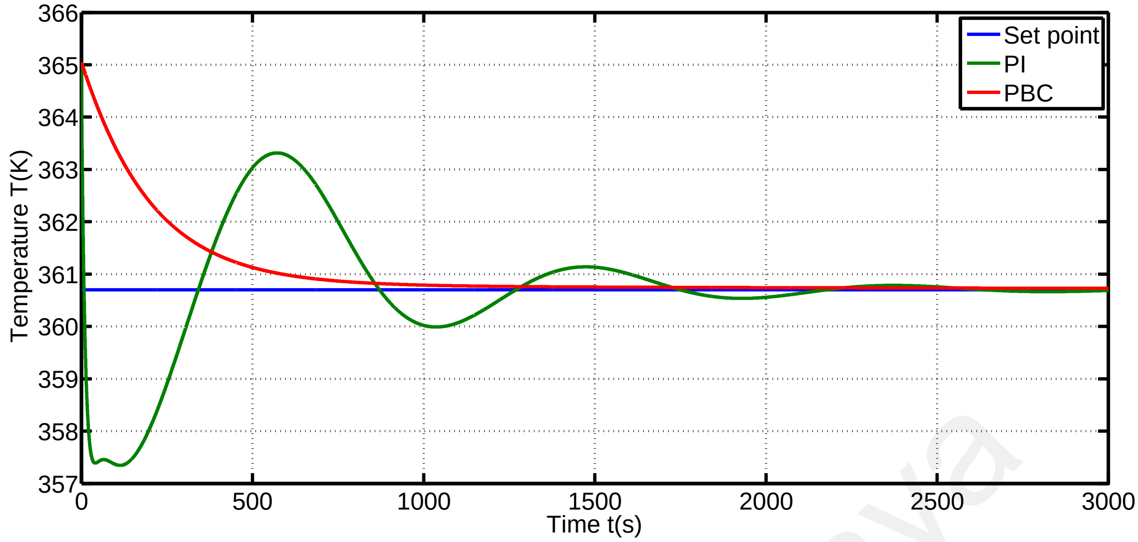
Figure 5.15: The control input when the system is affected by random noise of Q_{MF}



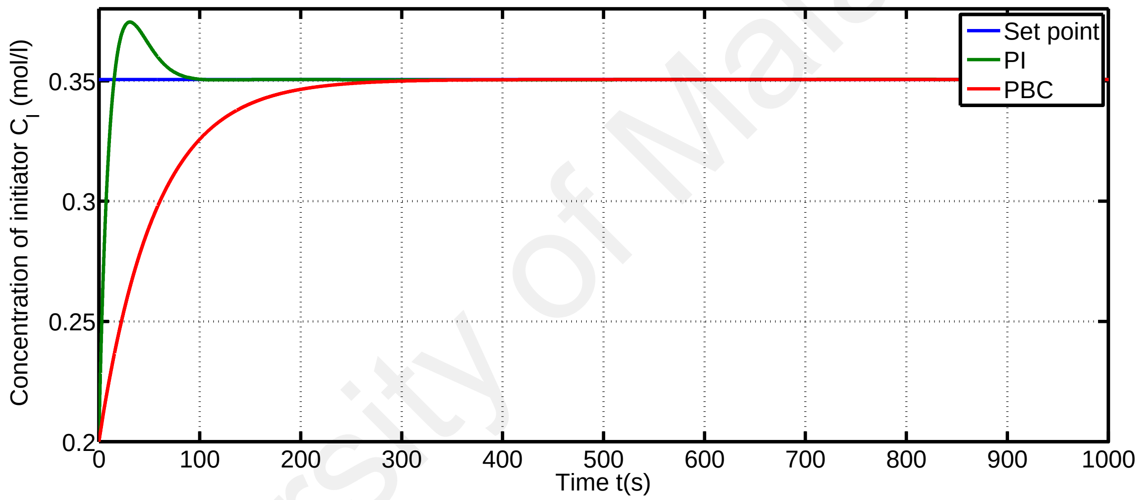
(a) Step response of $G_{11}(s)$



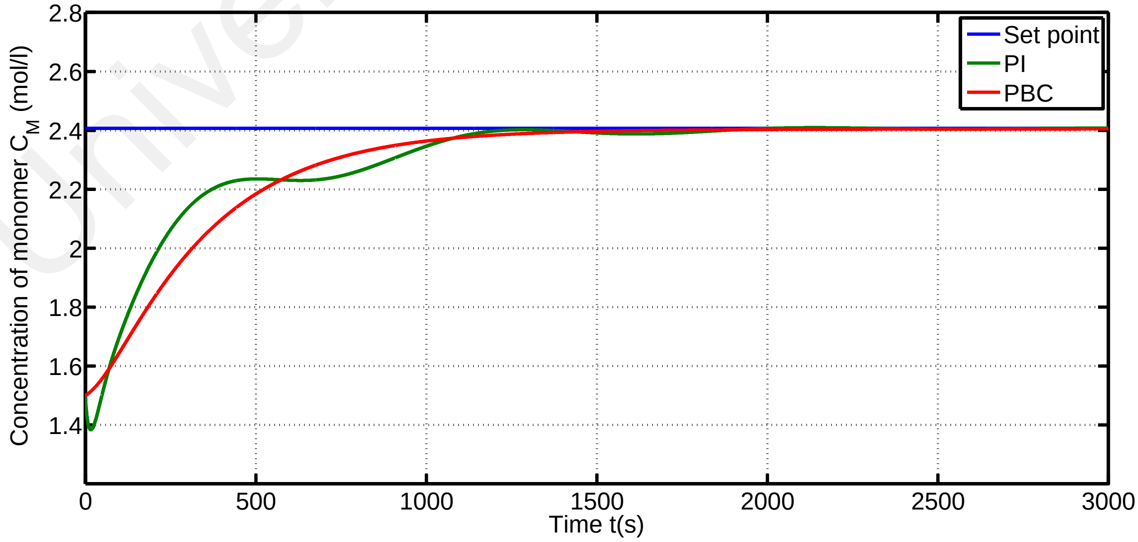
(b) Step response of $G_{22}(s)$



(a) Reactor temperature.

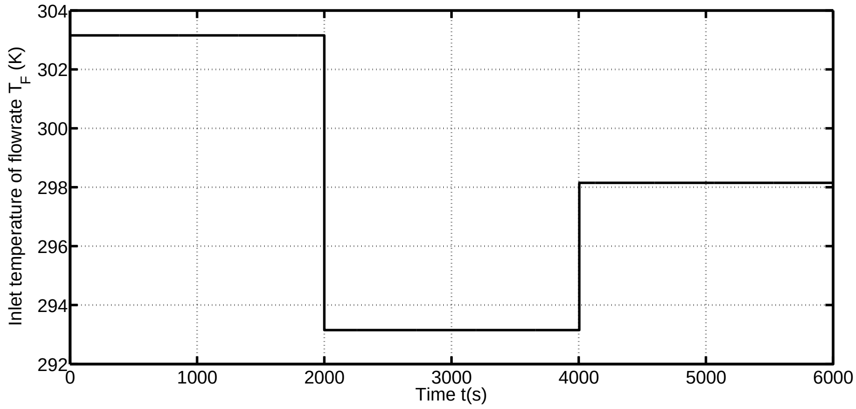


(b) The concentration of initiator.

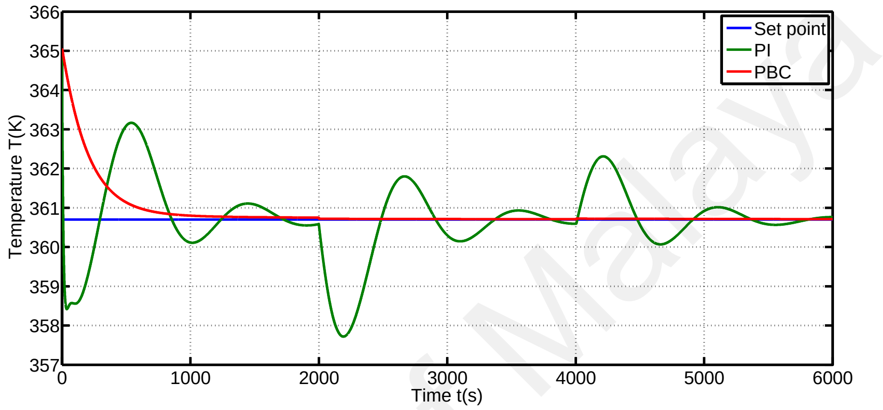


(c) The concentration of monomer.

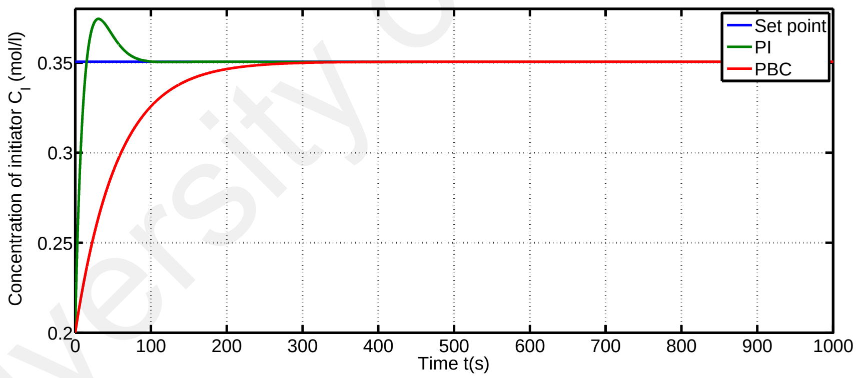
Figure 5.17: The control performance between PI control and PBC



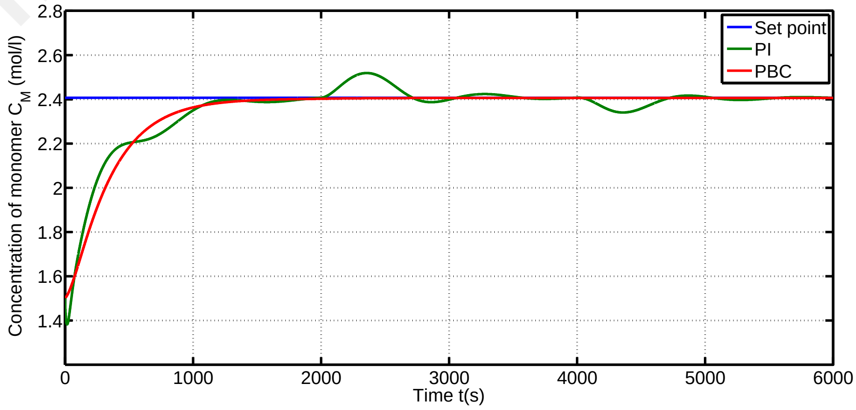
(a) Random noise in volumetric feedrate of monomer.



(b) Reactor temperature.



(c) The concentration of initiator.



(d) The concentration of monomer.

Figure 5.18: The control performance between PI control and PBC when the close-loop system is affected by disturbance in T_F

CHAPTER 6: CONCLUSION AND FUTURE WORKS

The final chapter of the dissertation aims to summarize the main contributions of this research work through the concluding remarks, focusing on the theoretical extensions of feedback passivation design from SISO systems to a class of MIMO ones. The methodology is divided into five parts as follow:

1. This research proposes the detailed stability analysis of continuous FRP reactor of styrene using the tools of system theory and the principle of heat balance. Both studies allow us to describe and explain the steady-state multiplicity behavior of the system dynamics. Although these approaches can be found in the literature for a class of nonlinear systems, they also play a central role in the clear determination of control problem for a particular chemical system.

2. The theoretical extensions for PBC contribute some interesting results including (1) rendering the MIMO system dynamics passive by using the input coordinate transformations and the natural decomposition of $f(x)$; (2) writing the resulting passive system into the canonical form strongly related to the so-called Port control Hamiltonian structure and (3) designing the multivariable feedback laws based on tracking error to stabilize exponentially the system trajectory at the desired equilibrium point. The design procedures can also be applied to any kind of the MIMO systems as soon as the assumptions are taken into account in the consideration.

3. The proposed PBC strategy is applied to design feedback laws for the stabilization of continuous polystyrene production process in the CSTR at the desired set-point (including the unstable-open-loop steady state).

4. The robustness of the closed-loop system under control of the proposed PBC with/without the effects of random noise and/or disturbance is illustrated and evaluated by numerical simulations.

5. The control performance of the proposed PBC scheme is compared with that of the conventional PI control in terms of the merit scores including ISE, IAE and ITAE.

6.1 Conclusion

In this research work, the steady-state multiplicity behavior of the polystyrene production process in the CSTR is firstly analyzed in two different ways where the first one is based on the tools of the system theory and the second one is strongly related to the principle of heat balance. The results show that at the unstable-open-loop equilibrium point, the approximately linearized system of the nonlinear chemical process has one eigenvalue which has the positive real part and this eigenvalue causes the instability of the system dynamics according to the system theory. In addition, the Van Heerden diagram gives that if any noise or disturbance move the system out of this unstable-open-loop equilibrium point, the system tends to run away from this equilibrium point and approach to another equilibrium point, which is locally stable, to meet the requirements of principle of heat balance (e.g. the system will approach the steady state with high temperature if the heat-generation rate Q_g is greater than the heat-removal rate Q_r, and vice versa the system will approach the low-temperature steady state). Additionally, the region of jacket temperature T_J where the multiplicity behavior takes place is found out when the volumetric flow rate of initiator Q_{IF} is fixed. Thanks to the stability analyses proposed, the strong connection between system theory and the principle of heat balance is derived and can be considered as one of the primary contributions in the work.

Furthermore, the numerical simulations are conducted to draw the bifurcation diagrams of the continuous styrene polymerization system where both the T_J and Q_{IF} are considered as the bifurcation parameters. In fact, such diagrams enable us to predict the appearance of steady-state multiplicity behavior in the wider operating domain (compared with the region derived from the Van Heerden diagram). Through the numerical simulations, it can be clearly seen that the domain of unstable-open-loop equilibrium points will be strongly influenced (increase or decrease) if T_J and Q_{IF} vary to meet the operating requirements. Consequently, in some specific operating conditions, the steady-state multiplicity behavior of FRP system of styrene in the CSTR will disappear and the system will have only one steady state. The steady-state multiplicity behavior and the bifurcation behavior are recognized as the theoretical challenge issues in the practical operation and they can prevent the styrene FRP process in the CSTR from obtaining acceptable performance to fulfill both the economic benefits and engineering constraints. Such stability analyses indeed lay a strong base for the control problem statement which is to stabilize exponentially the system at the unstable-open-loop equilibrium point because this steady state can compromise both economic benefits and engineering advantages..

Secondly, we extend the method of feedback passivation plus tracking error proposed by Sira-Ramírez (1998); Sira-Ramírez et al. (1997) for SISO systems and contribute the novel theoretical developments to passivate a class of MIMO nonlinear systems having m inputs and m outputs by using the input coordinate transformations. The resulting passive system is subsequently rewritten into the novel canonical form which is developed for any quadratic storage functions and strongly related to the Port-controlled Hamiltonian representation while the canonical form of (Sira-Ramírez et al., 1997) was established for only quadratic storage function $\mathbb{V}(x) = \frac{1}{2}x^\top x$ and its matrix $R(x)$ was not positive semidefinte symmetric, thereby not expressing fully the physical meanings of this representation. Next, the global exponential stabilization of the resulting passive system is developed through a tracking-error-based control, where the reference trajectory passing through the set-point (including the open-loop-unstable equilibrium point) is appropriately assigned[1]. Additionally, the proposed reference trajectory, which is completely different compared with reference trajectory in literature, allows us to show explicitly the physical meanings of the auxiliary reference system associated with the vector field x_d (i.e., the interconnection and damping injection terms). On the other hand, this simplifies the complexity of controller design in case of MIMO systems in general.

[1]Although the reference trajectory is able to be assigned as a constant function, it may make the control inputs overacting such as high overshooting

Thirdly, the theoretical extensions are applied to design the feedback laws for the stabilization of polystyrene production process in a CSTR at the desired equilibrium point which is the middle steady state, that is, $P_2 = (2.407; 0.351; 360.7)$. In fact, the numerical simulations show that the exponential stabilization of the system is globally guaranteed because the system trajectory converges exponentially to the desired set-point P_2. Furthermore, the dynamics of manipulated variables, i.e., the jacket temperature T_J and the volumetric feed rate of initiator (AIBN) Q_{IF}, are sufficiently smooth and physically admissible during the reaction course.

Fourthly, the robustness of closed-loop system under control of PBC scheme is tested via the simulation studies. More precisely, the external disturbance in the inlet temperature T_F, the inlet concentration of initiator C_{IF}, the uncertain heat transfer coefficient ΔH and the random noise in the volumetric feed rate of monomer Q_{MF} are assumed to disturb the closed-loop system during the reaction course. The simulation results show that the proposed PBC can still stabilize the system at the desired set point $P_2 = (2.407; 0.351; 360.7)$ by regulating the dynamics of manipulated variables T_J and Q_{IF} appropriately to handle different types of disturbance and/or noise. For example, under the impacts of external disturbance in T_F and C_{IF} at 500 s, 1500 s and 2500 s, the manipulated variables T_J and Q_{IF} show the corresponding step changes at 500 s, 1500 s and 2500 s while the oscillations are given in the dynamics of T_J and Q_{IF} when the closed-loop system is affected by the random noise in Q_{MF}.

Finally, the control performance of the proposed PBC is compared with that of the conventional PI control in terms of the merit scores of errors including IAE, ISE and ITAE. The numerical simulations show that the polymerization system under the proposed controller achieves the better control performance because the merit scores of errors for the closed-loop system under proposed PBC are lower than these of under PI control.

6.2 Future works

The dissipativity and passivity theories even considered as the extended Lyapunov theory (Ebenbauer, Raff, & Allgöwer, 2009) play central roles in the development of stability analysis and control design of nonlinear systems. Therefore, the theoretical researches on the dissipativity, passivity theories and their applications are vitally essential.

Firstly, the proposed control strategy based on the feedback passivation is limited by the necessary and sufficient conditions of passivation (Byrnes et al., 1991; Sepulchre et al., 1997), therefore, this approach cannot be applied directly to the chemical process systems exhibiting the non-minimum phase behavior, i.e., unstable zero dynamics, for instance, the Van de Vusse reacting system. To circumvent the structural obstacles, the method of synthesizing the outputs that are statically equivalent to the original process output and make the system minimum phase (this method can be found in the literature, see e.g., (Niemiec & Kravaris, 2003)) can be utilized together the feedback passivation. Additionally, the coordinated passivation design which is carried out in two steps: zero dynamics stabilization and feedback passivation is also a possible solution and several control systems designed by this method can be found in (Chen, Ji, Wang, & Xi, 2006; Larsen et al., 2000, 2003; Larsen & Kokotović, 1998; Sun, Zhao, & Dimirovski, 2009). As a result, these feedback-passivation-based approaches will become interesting topics in the future because they will enable the proposed PBC strategy to overcome the structural limitations of unstable zero dynamics.

Secondly, hardly can anyone of us deny the enormous advantages of nonlinear MPC to handle the constraints of optimal control problems in the practical applications. Therefore, the prospective future works firstly aim to combine the passivity theory with linear/nonlinear MPC strategies for the stabilization of chemical processes. Actually, this idea will be becoming the attractive issue in the area of process control, and although some first attempts have been made (Raff et al., 2007; Tan, Tippett, & Bao, 2016; Yu, Zhu, Xia, & Antsaklis, 2013), several questions remain open, especially when the irreversible thermodynamics have not been considered as the constraints of closed-loop system under the passivity-based nonlinear MPC.

Finally, the proposed control can be applied to a class of more complex nonlinear (bio)chemical processes such as microbial growth process model, particle nucleation, growth models and non-minimum phase reacting system. Additionally, the control performance of the proposed PBC will also be compared with that of other nonlinear controllers (see e.g., physics-based controllers (Hoang, Couenne, Jallut, & Le Gorrec, 2013)).

LIST OF PUBLICATIONS AND PAPERS PRESENTED

Nguyen, S., Hoang, H., & Hussain, M. A. (2016a). Analysis of the steady-state multiplicity behaviour for polystyrene production in CSTR. In *the 29th symposium of Malaysian chemical engineers (SOMChE).* Sarawak, Malaysia.

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APPENDIX A: THE OPERATING PARAMETERS OF POLYMERIZATION REACTOR

Quantity	**Symbol**	**Units**	**Value**
Flow rate of monomer (styrene) in the feed	Q_{MF}	l/s	1.0
Flow rate of initiator (AIBN) in the feed	Q_{IF}	l/s	0.75
Flow rate of solvent in the feed	Q_{SF}	l/s	1.0
Concentration of monomer (styrene) in the feed	C_{MF}	mol/l	9.2
Concentration of initiator (AIBN) in the feed	C_{SF}	mol/l	1.5
Concentration of solvent in the feed	C_{SF}	mol/l	4.0
Inlet temperature of feed	T_F	K	298.15
Jacket temperature	T_J	K	360.0
Reactor volume	V	l	1000
Ideal gas law constant	R	J/(mol.K)	8.314
Efficiency factor of initiator (AIBN)	f		0.6
The global hear transfer coefficient	UA	W.m^2/K	600
Heat of the polymerization reaction	ΔH	J/mol	-74400
Heat capacity of the reacting mixture in CSTR	c_p	J.kg/K	1855
Heat capacity of the feed	c_{pF}	J.kg/K	1978
	ρc_p	J/(l.K)	1507.248

APPENDIX B: THE INITIAL CONDITIONS OF THE CONTINUOUS STYRENE POLYMERIZATION REACTOR

	$C_{I\text{int}}$ (mol/ℓ)	$C_{M\text{int}}$ (mol/ℓ)	T_{int}(K)
SSI	0.20	1.5	365
SSII	0.22	2.2	370
SSIII	0.30	2.8	330
SSIV	0.01	1.3	390