

NEURO-ADAPTIVE CONTROL OF
CONTINUOUS POLYMERIZATION
REACTOR

BY
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Dedicated to my ever caring parents.

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THESIS ABSTRACT

NAME: MUHAMMAD MAARUF

TITLE OF STUDY: Neuro-adaptive control of continuous polymerization reactor

MAJOR FIELD: SYSTEMS AND CONTROL ENGINEERING

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The demand for high quality polymer elicits the application of nonlinear control methods to obtain a polymer of distinct properties. The properties (such as elasticity, tensile strength and so on) are determined by the molecular characteristics of the polymer which entirely depend on the reactor operating conditions (coolant flow rate, initiator type, monomer concentration, temperature and so on). The dynamic equations describing the polymerization reaction in a continuous stirred tank reactor (CSTR) are complex, nonlinear and strongly coupled. These pose a challenge in the control design. The presence of unknown external disturbances and input deadzone nonlinearities add more challenge to the control design. Different control techniques have been designed under different scenarios to ensure robust performances of the . A Neural-backstepping based fast terminal sliding mode (NBFSMC) controller is de-

signed to control the reactor temperature and average molecular weight of the polymer in the presence of unknown input deadzone. In addition, A Neural network based sliding mode controller (NNSMC) is designed to control the reactor temperature and the monomer concentration in the presence of unknown disturbances. Furthermore, a robust neuro-output feedback controller (NNFC) is designed to to control the reactor temperature and average molecular weight of the polymer in the presence of unknown disturbances.

ملخص الرسالة

الاسم: محمد معروف

عنوان الدراسة: التحكم العصبي في مفاعل البلمرة المستمر

التخصص: هندسة النظم والتحكم

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عند كتابة ملخص ، ضع في اعتبارك مجرد ملخص هويؤدي الطلب على البوليمر عالي الجودة إلى تطبيق طرق التحكم غير الخطي للحصول على بوليمر ذي خصائص مميزة. يتم تحديد الخصائص (مثل المرونة وقوة الشد وما إلى ذلك) من خلال الخصائص الجزيئية للبوليمر والتي تعتمد كليًا على ظروف تشغيل المفاعل (معدل تدفق المبرد ، نوع البادئ ، تركيز المونومر ، درجة الحرارة وما إلى ذلك). المعادلات الديناميكية التي تصف تفاعل البلمرة في مفاعل خزان متقلب مستمر (CSTR) معقدة وغير خطية ومقرونة بشدة. هذه تشكل تحديًا في تصميم التحكم. يضيف وجود اضطرابات خارجية غير معروفة ومدخلات منطقة غير خطية أكثر تحديًا إلى تصميم التحكم. تم وضع تقنيات تحكم مختلفة في سيناريوهات مختلفة لضمان أداء قوي. تم تصميم وحدة تحكم الوضع الانزلاقي الطرفي السريع (NBFSMC) على أساس العصبية الخلفية للتحكم في درجة حرارة المفاعل ومتوسط الوزن الجزيئي للبوليمر في وجود منطقة إدخال غير معروفة. بالإضافة إلى ذلك ، تم تصميم وحدة تحكم الوضع الانزلاقي القائمة على الشبكة العصبية (NNSMC) للتحكم في درجة حرارة المفاعل وتركيز المونومر في وجود اضطرابات غير معروفة. علاوة على ذلك ، تم تصميم وحدة تحكم تغذية مرتدة قوية للخرج العصبي (NNFC) للتحكم في درجة حرارة المفاعل ومتوسط الوزن الجزيئي للبوليمر في وجود اضطرابات غير معروفة.

CHAPTER 1

INTRODUCTION

1.1 Introduction

Polymerization reaction is a chemical process in which light chain hydro-carbons known as monomers react to form long chain hydro-carbons known as polymers [2]. Polymerization reactions are categorized into two reaction mechanisms; Step-growth polymerization and chain-growth polymerization [3]. The former involves the reaction of bi-functional or multi-functional monomers to first form a dimer (two bonded monomers), then trimer (three bonded monomers), up to oligomer (chain of few bonded monomers) and finally a polymer. The latter mechanism involves very fast inclusion of a sequence of monomers to the growing polymer chain initiated with the development of an active centre called free ion. These reactions usually take place in a chemical reactor which can be a batch, a continuous or a plug flow reactor [4].

Since the introduction of new commercial polymers such as epoxies, fluoropolymers, and polyesters in 1940s, new process technologies such as suspension polymerization process, slurry reactors and tubular reactors have been introduced [5]. The

advancement and evolution in process technologies have prompted large scale production of polymers, elemental understanding of polymerization reaction, development in reactor modelling, optimization and control [6].

Polymerization reactions proceeds at rapid rate and can cause fire and explosions if not sufficiently abated. As a result, it is imperative to regulate the operating conditions of the reactor. The operating conditions include but not limited to reaction rate, coolant flow rate, initiator type, monomer concentration, and temperature [7]. These conditions are manipulated depending on the desired end user specifications (such as elasticity, transparency, tensile strength and so on) of the polymer needed . The application of proper control methods to the polymerization reactor is requisite to obtaining polymers of specific properties. The properties include elasticity, flexibility, tensile strength, and toughness. These properties are associated with branching distributions, copolymer composition, and molecular weight [8]. Many authors have proposed different techniques from linear to nonlinear to regulate the operating conditions.

The dynamic equations of polymerization reactor are complex, multi-input-multi-output and strongly coupled nonlinear systems. The full mathematical model of the continuous polymerization reactor has been studied in [1]. The model is simplified under isothermal condition as the temperature dynamic equations are ignored [9], [10], [11].

1.2 Problem Formulation

Polymerization reactions are exothermic, progress at extreme rate and can cause thermal run away. As such, a sufficient temperature control mechanism must be put in place to cool the reactor and maintain a safe temperature. In addition, the concentration of the reactants determines the rate at which these reactions proceed and must be regulated for safety. Furthermore, controlling the reactor temperature and the concentration of the reactant ensures the production of polymers with specific qualities and physical properties. The physical properties as well as the quality of polymers depend on their average molecular weight. As such, a suitable control method must be put in place to control it.

Several researchers have proposed several control methods to address the aforesaid problems. It was discovered after a literature review that there are many open research areas in control of polymerization reactor. The control of polymerization reactors with Unstructured input nonlinearities such as deadzone and backlash nonlinearities were not reported in any literature. Moreover, no previous literature used backstepping method to control the average molecular weight of the polymer produced. In addition, the existing literature are based on asymptotic stability as the time reach infinity. Therefore, finite time based control is an interested area to investigate

1.3 Objectives

The contribution of this thesis are summarized by the following objectives

1. Designing a NBFSMC tracking controller for a polymerization reactor with input deadzone nonlinearity.
2. Designing a NNSMC tracking controller for a polymerization reactor with unknown disturbances.
3. Designing finite time robust NNFC tracking controller for a polymerization reactor with unknown disturbances.

1.4 Thesis Organisation

This thesis is arranged as follow: Chapter 2 presents the literature review. The mathematical Model of the polymerization reactor is presented in Chapter 3. chapter 4 presents the neuro-backstepping SMC for the polymerization reactor with input deadzone. In Chapter 5, neuro-SMC is presented for the polymerization reactor with unknown disturbances. Chapter 6 presents neuro-output feedback control of the polymerization reactor with time-varying disturbance observer. Chapter 7 presents the concluding remarks and future extension of the work.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter presents an overview of the previous works done to control the polymerization reactor. Many authors have proposed different techniques from linear to nonlinear to control the temperature, concentration of monomers, monomer conversion rate and average molecular weights of the polymers.

2.2 PID

The predominant control method in chemical industries is Proportional-Integral-Derivative (PID) due to its effectiveness and simplicity. Ogunye in [12] designed multi-loop Linear Quadratic Gaussian (LQG) and PID controllers for the control of average molecular weight and conversion rate in polymerization reactor. Altinten, et al. [13] applied self-tuning PID controller for the temperature tracking of jacketed batch polymerization reactor and further applied Genetic-Algorithm (GA) to obtain

optimal tuning parameters. Due to failure of PID to give satisfactory performance over the entire range of the process, [14] proposed Takagi-Sugeno Fuzzy Logic controller to control the temperature of batch polymerization reactor over the entire operation regions.

2.3 Feedforward control

The presence of disturbances in the reactor feed due to the recycle stream disturb the polymer properties. Congalidis & Richards in [15] proposed steady state feedforward control to compensate the disturbances, maintain continuous feed structure and flow to the reactor. Independent feedforward controllers with different set points are designed for each reactor feed streams (e.g transfer agent, initiator, monomers). However, in ratio control, One of the feed streams is selected as the set point [8]. The measured flow rate of the set point is passed on to the ratio station, which multiply the signal by the appropriate ratio to calculate the set point of the next feed stream and so on.

2.4 Sliding mode control

The uncertainties in a chemical processes can be sufficiently mitigated by a Sliding Mode Controller (SMC). SMC is a robust control scheme which trapped the trajectories of a system on the sliding surface where they asymptotically converge to zero [16]. Chen in [16] suggested SMC for tracking the temperature in batch process. Also, in [17], a variable structure SMC was applied to control a reactor in the laboratory. Kadu, et al. [18] have applied decentralised SMC for the control of two-input-two-

ouyput (TITO) chemical reactor and obtained excellent results both in simulation and experiment. A Sliding Mode Observer (SMO) was applied to estimate the average molecular weight and monomer concentration in a batch polymerization reactor [19] and to estimate substrate consumption in fermentation process [20]. A Robust Sliding Mode Observer has been in [21] using Differential Algebraic technique to estimate temperature of a chemical reactor subjected to sustained disturbances. Uçak & Günel in [22] introduced SVM to approximate the tunable parameters of adaptive SMC. In [23], an event triggered SMC control of CSTR was implemented.

2.5 Optimal control

The important objectives in polymer production are minimizing operating costs, improving productivity, quality and safety [24],[25]. These give room for optimization of polymerization reactor based on suitably defined objective function. Paulen, et al.[26] successfully reduced the total reaction time of emulsion copolymerization of α -methylstyrene and styrene by applying dynamic optimization. [27] applied Control vector parametrization to solve quadratic programming for maximizing the average molecular weight in one case and monomer conversion in the second case. Similarly, multiobjective dynamic optimization has been employed in semibatch styrene polymerization process to set up optimal feeding policies and operating temperature to minimize the excess initiator and maximize the monomer conversion in the final products [28]. [29] designed and implemented online multiobjective optimal control of the average molar mass of the product in the free radical polymerization of acrylamide in

water using potassium persulfate as an initiator.

2.6 Model predictive control

The nonminimum phase behaviors of reactors at low operating conditions resulted in poor operations. This problem was solved by [30] using Linear Model Predictive Control (MPC) based on parameter varying system. MPC executes specific control action by predicting future states and outputs [28]. Maner & Doyle in [31], designed nonlinear MPC using autoregressive-plus Volterra model. This control scheme gave superior performance compared to Linear MPC and feedback Proportional-Integral Control. Identification of autoregressive-plus Volterra model increases the computation and is approximated model. [32] employed nonlinear MPC to maintain the quality of the polymer at different production rates. In [33], a linear multi-variable Model Predictive Controller was applied to the identified linear model of polymerization reactor. When the system deviates from the operating point in which the model was identified, the reactor model is re-identified in closed loop to guarantees the robustness of the scheme. Sheng, et al. [34] proposed a new process model that makes possible the augmentation of process states and tracking errors. Subsequently, an improved robust linear MPC was designed to improve tracking control in a moulding process. A nonlinear MPC has been designed to control the average molecular weight of Methyl-Methacrylate [35]. Since the average molecular weight is unmeasured, a receding horizon estimator was applied to estimate it. A robust nonlinear MPC with Kalman filter for uncertainty estimation was employed in crystallization batch process [5]. Lucia et al. [36] presented

a robust multi-stage nonlinear MPC for the semi-batch polymerization reactor in the presence of uncertainties.

2.7 Gain scheduling

Chemical processes exhibit complex nonlinearities and fast changing operating conditions. Linearizing the model at different operating conditions enable the design of fast response changing control. Gain Scheduling provides fast response linear controller for each operating condition. Scheduling variables determine the appropriate linear controller for the current operating condition of the system [37]. The scheduling MPC for a nonlinear system represented by piecewise linear models at different operating conditions has been studied in [38]. The scheme was applied to stabilize the states of a chemical reactor. Another study, [39] linearized the nonlinear model of the chemical reactor at each operating condition, and designed a local Quantified Feedback Theory (QFT) controller. From the local controllers, a global controller effective over all the operating range was designed using gap-metric concept. Zhuge & Ierapetritou in [40] integrated scheduling with dynamic optimization.

2.8 Automatic continuous online monitoring

It is difficult to accurately monitor or directly control the polymerization process due to the contamination of the measurements by uncertainties arising from sensor noises, degree of mixing, purity of products and variation in feed conditions [41]. The most recent sensor, the Automatic Continuous Online Monitoring of Polymer-

ization reactions (ACOMP), provides real-time measurements of the polymerization dynamic states [42]. Some of the applications of ACOMP include online monitoring of polymerization of acrylamide [43], online verification of average mass distribution in homo-polymerization of acrylamide [44]. Despite the fact that ACOMP can overcome many measurement limitations, the complete state vector is hardly measured. Therefore, an observer that can estimate all the states is necessary for a comprehensive control of the process [45].

2.9 Extended Kalman filter

An Extended Kalman Filter (EKF) is the most widely used estimation technique in chemical industries [46]. EKF is based on the linearized model of the plant and it is easy to design once the linearized plant is observable. Even so, tuning EKF is time consuming and requires a lot of trial and errors. To overcome this limitation, Salas, et al. [47] proposed an auto-tuning EKF using global optimization method to attain target average molecular weight trajectories. The unknown composition of the biogas in a Continuous Stirred Tank Reactor (CSTR) were estimated using EKF [48]. In the production of ethylene-propylene-diene polymer (EPDM) in continuous reactor, a hierarchical EKF has been used to estimate the kinetic parameters and the unmeasured states [49]. The states of Methyl-Methacrylate (MMA) copolymerization reactor were estimated using the conventional EKF [50]. Cheng & Liu in [51] estimated the melt index (MI) of propylene polymerization process using least squares support vector machine (LS-SVM).

2.10 Adaptive control

The operating conditions of polymerization process (such as temperature, initiator concentration, e.t.c) are varying continuously. An adaptive controller continuously update its parameters as the parameters of the system varies. An adaptive controller was employed in [52] to control the temperature of a batch suspension poly-vinylchloride reactor and it outperformed Proportional-Integral-Derivative (PID) controller. Tyner, et al. [53] presented adaptive control system consisting of cascade temperature control and an estimator that estimate the varying reaction rate and heat transfer coefficient for a jacketed stirred tank reactor. Vasanthi, et al. [?] did similar work as [53], but obtained excellent tracking of the temperature trajectory by adding cascade feedforward controller. Model-free adaptive control has been implemented in [54] to control the temperature of the polymerization reactor. The authors used particle swarm optimization to optimized the controller parameters. Sarthak, et al [55] controlled the average molecular weight of in free radical polymerization of MMA using Internal Model Control (IMC) based on weight updated Radial Basis Function Network (RBFN). In order to tackle time varying parameters in batch process, a recursive least squares algorithm with forgetting factor was applied to update the controller parameters [56]. Haiyan, et al. [57] demonstrated Model Free Adaptive Control (MFAC) of molecular weight distribution in styrene polymerization. An adaptive control scheme for nonlinear wiener model has been proposed in [58] and its effectiveness was demonstrated for composition control in CSTR.

2.11 Neural network

In the last two decades, the use of neural network for modelling and control of polymerization processes has become increasingly popular. Detail explanations and applications of neural network can be found in [59]. Hagan, et al. in [60] presented gain scheduling control of a nonlinear system approximated by neural network. The authors tested the effectiveness of the scheme on continuous stirred tank reactor and obtained an excellent results in controlling the outflow temperature and concentration of the products. [61], [62], and [63] proposed neural network to approximate the mechanistic model of batch-to-batch reactor. The authors designed optimal controller based on the linearized neural network model. The neural network improved the model prediction confidence bounds of the batch-to-batch polymerization process. Dias, et al. in [64] proposed virtual sensor consisting of particle filter and artificial neural network to observe latent variables and predict the final properties of the polymer respectively. Similarly, in [65], the nonlinear part of the CSTR Wiener model was approximated by NN. The NN approximated part was then linearized online at each sampling instant and used for linear MPC.

CHAPTER 3

MATHEMATICAL MODELLING

3.1 Introduction

This thesis considers the free radical polymerization of Methyl-metacrylate MMA in CSTR with toluene as solvent and azo-bis-isobutyronitrile as initiator. The reaction is exothermic and a cooling jacket continuously removes the heat generated. The detail mechanism of the process was given in [10]. The schematic diagram of the polymerization reactor is shown in fig. 3.1 obtained from [66].

3.2 Full order model

The mathematical model describing the dynamics of the polymerization reaction in CSTR is derived from mass and balance equations under the following assumptions [1]

1. The volume and heat capacity of the reacting mixture do not change.
2. No gel effect.

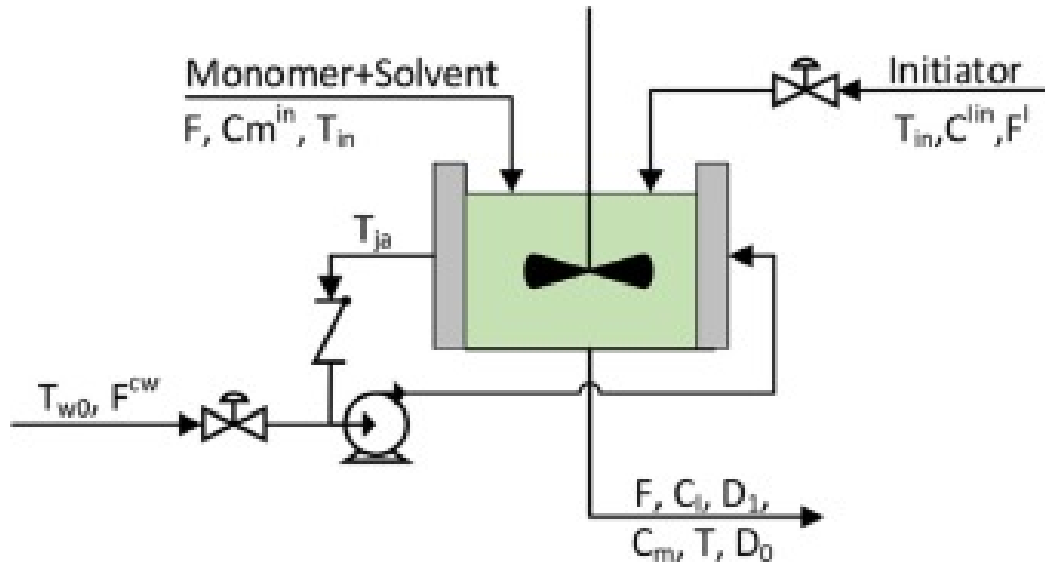


Figure 3.1: Schematic diagram of CSTR

3. The coolant temperature is Uniform in the cooling jacket.
4. The reactor is insulated.
5. No polymer in the inlet streams
6. The reactant are perfectly mixed

The nonisothermal full order model is represented by a set of six coupled nonlinear

equations [1] below

$$\frac{dC_m}{dt} = - \left[Z_{fm} \exp \left(\frac{-E_{fm}}{RT} \right) + Z_p \exp \left(\frac{E_I}{RT} \right) C_m k_0 \right] + \frac{F}{V} (C_m^{in} - C_m) \quad (3.1)$$

$$\frac{dC_I}{dt} = - Z_I \exp \left(\frac{E_I}{RT} \right) C_I + \frac{F_I C_I^{in} - F C_I}{V} \quad (3.2)$$

$$\frac{dD_O}{dt} = - \left[Z_{Td} \exp \left(\frac{-E_{Td}}{RT} \right) + 0.5 Z_{Tc} \exp \left(\frac{E_{Tc}}{RT} \right) \right] C_m k_0 - \frac{F}{V} D_0 \quad (3.3)$$

$$\frac{dD_L}{dt} = - \left[Z_{fm} \exp \left(\frac{-E_{fm}}{RT} \right) + Z_p \exp \left(\frac{-E_p}{RT} \right) \right] M_m C_m k_0 - \frac{F}{V} D_0 \quad (3.4)$$

$$\frac{dT}{dt} = Z_P \exp \left(\frac{-E_P}{RT} \right) C_M \frac{-\Delta H_p}{\rho C_p} - \frac{U A}{\rho C_p V} (T - T_{cj}) + \frac{F}{V} (T_{in} - T) \quad (3.5)$$

$$\frac{dT_{cj}}{dt} = \frac{F_{cw}}{V_{cw}} (T_{cw} - T_{cj}) + \frac{U A}{\rho_w C_w V_{cw}} \quad (3.6)$$

$$k_0 = \left(\frac{C_I Z_I \exp(E_I/RT)}{Z_{Tc} \exp(E_{Tc}/RT) + Z_{Td} \exp(E_{Td}/RT)} \right)^0 .5$$

Let $\chi_1 = C_m$, $\chi_2 = C_I$, $\chi_3 = D_0$, $\chi_4 = D_i$, $\chi_5 = T$, $\chi_6 = T_{cj}$

$$K_{fm} = Z_{fm} \exp \left(\frac{-E_{fm}}{RT} \right); \quad K_p = Z_p \exp \left(\frac{E_I}{RT} \right)$$

$$K_I = Z_I \exp \left(\frac{E_I}{RT} \right); \quad K_{Tc} = 0.5 Z_{Tc} \exp \left(\frac{E_{Tc}}{RT} \right)$$

$$K_{Td} = Z_{Td} \exp \left(\frac{-E_{Td}}{RT} \right)$$

The full order model can be rewritten as [67]

$$\frac{d\chi_1}{dt} = -(k_p + k_{fm})k_0\chi_1 + \frac{F(C_m - \chi_1)}{v} \quad (3.7)$$

$$\frac{d\chi_2}{dt} = -k_I\chi_2 + \frac{F_IC_I - F\chi_2}{v} \quad (3.8)$$

$$\frac{d\chi_3}{dt} = (0.5k_{Tc} + k_{Td})k_0^2 + K_{fm}k_0\chi_1 - \frac{F\chi_3}{v} \quad (3.9)$$

$$\frac{d\chi_4}{dt} = M_m(k_p + k_{fm})k_0\chi_1 - \frac{F\chi_4}{v} \quad (3.10)$$

$$\frac{d\chi_5}{dt} = k_p \frac{(-\Delta H_p)}{\rho c_p} \chi_1 k_0 - \frac{UA}{\rho c_p v} (\chi_5 - \chi_6) + \frac{F(T_{in} - \chi_5)}{v} \quad (3.11)$$

$$\frac{d\chi_6}{dt} = \frac{F_w T_w - F\chi_6}{V_w} + \frac{UA}{\rho_w c_w v_w} (\chi_5 - \chi_6) \quad (3.12)$$

$$k_0 = \left[\frac{2fk_I}{k_{Tc} + k_{Td}} \right]^{1/2} \sqrt{\chi_2}$$

3.3 Isothermal model

When the reactor temperature is constant (isothermal), the temperature dynamic equations are ignored and the model reduces to [11]

$$\frac{d\chi_1}{dt} = -(k_p + k_{fm})k_0\chi_1 + \frac{F(C_m - \chi_1)}{v} \quad (3.13)$$

$$\frac{d\chi_2}{dt} = -k_I\chi_2 + \frac{F_IC_I - F\chi_2}{v} \quad (3.14)$$

$$\frac{d\chi_3}{dt} = (0.5k_{Tc} + k_{Td})k_0^2 + K_{fm}k_0\chi_1 - \frac{F\chi_3}{v} \quad (3.15)$$

$$\frac{d\chi_4}{dt} = M_m(k_p + k_{fm})k_0\chi_1 - \frac{F\chi_4}{v} \quad (3.16)$$

The physical meaning and values of the parameters of the model are given in Table

3.1

Table 3.1: Summary and definition of the parameters of polymerization of MMA in CSTR [1]

Parameters	Values	Definition
v	$1.0m^3$	Reactor volume
T	$335K$	Reactor temperature
F	$10.0m^3/h$	Monomer flow rate
f^*	0.58	Initiator efficiency
k_p	$2.50 \times 10^6 m^3/(kmol.h)$	Propagation rate constant
k_{Tc}	$1.33 \times 10^{10} m^3/(kmol.h)$	Termination by coupling rate constant
k_{Td}	$1.09 \times 10^{11} m^3/(kmol.h)$	Termination by disproportionation rate constant
C_m	$6.00 kmol/m^3$	Inlet monomer concentration
C_I	$8.00 kmol/m^3$	Inlet monomer concentration
K_I	$1.02 \times 10^{-1} h^{-1}$	Initiation rate constant
k_{fm}	$2.45 \times 10^3 m^3/(kmol.h)$	Chain transfer to monomer rate constant
M_m	$100.12 kg/kmol$	Molecular weight of the monomer
ρ	$866 kg/m^3$	Density of the reacting mixture
ρ_w	$1000 kg.m^3$	Density of water
c_p	$2.0 kJ.kg^{-1}.K^{-1}$	Heat capacity of the reacting mixture
$-\Delta H_p$	$57800 kJ.kmol^{-1}$	Heat of propagation reaction
U	$720 kJ.h^{-1}.K^{-1}$	Overall heat transfer coefficient
A	$2.0 m^2$	Heat transfer area
c_w	$4.2 kJ.kg^{-1}.K^{-1}$	Heat capacity of water
T_{in}	$350 K$	Temperature of the inlet streams in the reactor
T_w	$293.2 K$	Temperature of the inlet coolant stream

CHAPTER 4

NEURO-ADAPTIVE BACKSTEPPING FAST TERMINAL SLIDING MODE CONTROL

4.1 Introduction

In this chapter, a backstepping based fast terminal SMC is developed to control the average molecular weight ($A = \chi_4/\chi_3$) of the polymer and the reactor temperature ($T = \chi_5$). Also, the effect of the input deadzone has been taken into account in the control design. In addition, the complex dynamics of the polymerization reactor are approximated with NN. Moreover, a proportional derivative (PD) controller is constructed for comparison sake.

4.2 Output Dynamics

The outputs A and T are differentiated continuously until the inputs appear. The control input are selected to drive the outputs to track the desired trajectories. The first time-derivatives of the outputs are

$$\begin{cases} \dot{A} = \frac{\partial A}{\partial \chi_3} \dot{\chi}_3 + \frac{\partial A}{\partial \chi_4} \dot{\chi}_4 \\ \dot{T} = \frac{\partial T}{\partial \chi_3} \dot{\chi}_3 \end{cases} \quad (4.1)$$

Equation. (4.1) is further differentiated leading to

$$\begin{cases} \ddot{A} = \frac{\partial(\dot{A})}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial(\dot{A})}{\partial \chi_2} \dot{\chi}_2 + \frac{\partial(\dot{A})}{\partial \chi_3} \dot{\chi}_3 + \frac{\partial(\dot{A})}{\partial \chi_4} \dot{\chi}_4 \\ \ddot{T} = \frac{\partial(\dot{T})}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial(\dot{T})}{\partial \chi_2} \dot{\chi}_2 + \frac{\partial(\dot{T})}{\partial \chi_5} \dot{\chi}_5 + \frac{\partial(\dot{T})}{\partial \chi_6} \dot{\chi}_6 \end{cases} \quad (4.2)$$

Equation. 4.2 can be expressed as

$$\begin{cases} \ddot{A} = F_1(\chi) + g_1(\chi)Z_1(u_1) \end{cases} \quad (4.3a)$$

$$\begin{cases} \ddot{T} = \bar{F}_2(\chi) + \bar{g}_2(\chi)Z_1(u_1) + g_2(\chi)Z_2(u_2) \end{cases} \quad (4.3b)$$

Where:

$$\begin{aligned}
F_1(\chi) &= \frac{\partial(\dot{A})}{\partial\chi_1} \dot{\chi}_1 + \frac{\partial(\dot{A})}{\partial\chi_2} \left[-k_I \chi_2 + \frac{-F\chi_2}{v} \right] + \frac{\partial(\dot{A})}{\partial\chi_3} \dot{\chi}_3 + \frac{\partial(\dot{A})}{\partial\chi_4} \dot{\chi}_4 \\
\bar{F}_2(\chi) &= \frac{\partial(\dot{T})}{\partial\chi_1} \dot{\chi}_1 + \frac{\partial(\dot{T})}{\partial\chi_2} \left[-k_I \chi_2 + \frac{-F\chi_2}{v} \right] + \frac{\partial(\dot{T})}{\partial\chi_5} \dot{\chi}_5 \\
&\quad + \frac{\partial(\dot{T})}{\partial\chi_6} \left[\frac{-F\chi_6}{V_w} + \frac{UA}{\rho_w c_w v_w} (\chi_5 - \chi_6) \right] \\
g_1(\chi) &= \frac{C_I}{v} \frac{\partial(\dot{A})}{\partial\chi_2}, \quad g_2(\chi) = \frac{\partial(\dot{T})}{\partial\chi_6} \frac{T_w}{V_w}, \quad \bar{g}_2(\chi) = \frac{\partial(\dot{T})}{\partial\chi_2} \frac{C_I}{v}
\end{aligned}$$

The deadzone output $Z_i(u_i)$ (i=1,2) is given by

$$Z_i(u_i(t)) = \begin{cases} s_{ri}[u_i(t) - b_{ri}], & u_i(t) \geq b_{ri} \\ 0, & -b_{li} < u_i(t) < b_{ri} \\ s_{li}[u_i(t) + b_{li}], & u_i(t) \leq -b_{li} \end{cases}$$

s_{li} and s_{ri} represent the unknown left and right slopes, $b_{li} > 0$ and $b_{ri} > 0$ denote the unknown left and right thresholds deadzone outputs. The deadzone can be expressed as a slow time varying input-dependent function.

$$Z_i(u_i) = s_i u_i(t) + \delta_i(t) \tag{4.4}$$

Where

$$s_i = \begin{cases} s_{ri}, & u_i(t) > 0 \\ s_{li} & u_i(t) \leq 0 \end{cases}$$

$$\delta_i(t) = \begin{cases} -s_{ri}b_{ri}, & u_i(t) \geq b_{ri} \\ -s_i u_i(t), & -b_{li} < u_i(t) < b_{ri} \\ s_{li}b_{li}, & u_i(t) \leq -b_{li} \end{cases}$$

It can be easily obtained that

$$|\delta_i| \leq \bar{s}_i \bar{b}_i \quad (4.5)$$

Where $\bar{b}_i = \max\{b_{ri}, b_{li}\}$, $\bar{s}_i = \max\{s_{ri}, s_{li}\}$. Therefore, one has

$$\begin{cases} \ddot{A} = F_1(\chi) + g_1(\chi)[s_1 u_1 + \delta_1] \\ \ddot{T} = \bar{F}_2(\chi) + \bar{g}_2(\chi)[s_1 u_1 + \delta_1] + g_2(\chi)[s_2 u_2 + \delta_2] \end{cases} \quad (4.6)$$

Let $G_i(\chi) = g_i(\chi)s_i, (i = 1, 2)$, $\bar{G}_2(x) = \bar{g}_2(x)s_1$, $d_1 = g_1(\chi)\delta_1$, $d_2 = g_1(\chi)\delta_1 + \bar{g}_2(\chi)\delta_1$, $A_1 = A$, $A_2 = \dot{A}$, $T_1 = T$ and $T_2 = \dot{T}$, then Eq. (4.6) can be written in state space form as

$$\dot{A}_1 = A_2 \quad (4.7)$$

$$\dot{A}_2 = F_1(\chi) + G_1(\chi)u_1 + d_1 \quad (4.8)$$

$$\dot{T}_1 = T_2 \quad (4.9)$$

$$\dot{T}_2 = \bar{F}_2(\chi) + \bar{G}_2(x)u_1 + G_2(\chi)u_2 + d_2 \quad (4.10)$$

4.2.1 NN approximation

The universal approximation property of NN is utilised to approximation F_1 , F_2 , G_1 and G_2 in a compact set

$$\begin{cases} F_i(\chi_i) = V_i^T \Phi_i(\chi_i) + \varepsilon_{Fi} \\ G_i(\chi_i) = W_i^T \Phi_i(\chi_i) + \varepsilon_{Gi} \end{cases} \quad (i = 1, 2) \quad (4.11)$$

Where

$$\Phi_i(\chi_i) = \frac{1}{1 + e^{\chi_i}}, \quad (i = 1, 2)$$

$\chi_i \in \mathcal{R}^n$ is the NN input vector, $\Phi_i(.) : \mathcal{R}^n \rightarrow \mathcal{R}^L$ is a Sigmoid activation function, $V_i, W_i \in \mathcal{R}^{L \times m}$ are the NN weight vectors, $F_i(\chi_i), G_i(\chi_i) \in \mathcal{R}^m$ are the outputs, $\varepsilon_{Fi} < \bar{\varepsilon}_{Fi}$ and $\varepsilon_{Gi} < \bar{\varepsilon}_{Gi}$ are the NN approximation errors with bounds $\bar{\varepsilon}_{Fi}$ and $\bar{\varepsilon}_{Gi}$ respectively. The NN estimation of $F_i(\chi)$ and $G_i(\chi)$ can be written as

$$\begin{cases} \hat{F}_i(\chi_i) = \hat{V}_i^T \Phi_i(\chi_i) \\ \hat{G}_i(\chi_i) = \hat{W}_i^T \Phi_i(\chi_i) \end{cases} \quad (4.12)$$

The NN estimation errors are given as

$$\begin{cases} \tilde{F}_i(\chi) = F_i(\chi) - \hat{F}_i(\chi) = \tilde{V}_i^T \Phi_i(\chi_i) + \varepsilon_{Fi} \\ \tilde{G}_i(\chi) = G_i(\chi) - \hat{G}_i(\chi) = \tilde{W}_i^T \Phi_i(\chi_i) + \varepsilon_{Gi} \end{cases} \quad (4.13)$$

Where $\tilde{V}_i = V_i - \hat{V}_i$ and $\tilde{W}_i = W_i - \hat{W}_i$ are NNs' weight estimation errors.

4.3 Backstepping sliding mode controller

A backstepping sliding mode controllers are designed to track the desired trajectories A_d & T_d and mitigate the effect of the deadzone. The controller is designed in the following steps

Step 1 *Define the tracking of the average molecular weight as*

$$e_1 = A_1 - A_d \quad (4.14)$$

Then, the derivative of e_1 is

$$\dot{e}_1 = \dot{A}_1 - \dot{A}_d = \dot{A}_2 - \dot{A}_d \quad (4.15)$$

Choose the Lyapunov candidate function as

$$L_1 = \frac{1}{2}e_1^2 \quad (4.16)$$

It follows that the time-derivative of L_1 is

$$\dot{L}_1 = e_1\dot{e}_1 = e_1(A_2 - \dot{A}_d) \quad (4.17)$$

Where S_1 is the sliding surface. Choosing the virtual input as $A_2 = S_1 + \dot{A}_d - k_1e_1$, Eq. (4.17) becomes

$$\dot{L}_1 = -k_1e_1^2 + S_1e_1 \quad (4.18)$$

Step 2 *Let the following Lyapunov function be*

$$L_2 = \frac{1}{2}e_1^2 + \frac{1}{2}S^2 + \frac{1}{2\gamma_1}\tilde{V}^T\tilde{V} + \frac{1}{2\Gamma_1}\tilde{W}^T\tilde{W} + \frac{1}{2\alpha_1}\tilde{d}_1^2 \quad (4.19)$$

$$\dot{L}_2 = e_1\dot{e}_1 + S_1\dot{S}_1 + \frac{1}{\gamma_1}\tilde{V}^T\dot{\tilde{V}} + \frac{1}{\Gamma_1}\tilde{W}^T\dot{\tilde{W}} + \frac{1}{\alpha_1}\tilde{d}_1\dot{\tilde{d}}_1 \quad (4.20)$$

Onward, the sliding surface is selected as

$$S_1 = \dot{e}_1 + k_1e_1 + \theta e_1^{p/q} \quad (4.21)$$

Where $\theta > 0$, $q > p$, $0 < p/q < 1$. The time derivative of S_1 is derived as follows

$$\begin{aligned}\dot{S}_1 &= \dot{A}_2 - \ddot{A}_d + k_1 \dot{e}_1 + \theta \frac{p}{q} e_1^{p/q-1} \\ &= F_1(\chi) + G_1(\chi)u_1 + d_1 - \ddot{A}_d + k_1 \dot{e}_1 + \theta \frac{p}{q} e_1^{p/q-1}\end{aligned}\quad (4.22)$$

Substituting Eq. (4.18) and Eq. (4.22) into Eq. (4.20) yields

$$\begin{aligned}\dot{L}_2 &= -k_1 e_1^2 + S_1[F_1 + \hat{G}_1 u_1 + (G_1 - \hat{G}_1)u_1 + d_1 + v_1] \\ &\quad + \frac{1}{\gamma_1} \tilde{V}^T \dot{\tilde{V}} + \frac{1}{\Gamma_1} \tilde{W}^T \dot{\tilde{W}} + \frac{1}{\alpha_1} \tilde{d} \dot{\tilde{d}}\end{aligned}\quad (4.23)$$

Where $v_1 = -\ddot{A}_d + k_1 \dot{e}_1 + e_1 + \theta \frac{p}{q} e_1^{p/q-1}$. The following control law is selected

$$u_1 = \frac{1}{\hat{G}_1} \left[-\hat{F}_1 - \hat{d}_1 \text{sign}(S_1) - \lambda_1 S_1 - v_1 \right] \quad (4.24)$$

Substituting the control law u_1 into Eq. (4.23), one gets

$$\begin{aligned}\dot{L}_2 &= -k_1 e_1^2 - \lambda_1 S_1^2 + S_1 \epsilon_F + S_1 \epsilon_G u_1 \\ &\quad + \tilde{V}_1 \left[S_1 \Phi_1(\chi_1) - \frac{1}{\gamma_1} \dot{\tilde{V}} \right] + \tilde{W}_1 \left[S_1 \Phi_1(\chi_1) u_1 - \frac{1}{\Gamma_1} \dot{\tilde{W}} \right] \\ &\quad + \tilde{d} \left[|S_1| - \frac{1}{\alpha_1} \dot{\tilde{d}} \right]\end{aligned}\quad (4.25)$$

Note that $\hat{d}_1 S_1 \text{sign}(S_1) = \hat{d}_1 |S_1|$, $d_1 S_1 \leq d_1 |S_1|$. The following adaptation laws

are proposed

$$\dot{\hat{V}}_1 = \gamma_1 \left[S_1 \Phi_1(\chi_1) - \eta_1 \hat{V}_1 \right] \quad (4.26)$$

$$\dot{\hat{W}}_1 = \Gamma_1 \left[S_1 \Phi_1(\chi_1) u_1 - \eta_1 \hat{W}_1 \right] \quad (4.27)$$

$$\dot{\hat{d}}_1 = \alpha_1 \left[|S_1| - \eta_1 \hat{d}_1 \right] \quad (4.28)$$

Using the adaptation laws Eq. (4.26)-(4.28), Eq. (4.25) becomes

$$\begin{aligned} \dot{L}_2 = & -k_1 e_1^2 - \lambda_1 S_1^2 + S_1 \epsilon_F + S_1 \epsilon_G u_1 \\ & + \eta_1 \tilde{V}_1 \hat{V}_1 + \eta_1 \tilde{W}_1 \hat{W}_1 + \eta_1 \tilde{d}_1 \hat{d}_1 \end{aligned} \quad (4.29)$$

The following Young's inequalities are substituted into Eq. (4.29) and leads to Eq.

(4.30)

$$\begin{aligned} \tilde{d}_1 \hat{d}_1 = \tilde{d}_1 [d_1 - \tilde{d}_1] & \leq \frac{\|d\|^2}{2} - \frac{\|\tilde{d}\|^2}{2}; \quad S_1 \epsilon_G \leq \frac{S_1^2}{2} + \frac{\epsilon_G^2}{2} \\ \tilde{V}_1 \hat{V}_1 = \tilde{V}_1 [V_1 - \tilde{V}_1] & \leq \frac{V^2}{2} - \frac{\tilde{V}^2}{2}; \quad S_1 \epsilon_F \leq \frac{S_1^2}{2} + \frac{\epsilon_F^2}{2} \\ \tilde{W}_1 \hat{W}_1 = \tilde{W}_1 [W_1 - \tilde{W}_1] & \leq \frac{W^2}{2} - \frac{\tilde{W}^2}{2} \end{aligned}$$

$$\begin{aligned} \dot{L}_2 = & -\beta_1 \frac{e_1^2}{2} - \beta_1 \frac{S_1^2}{2} - \beta_1 \frac{\|\tilde{V}_1\|^2}{2} - \beta_1 \frac{\|\tilde{W}_1\|^2}{2} + \beta_2 \\ & \leq -\beta_1 L_2 + \beta_2 \end{aligned} \quad (4.30)$$

Where $\beta_1 = \min\{2k_1, (2\lambda_1 - 2\eta_1), \eta_1, \eta_1, \eta_1\}$, $\beta_2 = \eta_1 \frac{W_1^2}{2} + \eta_1 \frac{V_1^2}{2} + \eta_1 \frac{d_1^2}{2} + \frac{\epsilon_F^2}{2} + \frac{\epsilon_G^2}{2}$.

From Eq. (4.30), one can derive

$$\begin{aligned}
\dot{L}_2 + \beta_1 L_2 &\leq \beta_2 \\
\int_0^t (\dot{L}_2 + \beta_1 L_2) e^{\beta_1 t} dt &\leq \beta_2 \int_0^t e^{\beta_1 t} dt \\
L_2 e^{\beta_1 t} - L_2(0) &\leq \frac{\beta_2 e^{\beta_1 t}}{\beta_1} - \frac{\beta_2}{\beta_1} \\
L_2 &\leq \frac{\beta_2}{\beta_1} + \left(L_2(0) - \frac{\beta_2}{\beta_1} \right) e^{-\beta_1 t}
\end{aligned} \tag{4.31}$$

When $t \rightarrow \infty$, $L_2 \leq \frac{\beta_2}{\beta_1}$. Hence, the closed loop signals are uniformly ultimately bounded in the compact set $\Upsilon_1 = \{L_2 : L_2 \leq \frac{\beta_2}{\beta_1}\}$

Step 3 *Define the tracking error of the reactor temperature as*

$$e_3 = T_1 - T_d \tag{4.32}$$

$$\dot{e}_3 = \dot{T}_1 - \dot{T}_d = T_2 - \dot{T}_d \tag{4.33}$$

Let the Lyapunov function be

$$L_3 = \frac{1}{2} e_3^2 \tag{4.34}$$

Differentiating L_3 with respect to time produces

$$\dot{L}_3 = e_3 \dot{e}_3 = e_3 (T_2 - \dot{T}_d) \tag{4.35}$$

Where S_2 is the sliding surface. Using the virtual input $T_2 = S_2 + \dot{T}_d - k_2 e_3$, Eq. (4.35) becomes

$$\dot{L}_3 = -k_2 e_3^2 + S_2 e_3 \quad (4.36)$$

Step 4 *Select the Lyapunov function as*

$$L_4 = \frac{1}{2} e_3^2 + \frac{1}{2} S_2^2 + \frac{1}{2\gamma_2} \tilde{V}_2^T \tilde{V}_2 + \frac{1}{2\Gamma_2} \tilde{W}_2^T \tilde{W}_2 + \frac{\tilde{d}_2^2}{\alpha_2} \quad (4.37)$$

$$\dot{L}_4 = e_3 \dot{e}_3 + S_2 \dot{S}_2 + \frac{1}{\gamma_2} \tilde{V}_2^T \dot{\tilde{V}}_2 + \frac{1}{\Gamma_2} \tilde{W}_2^T \dot{\tilde{W}}_2 + \frac{\tilde{d}_2 \dot{\tilde{d}}_2}{\alpha_2} \quad (4.38)$$

Let the sliding surface be of the form

$$S_2 = \dot{e}_3 + k_2 e_3 + \theta e_3^{p/q} \quad (4.39)$$

The time derivative of S_2 is thus

$$\begin{aligned} \dot{S}_2 &= \dot{T}_2 - \ddot{T}_d + k_2 \dot{e}_3 + \theta \frac{p}{q} e_3^{p/q-1} \\ &= \bar{F}_2(\chi) + \bar{G}_2(x) u_1 + G_2(\chi) u_2 + d_2 - \ddot{T}_d + k_2 \dot{e}_3 + \xi \frac{p}{q} e_3^{p/q-1} \\ &= F_2(\chi) + G_2(\chi) u_2 + d_2 - \ddot{T}_d + k_2 \dot{e}_3 + \xi \frac{p}{q} e_3^{p/q-1} \end{aligned} \quad (4.40)$$

Where $F_2(\chi) = \bar{F}_2(\chi) + \bar{G}_2(\chi) u_1$. Using Eq. (4.36) and Eq. (4.40), Eq. (4.38)

becomes

$$\begin{aligned}\dot{L}_4 = & -k_2 e_3^2 + S_2[F_2 + \hat{G}_2 u_2 + (G_2 - \hat{G}_2)u_2 + d_2 + v_2] \\ & + \frac{1}{\gamma_2} \tilde{V}_2^T \dot{\tilde{V}}_2 + \frac{1}{\Gamma_2} \tilde{W}_2^T \dot{\tilde{W}}_2 + \frac{1}{\alpha_2} \tilde{d}_2 \dot{\tilde{d}}_2\end{aligned}\quad (4.41)$$

Where $v_2 = -\ddot{T}_d + k_2 \dot{e}_3 + e_3 + \theta_q^p e_3^{p/q-1}$. Set the control law as

$$u_2 = \frac{1}{\hat{G}_2} \left[-\hat{F}_2 - \hat{d}_2 \text{sign}(S_2) - \lambda_2 S_2 - v_2 \right] \quad (4.42)$$

Using the control law u_2 , Eq. (4.36) becomes

$$\begin{aligned}\dot{L}_4 = & -k_2 e_3^2 - \lambda_2 S_2^2 + S_2 \epsilon_F + S_2 \epsilon_G u_2 \\ & + \tilde{V}_2 \left[S_2 \Phi_2(\chi_2) - \frac{\dot{\tilde{V}}_2}{\gamma_2} \right] + \tilde{W}_2 \left[S_2 \Phi_2(\chi_2) u_2 - \frac{\dot{\tilde{W}}_2}{\Gamma_2} \right] \\ & + \tilde{d}_2 \left[|S_2| - \frac{1}{\alpha_2} \dot{\tilde{d}}_2 \right]\end{aligned}\quad (4.43)$$

Note that $\hat{d}_2 S_2 \text{sign}(S_2) = \hat{d}_2 |S_2|$, $d_2 S_2 \leq d_2 |S_2|$. The adaptation laws chosen are

$$\dot{\tilde{V}}_2 = \gamma_2 \left[S_2 \Phi_2(\chi_2) - \eta_2 \hat{V}_2 \right] \quad (4.44)$$

$$\dot{\tilde{W}}_2 = \Gamma_2 \left[S_2 \Phi_2(\chi_2) u_2 - \eta_2 \hat{W}_2 \right] \quad (4.45)$$

$$\dot{\tilde{d}}_2 = \alpha_2 \left[|S_2| - \eta_2 \hat{d}_2 \right] \quad (4.46)$$

Using the adaptation laws above, Eq. (4.43) becomes

$$\begin{aligned}\dot{L}_4 = & -k_2 e_3^2 - \lambda_2 S_2^2 + S_2 \epsilon_{F2} + S_2 \epsilon_{[G2]} u_2 \\ & + \eta_2 \tilde{V}_2 \hat{V}_2 + \eta_2 \tilde{W}_2 \hat{W}_2 + \eta_2 \tilde{d}_2 \hat{d}_2\end{aligned}\quad (4.47)$$

Based on Young's inequalities, one obtains

$$\begin{aligned}\tilde{d}_2 \hat{d}_2 = \tilde{d}_2 [d_2 - \tilde{d}_2] & \leq \frac{d_2^2}{2} - \frac{\tilde{d}_2^2}{2}; \quad S_2 \epsilon_G \leq \frac{S_2^2}{2} + \frac{\epsilon_G^2}{2} \\ \tilde{V}_2 \hat{V}_2 = \tilde{V}_2 [V_2 - \tilde{V}_2] & \leq \frac{V_2^2}{2} - \frac{\tilde{V}_2^2}{2}; \quad S_2 \epsilon_F \leq \frac{S_2^2}{2} + \frac{\epsilon_F^2}{2} \\ \tilde{W}_2 \hat{W}_2 = \tilde{W}_2 [W_2 - \tilde{W}_2] & \leq \frac{W_2^2}{2} - \frac{\tilde{W}_2^2}{2}\end{aligned}$$

By substituting the derived Young's inequalities into Eq. (4.47), we achieve

$$\begin{aligned}\dot{L}_4 = & -\beta_3 \frac{e_3^2}{2} - \beta_3 \frac{S_2^2}{2} - \beta_3 \frac{\|\tilde{V}_2\|^2}{2} - \beta_3 \frac{\|\tilde{W}_2\|^2}{2} + \beta_4 \\ & \leq -\beta_3 L_4 + \beta_4\end{aligned}\quad (4.48)$$

Where $\beta_3 = \min\{2k_2, (2\lambda_2 - 2\eta_2), \eta_2, \eta_2, \eta_2\}$, $\beta_4 = \eta_2 \frac{\|W_2\|^2}{2} + \eta_2 \frac{\|V_2\|^2}{2} + \eta_2 \frac{d_2^2}{2} + \frac{\epsilon_F^2}{2} + \frac{\epsilon_G^2 u_2^2}{2}$. The general solution of Eq. (4.48) is realised as follows

$$\begin{aligned}
\dot{L}_4 + \beta_3 L_4 &\leq \beta_4 \\
\int_0^t (\dot{L}_4 + \beta_3 L_4) e^{\beta_3 t} dt &\leq \beta_4 \int_0^t e^{\beta_3 t} dt \\
L_4 e^{\beta_3 t} - L_4(0) &\leq \frac{\beta_4 e^{\beta_3 t}}{\beta_3} - \frac{\beta_4}{\beta_3} \\
L_4 &\leq \frac{\beta_4}{\beta_3} + \left(L_4(0) - \frac{\beta_4}{\beta_3} \right) e^{-\beta_3 t}
\end{aligned} \tag{4.49}$$

When $t \rightarrow \infty$, $L_4 \leq \frac{\beta_4}{\beta_3}$. Thus the closed loop signals are uniformly bounded in the compact $\Upsilon_2 = \{L_4 : L_4 \leq \frac{\beta_4}{\beta_3}\}$

4.4 Proportional derivative control

The PD controller is constructed as follows: $u_1 = K_{p1}(A_1 - A_d) + K_{d1}(\dot{A}_1 - \dot{A}_d)$,
 $u_2 = K_{p2}(T_1 - T_d) + K_{d2}(\dot{T}_1 - \dot{T}_d)$

4.5 Simulation results and discussions

The controller tuning parameters are $K_1 = 8$, $K_2 = 30$, $\lambda_1 = 5$, $\lambda_2 = 20$ p=3, q=5, $\theta = 0.001$ and the desired outputs are $A_d = 2.50 \times 10^4 \text{ kg/kmol}$, $T_d = 350^0 \text{ K}$. The deadzone parameters are $s_{l1} = 0.5$, $s_{r1} = 1$, $s_{l2} = 2$, $s_{r1} = 1$ $b_{r1} = 0.01$, $b_{l1} = -0.03$, $b_{r2} = 0.2$, $b_{l2} = -0.4$, $\alpha_1 = 10$, $\alpha_2 = 400$, $\eta_1 = 50$ and $\eta_2 = 100$. The NN learning rate $\gamma_1 = \Gamma_1 = 0.0001$, $\gamma_2 = 0.125$, $\Gamma_2 = 0.01$, $\eta 0.01$, $L = 10$, and the input vector $X_i = [1, e_i, \dot{e}_i]$. The PD controller tuning parameters are $K_{d1} = 10$, $K_{p1} = 120$, $K_{p2} = 30$, $K_{d2} = 600$.

The simulation results are depicted in Figs. 4.1-4.13. As shown in Fig. 4.1, The

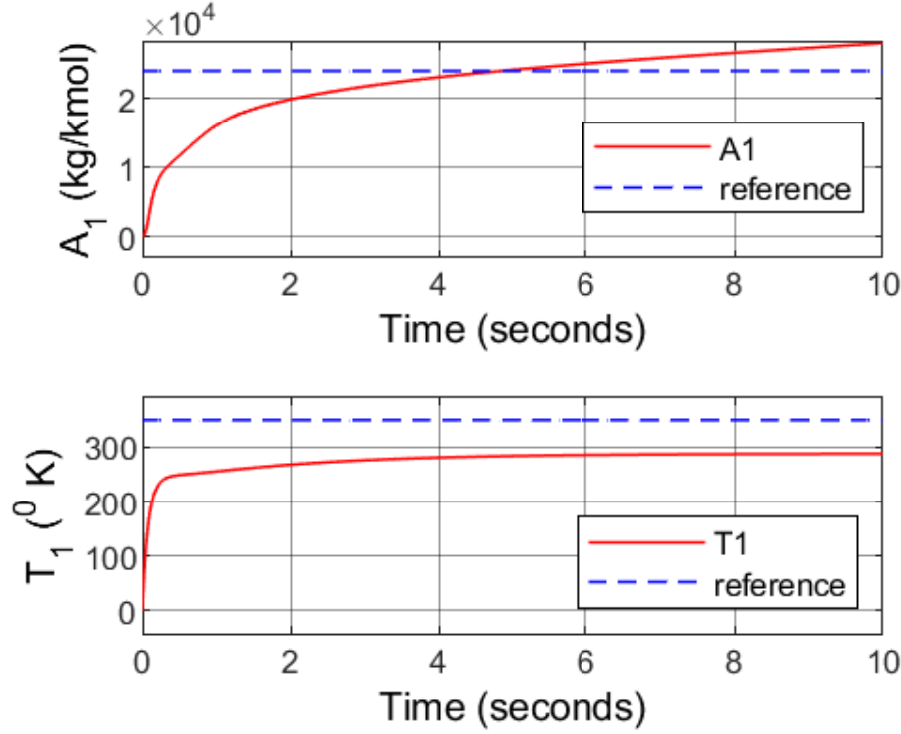


Figure 4.1: AMW (above)
and reactor temperature (below): PD control

outputs under PD controller failed to track the desired signals due to the deadzone effects. The tracking errors are large and unacceptable as depicted in Fig. 4.2. The distorted control inputs are shown in Fig. 4.3.

The outputs, A and T , under NN-BFTSMC have satisfactorily tracked the desired trajectories despite the input deadzone nonlinearity as shown in Fig. 4.4. The tracking errors are presented in Fig. 4.5. The compensated inputs are shown in Fig. 4.6. The fast terminal sliding mode surfaces are depicted in Fig. 4.7. The states of the process are shown in Figs. 4.8-4.13

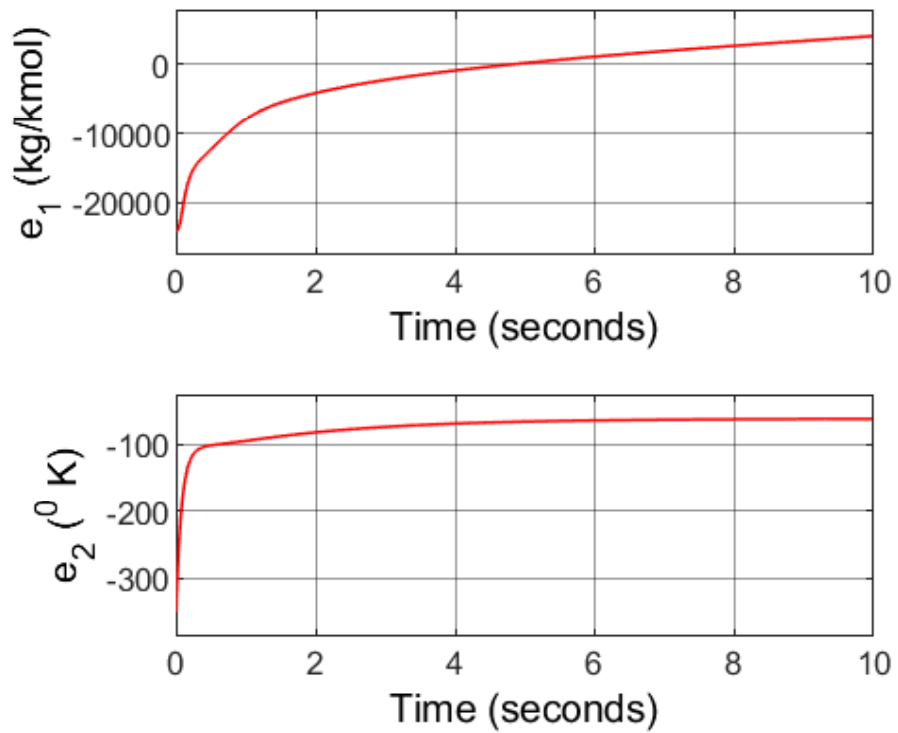


Figure 4.2: Average molecular weight tracking error (top) and the reactor temperature tracking error (below): PD controller

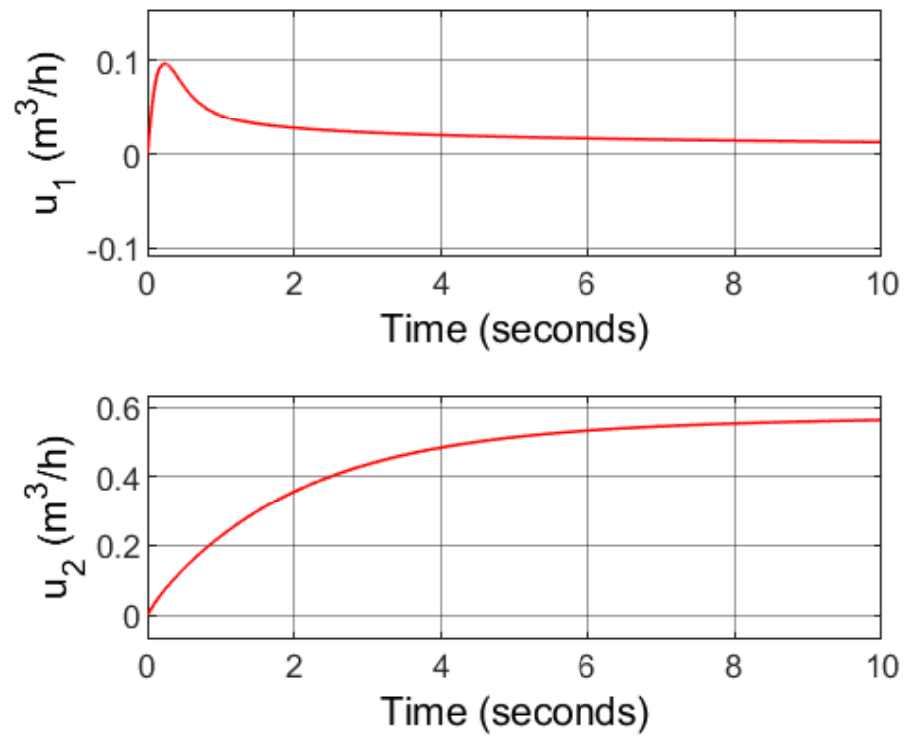


Figure 4.3: The initiator flow rate (above) and the coolant flow rate (below): PD controller

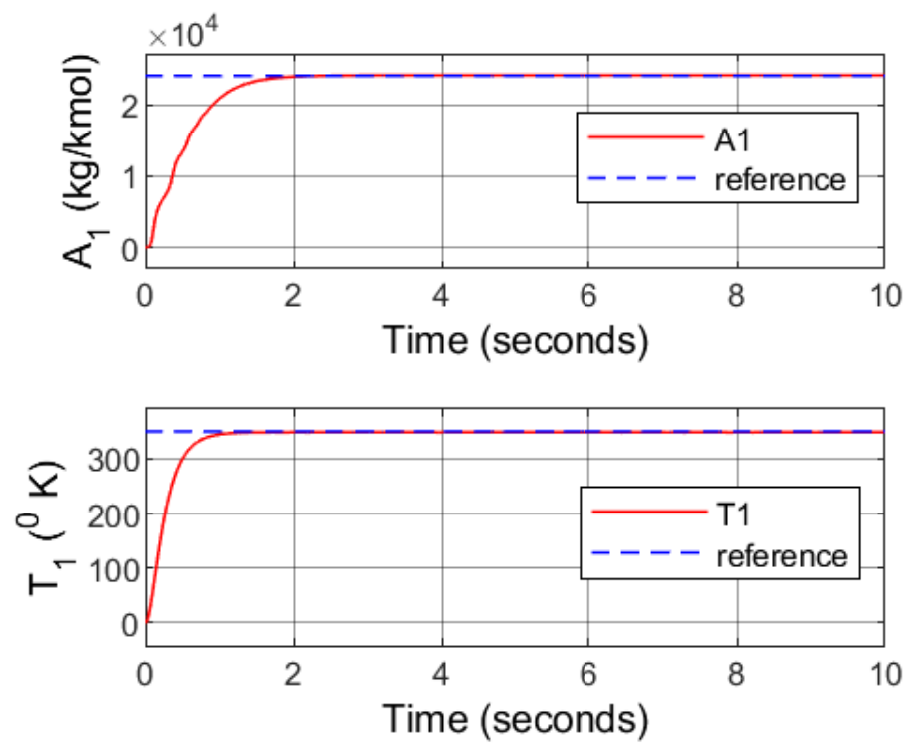


Figure 4.4: AMW (above)
and reactor temperature (below)

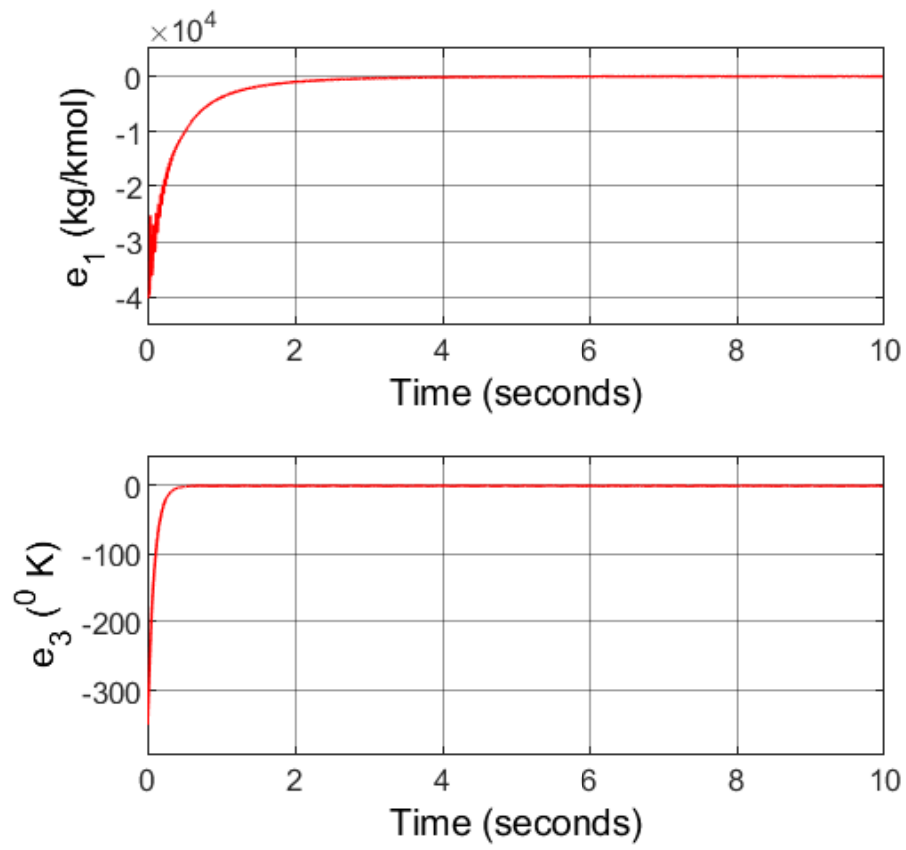


Figure 4.5: Average molecular weight tracking error (top) and the reactor temperature tracking error (below)

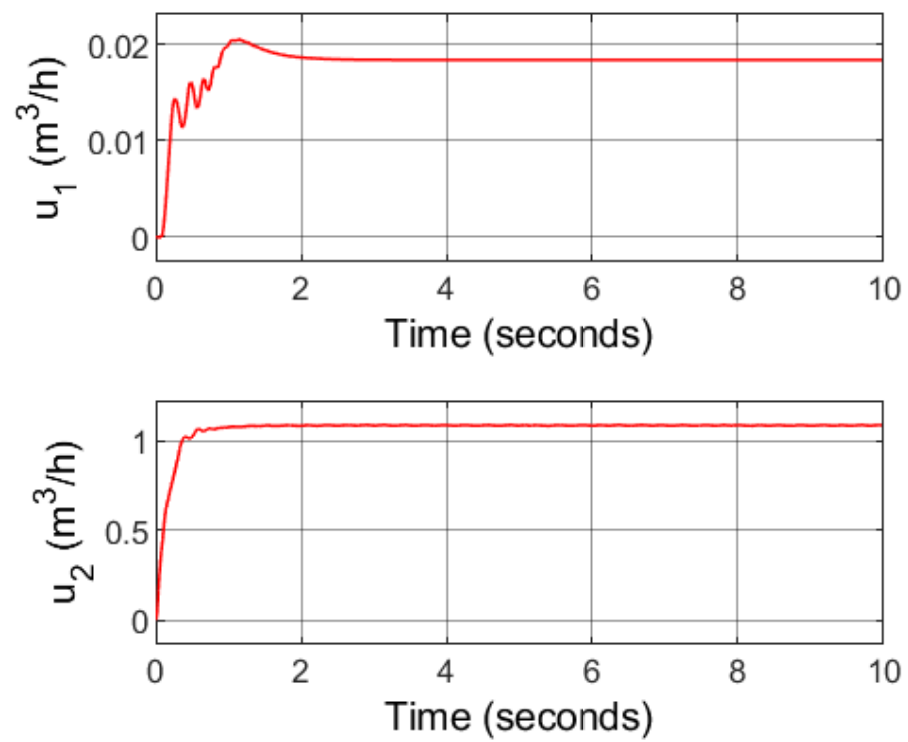


Figure 4.6: The initiator flow rate (above)
and the coolant flow rate (below)

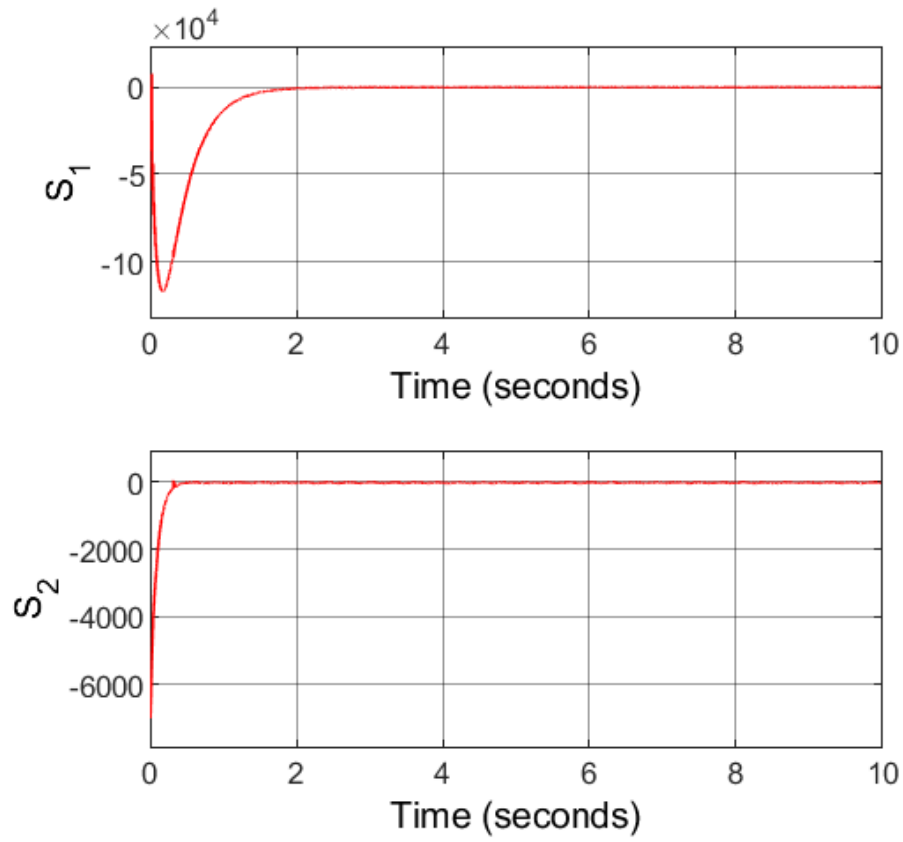


Figure 4.7: Fast terminal sliding surfaces

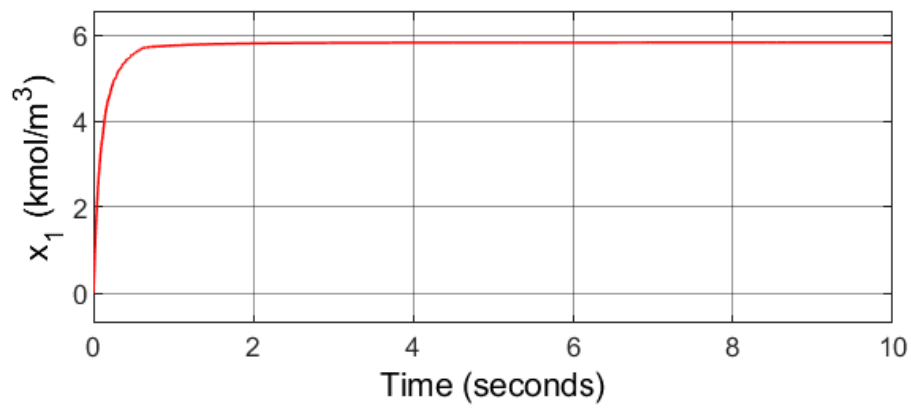


Figure 4.8: The monomer concentration

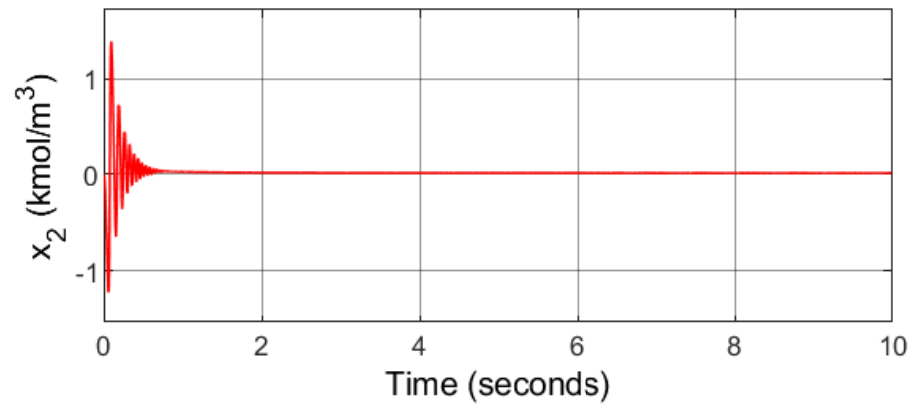


Figure 4.9: Initiator concentration

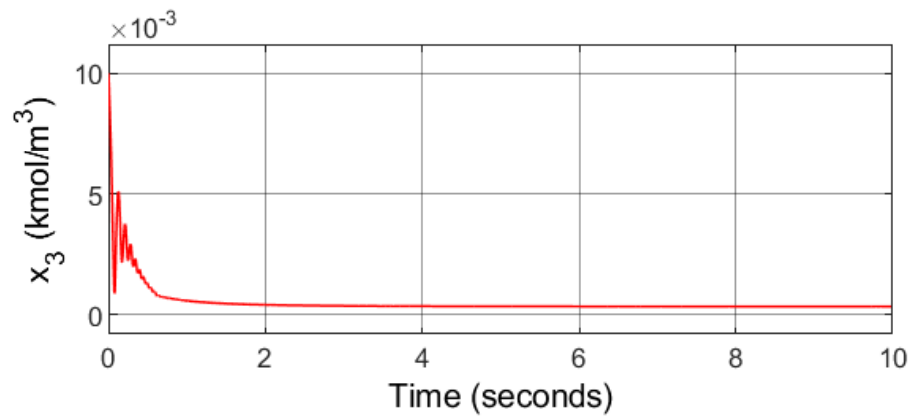


Figure 4.10: Molar concentration of death polymer chains.

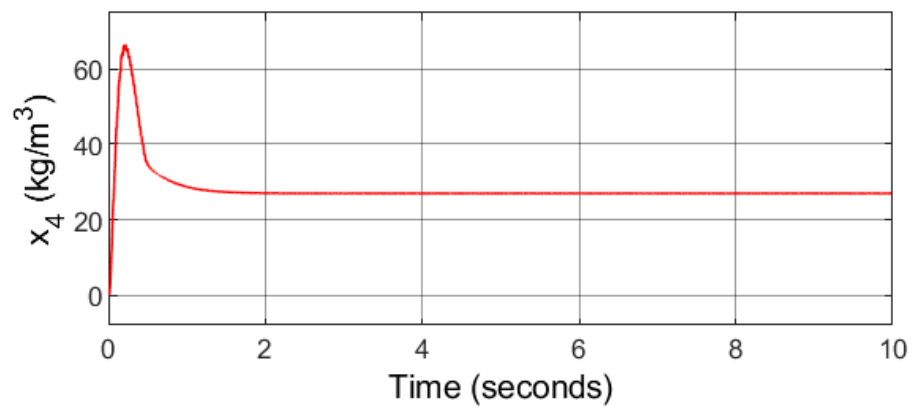


Figure 4.11: Mass concentration of death polymer chains.

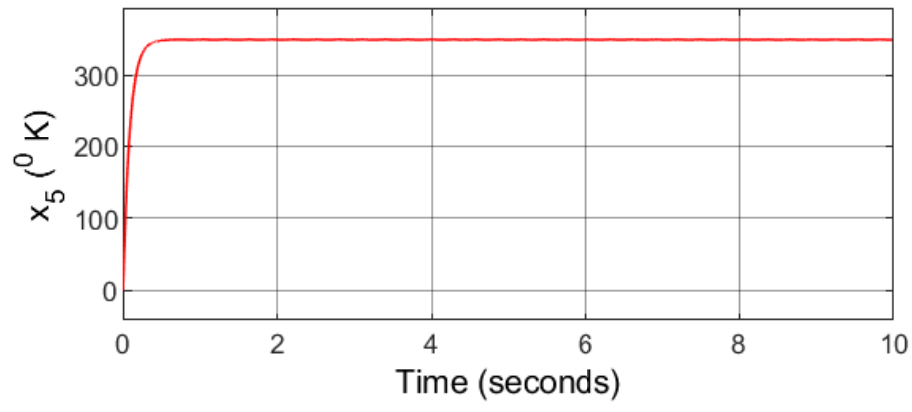


Figure 4.12: Reactor temperature.

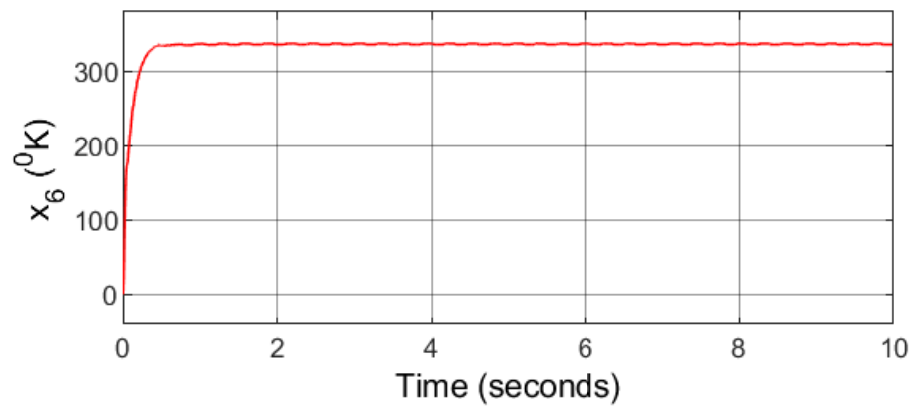


Figure 4.13: Coolant's temperature.

CHAPTER 5

NEURO-ADAPTIVE SLIDING MODE CONTROL

5.1 Introduction

In this chapter, a robust NN-SMC is deigned to force the monomer concentration ($M = \chi_1$) and the reactor temperature ($T = \chi_5$) to follow the desired trajectories in the presence of unknown disturbances. The unknown disturbances are estimated using an adaptive laws. Furthermore, the nonlinear functions of the reactor dynamics are approximated using NN. The performance of the NN-SMC is compared with that of PID controller.

5.2 Output dynamics

In this section, the input-output equations describing the dynamics of M and T are derived. The outputs are differentiated continuously with respect to time until the

inputs emerge. The first time-derivatives are thus

$$\begin{cases} \dot{M} = \frac{\partial M}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial M}{\partial \chi_2} \dot{\chi}_2 \\ \dot{T} = \frac{\partial T}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial T}{\partial \chi_2} \dot{\chi}_2 + \frac{\partial T}{\partial \chi_5} \dot{\chi}_5 + \frac{\partial T}{\partial \chi_6} \dot{\chi}_6 \end{cases} \quad (5.1)$$

Differentiating Equation. (5.1) with respect to time yields

$$\begin{cases} \ddot{M} = \frac{\partial(\dot{M})}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial(\dot{M})}{\partial \chi_2} \dot{\chi}_2 \\ \ddot{T} = \frac{\partial(\dot{T})}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial(\dot{T})}{\partial \chi_2} \dot{\chi}_2 + \frac{\partial(\dot{T})}{\partial \chi_5} \dot{\chi}_5 + \frac{\partial(\dot{T})}{\partial \chi_6} \dot{\chi}_6 \end{cases} \quad (5.2)$$

It is obvious that the inputs can be extracted from Equation. 5.2. So, the differentiation is stopped and hence each of the outputs has a relative degree of two. The input-output dynamics are as follows

$$\begin{cases} \ddot{M} = F_1(\chi) + G_1(\chi)u_1 \\ \ddot{T} = \bar{F}_2(\chi) + \bar{G}_2(\chi)u_1 + G_2(\chi)u_2 \end{cases} \quad (5.3)$$

Where:

$$\begin{aligned} F_1(\chi) &= \frac{\partial(\dot{M})}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial(\dot{M})}{\partial \chi_2} \left[-k_I \chi_2 + \frac{-F \chi_2}{v} \right] \\ \bar{F}_2(\chi) &= \frac{\partial(\dot{T})}{\partial \chi_1} \dot{\chi}_1 + \frac{\partial(\dot{T})}{\partial \chi_2} \left[-k_I \chi_2 + \frac{-F \chi_2}{v} \right] + \frac{\partial(\dot{T})}{\partial \chi_5} \dot{\chi}_5 \\ &\quad + \frac{\partial(\dot{T})}{\partial \chi_6} \left[\frac{-F \chi_6}{V_w} + \frac{U A}{\rho_w c_w v_w} (\chi_5 - \chi_6) \right] \\ G_1(\chi) &= \frac{C_I}{v} \frac{\partial(\dot{M})}{\partial \chi_2}, \quad \bar{G}_2(\chi) = \frac{\partial(\dot{T})}{\partial \chi_2} \frac{C_I}{v}, \quad G_2(\chi) = \frac{\partial(\dot{T})}{\partial \chi_6} \frac{T_w}{V_w} \end{aligned}$$

Therefore, the input-output dynamic equations Eq. (5.3), becomes a single-input-single-output as follows

$$\begin{cases} \ddot{M} = F_1(\chi) + G_1(\chi)U_1 + \Delta_1 \\ \ddot{T} = F_2(\chi) + G_2(\chi)U_2 + \Delta_2 \end{cases} \quad (5.4)$$

Where $F_2(\chi) = \bar{F}_2(\chi) + \bar{G}_2(\chi)u_1$, Δ_1 and Δ_2 represent lumped uncertainties/disturbances terms. For easier analysis and control design, Eq. (5.4), can be expressed as

$$\dot{\Pi}_1 = \Pi_2 \quad (5.5)$$

$$\dot{\Pi}_2 = F(\chi) + G(\chi)U + \Delta \quad (5.6)$$

Where

$$\begin{aligned} \Pi_1 &= \begin{bmatrix} M \\ T \end{bmatrix}, \quad \Pi_2 = \begin{bmatrix} \dot{M} \\ \dot{T} \end{bmatrix}, \quad F(\chi) = \begin{bmatrix} F_1(\chi) \\ F_2(\chi) \end{bmatrix} \\ U &= \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad \Delta = \begin{bmatrix} \Delta_1 \\ \Delta_2 \end{bmatrix}, \quad G(\chi) = \begin{bmatrix} G_1(\chi) & 0 \\ 0 & G_2(\chi) \end{bmatrix} \end{aligned}$$

5.3 Neuro-adaptive sliding mode control

In this section, robust sliding mode controllers are deigned to attracts the outputs trajectories towards their respective sliding surfaces. Once the outputs reach the

surfaces, they remained their (tracking error converge to zero) and become free from uncertainties/disturbances. Define the tracking error variables as

$$\begin{aligned} z_1 &= \Pi_1 - \Pi_{1d}, & \dot{z}_1 &= \dot{\Pi}_1 - \dot{\Pi}_{1d} = \Pi_2 - \dot{\Pi}_{1d} \\ z_2 &= \Pi_2 - \dot{\Pi}_{1d}, & \dot{z}_2 &= \dot{\Pi}_2 - \ddot{\Pi}_{1d} \end{aligned}$$

Where $z_1 = [z_{m1} \ z_{T1}]^T$, $z_2 = [z_{m2} \ z_{T2}]^T$ are the vectors of tracking errors and $\Pi_d = [M_d \ T_d]^T$ is the vector of the desired trajectory. The sliding surface is define as

$$S = z_2 + \lambda z_1 \quad (5.7)$$

Where

$$S = \begin{bmatrix} S_M \\ S_T \end{bmatrix}; \quad \lambda = \begin{bmatrix} \lambda_M & 0 \\ 0 & \lambda_T \end{bmatrix}$$

$\lambda_M > 0$, $\lambda_T > 0$, are design parameters. The convergence speed of the error trajectories is determined by the constant rate continuous reaching law.

$$\dot{S} = -KS = - \begin{bmatrix} k_M & 0 \\ 0 & k_T \end{bmatrix} \begin{bmatrix} S_M \\ S_T \end{bmatrix} \quad (5.8)$$

Where $k_M > 0$ $k_T > 0$ are chosen to compensate the disturbances in the system.

The error trajectories will remain on the surface as long as

$$S^T \dot{S} \leq 0 \quad (5.9)$$

The derivative of the sliding surface Eq. 5.7 yields

$$\begin{aligned} \dot{S} &= \dot{z}_2 + \lambda \dot{z}_1 = \ddot{\Pi}_2 - \ddot{\Pi}_{2d} + \lambda \dot{z}_1 \\ &= F(\chi) + \hat{G}(\chi)U + [G(\chi) - \hat{G}(\chi)]U + \Delta - \ddot{\Pi}_{2d} + \lambda \dot{z}_1 \end{aligned} \quad (5.10)$$

The tracking error trajectories converge and remain on the sliding surface $S = \dot{S} = 0$. The control laws to keep the trajectories always on the sliding surfaces are

$$U_{eqv} = -\hat{G}(\chi)^{-1} \left(\hat{F}(\chi) + \hat{\Delta} - \ddot{\Pi}_{2d} + \lambda \dot{z}_1 \right) \quad (5.11)$$

and the reaching laws for compensating the disturbances are

$$u_r = -\hat{G}(\chi)^{-1} K S \quad (5.12)$$

Therefore, the control laws for reaching and remaining on the surfaces are

$$u = u_{eqv} + u_r = -\hat{G}(\chi)^{-1} \left(\hat{F}(\chi) + \hat{\Delta} - \ddot{\Pi}_{2d} + \lambda \dot{z} + K S \right) \quad (5.13)$$

Where $\hat{F}(\chi)$, $\hat{G}(\chi)$ and $\hat{\Delta}$ are the estimates of $F(\chi)$, $G(\chi)$ and Δ respectively. Since $\det(G(\chi)) = G_1(\chi)G_2(\chi) \neq 0$, then $B^{-1}(\chi)$ exists.

5.3.1 NN approximation

The nonlinear functions $F(\chi)$ and $G(\chi)$ can be approximated by a feed forward NN in a compact set. The NN approximations for $F(\chi)$ and $G(\chi)$ are

$$\begin{cases} F(\chi) = V^T \phi(\chi) + \epsilon_F \\ G(\chi) = W^T \phi(\chi) + \epsilon_G \end{cases} \quad (5.14)$$

Where

$$\phi(\chi) = \frac{1}{1 + e^{-X}}$$

$X \in \mathcal{R}^n$ is the NN input vector, $\phi(.) : \mathcal{R}^n \rightarrow \mathcal{R}^L$ is a compact set activation function, $V_i, W \in \mathcal{R}^{L \times m}$ is the NN weight vector, $A(\chi_i), B(\chi_i) \in \mathcal{R}^m$ are the NN outputs, ϵ_F and ϵ_G are the NN bounded approximation errors.

The adaptive NN for the estimation of the nonlinear function can be written as

$$\hat{F}(\chi) = \hat{V}^T \phi(\chi); \quad \hat{G}(\chi) = \hat{W}^T \phi(\chi) \quad (5.15)$$

and the NN estimation errors are expressed as

$$\tilde{F}(\chi) = F(\chi) - \hat{F}(\chi) = \tilde{V}^T \phi(\chi) + \epsilon_F; \quad \tilde{G}(\chi) = G(\chi) - \hat{G}(\chi) = \tilde{W}^T \phi(\chi) + \epsilon_G \quad (5.16)$$

Where $\tilde{F}$ and $\tilde{G}$ are the NN function approximation errors, $\tilde{V} = V - \hat{V}$ and

$\tilde{W} = W - \hat{W}$ are the NN weight errors. Substituting Eq. (5.13) into Eq. (5.10) gives

$$\begin{aligned}
\dot{S} &= F - \hat{G}\hat{G}^{-1} \left(\hat{F} + \hat{\Delta} - \ddot{\Pi}_{2d} + \lambda\dot{z} + KS \right) + [G - \hat{G}]U + \Delta - \ddot{\Pi}_{2d} + \lambda\dot{z}_1 \\
&= \tilde{F} + \tilde{G}U + \tilde{\Delta} - KS \\
&= -KS + \tilde{V}^T \phi(\chi) + \epsilon_F + [\tilde{W}^T \phi(\chi) + \epsilon_G]U + \tilde{\Delta}
\end{aligned} \tag{5.17}$$

Theorem 5.1 *Consider the input-output system Eqs. (??)-(??), the sliding mode surface Eq. (5.7), the control input Eq. (5.13), and if the adaptation algorithms are*

$$\begin{cases} \dot{\hat{\Delta}} = \alpha S - \kappa_1 \alpha \|S\| \hat{\Delta} \\ \dot{\hat{V}} = S^T \gamma \phi(\chi) - \kappa_2 \gamma \|S\| \hat{V} \\ \dot{\hat{W}} = S^T \Gamma \phi(\chi) - \kappa_2 \Gamma \|S\| \hat{W} \end{cases} \tag{5.18}$$

with $\gamma = \gamma^T > 0$, $\Gamma = \Gamma^T > 0$, $\alpha = \alpha^T > 0$ are constant diagonal matrices, $\kappa_1 > 0$, $\kappa_2 > 0$. Then, S , $\tilde{\Delta}$, $\tilde{V}$, and $\tilde{W}$ are ultimately uniformly bounded.

Proof. Selecting a candidate Lyapunov function

$$L = \frac{1}{2} S^T S + \frac{1}{2\gamma} \tilde{V}^T \tilde{V} + \frac{1}{2\Gamma} \tilde{W}^T \tilde{W} + \frac{1}{2\alpha} \tilde{\Delta}^T \tilde{\Delta} \tag{5.19}$$

whose derivative is

$$\dot{L} = S^T \dot{S} - \gamma^{-1} \tilde{V}^T \dot{\tilde{V}} - \Gamma^{-1} \tilde{W}^T \dot{\tilde{W}} - \alpha^{-1} \tilde{\Delta}^T \dot{\tilde{\Delta}} \tag{5.20}$$

Note that $\dot{W} = \dot{V} = \dot{D} = 0$. Substituting Eq. (5.18) into Eq. (5.20) and noting that $\hat{V} = V - \tilde{V}$, $\hat{W} = W - \tilde{W}$ and $\hat{\Delta} = \Delta - \tilde{\Delta}$

$$\begin{aligned}
\dot{L} &\leq -S^T K S + S^T [\epsilon_F + \epsilon_C U] + \kappa_2 \|S\| \tilde{V}^T \hat{V} + \kappa_2 \|S\| \tilde{W}^T \hat{W} + \kappa_1 \|S\| \tilde{\Delta} \Delta \\
&\leq -S^T K S + S^T [\epsilon_F + \epsilon_C U] + \kappa_1 \|S\| \tilde{\Delta} (\Delta - \tilde{\Delta}) \\
&\quad + \kappa_2 \|S\| \tilde{V}^T (V - \tilde{V}) + \kappa_2 \|S\| \tilde{W}^T (W - \tilde{W}) \\
&\leq -K \|S\|^2 + \|S\| [\epsilon_F + \epsilon_C U] - \kappa_1 \|S\| (\|\tilde{\Delta}\|^2 - \|\tilde{\Delta}\| \Delta) \\
&\quad - \kappa_2 \|S\| \left[(\|\tilde{V}\|^2 - \|\tilde{V}\| V) + (\|\tilde{W}\|^2 - \|\tilde{W}\| W) \right] \tag{5.21}
\end{aligned}$$

Completing the squares in Eq. (5.21) result in

$$\begin{aligned}
\dot{L} &\leq -\kappa_2 \|S\| \left[\left(\|\tilde{V}\| - \frac{V}{2} \right)^2 + \left(\|\tilde{W}\| - \frac{W}{2} \right)^2 \right] \\
&\quad - \kappa_1 \|S\| \left(\|\tilde{\Delta}\| - \frac{\Delta}{2} \right)^2 \\
&\quad - \|S\| \left[K \|S\| - \frac{\kappa_2 W^2}{4} - \frac{\kappa_2 V^2}{4} - \frac{\Delta^2}{4} - (\epsilon_F + \epsilon_C U) \right] \tag{5.22}
\end{aligned}$$

Therefore, $\dot{L} \leq 0$ if and only if

$$\|S\| > \frac{\kappa_2 W^2}{4K} + \frac{\kappa_2 V^2}{4K} + \frac{\kappa_1 \Delta^2}{4K} + \frac{\epsilon_F + \epsilon_C U}{K} \equiv \mu_s \tag{5.23}$$

Selecting appropriate K guarantees that the compact set given by $\|S\| \leq \mu_s$ is bounded. Hence, the approximation property is valid throughout and ensures the uniformly ultimate bound for $\|S\|$, $\|\tilde{W}\|$, $\|\tilde{V}\|$, and $\|\tilde{\Delta}\|$. ■

5.4 PID controller

The controller is designed as follows: $u_1 = K_{p1}(A_1 - A_d) + K_{d1}(\dot{A}_1 - \dot{A}_d) + K_{i1} \int (A_1 - A_d)dt$, $u_2 = K_{p2}(T_1 - T_d) + K_{d2}(\dot{T}_1 - \dot{T}_d) + K_{i2} \int (T_1 - T_d)dt$.

5.5 Simulation results and discussions

The controller parameters are $\lambda_M = 25$, $\lambda_T = 30$, $K_M = 14$, $K_T = 20$ and the desired trajectories are $M_d = 5 \text{ kmol/m}^3$ and $T_d = 350^\circ \text{K}$. The parameters of the adaptive disturbance estimator are $\alpha_M = \alpha_T = 0.2$. The constant input disturbances are $\Delta_1 = 1$ and $\Delta_2 = 70$. The NN tuning parameters are $\gamma_M = \Gamma_M = 0.01$, $\gamma_T = 0.125$, $\Gamma_T = 0.01$, $\kappa = 0.01$ and the number of nodes of the hidden layer $L = 10$.

The simulation results are presented in Figs. 5.1-5.10. The outputs, M and T, have satisfactorily traced the desired trajectories with short settling time and no overshoot under the action NN-SMC as shown in Fig. 5.1. The tracking errors converged to zero faster under NN-SMC than PID as depicted in Fig. 5.2. The control inputs are smoother and settle faster under the action of NN-SMC as shown in Fig. 5.3. The sliding mode surfaces are shown in Fig. 5.4. The states' responses of the process are shown in Figs. 5.5-5.10.

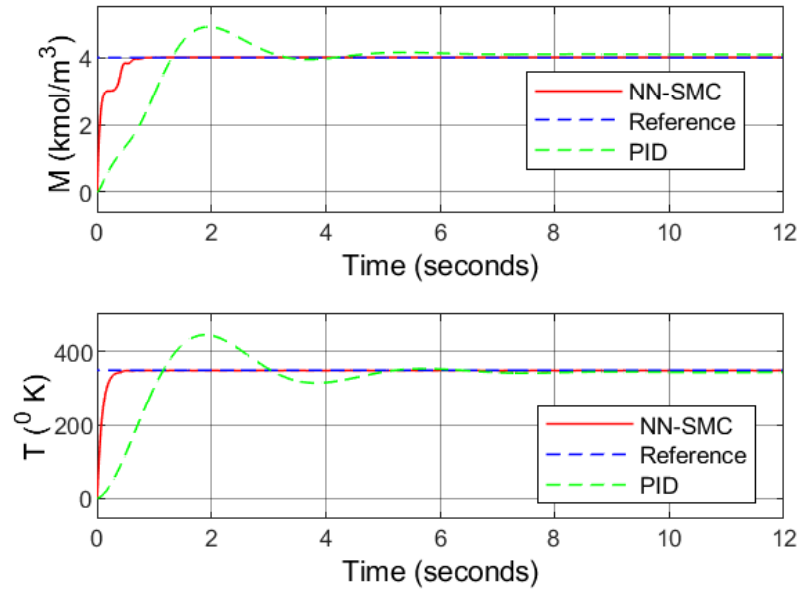


Figure 5.1: Monomer concentration (above) and reactor temperature (below)

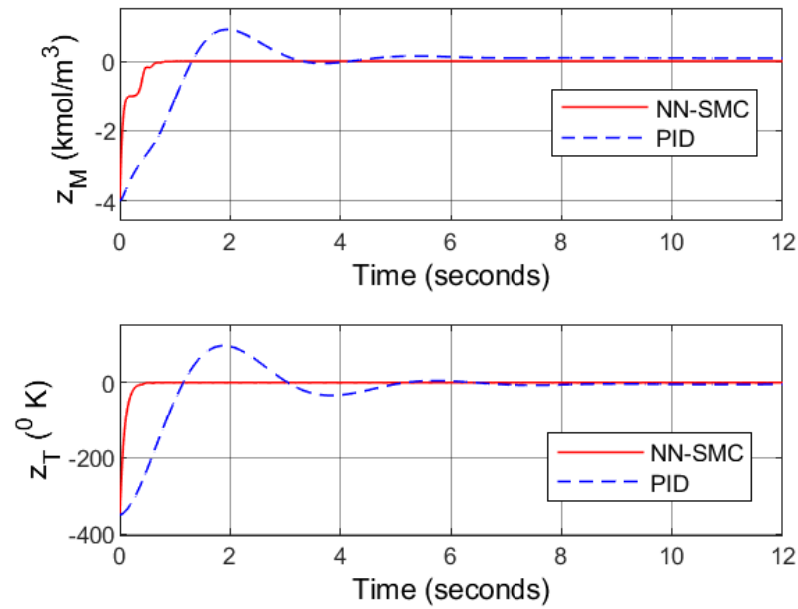


Figure 5.2: Monomer concentration tracking error (top) and the reactor temperature tracking error (below)

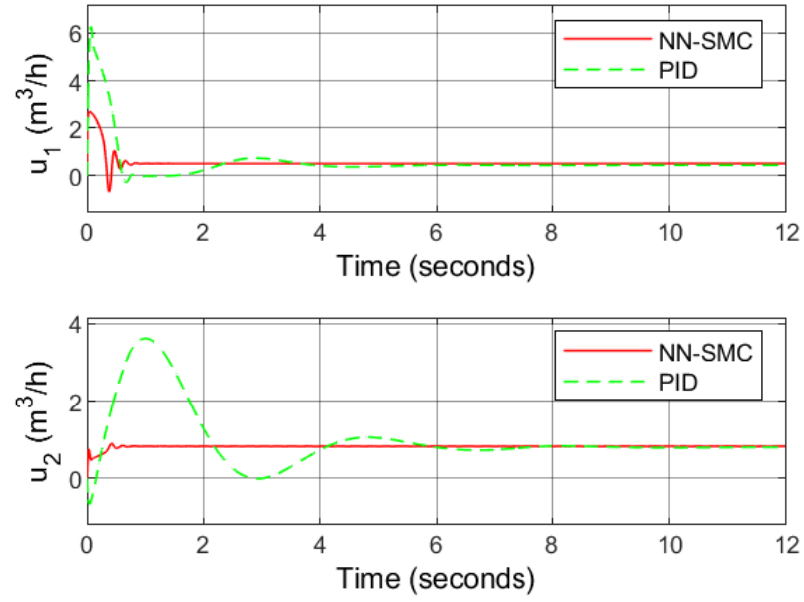


Figure 5.3: The initiator flow rate (above) and the coolant flow rate (below)

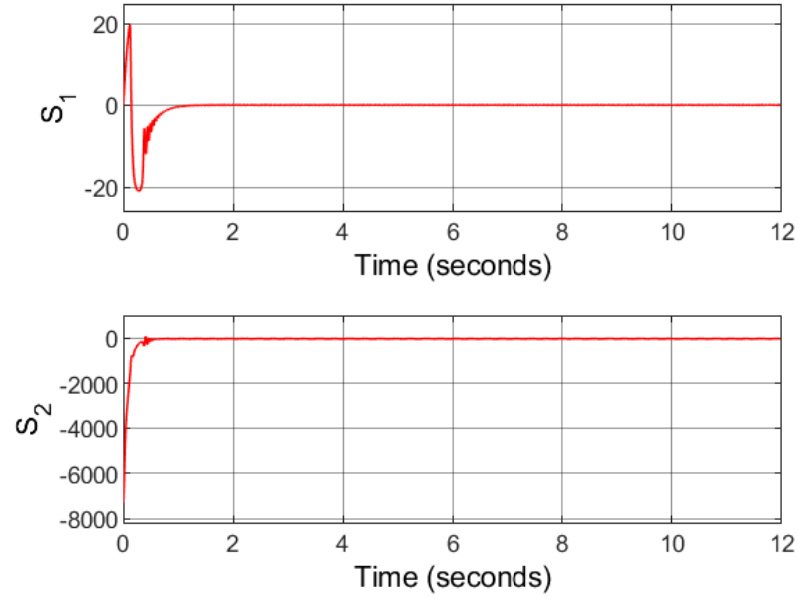


Figure 5.4: Fast terminal sliding surfaces

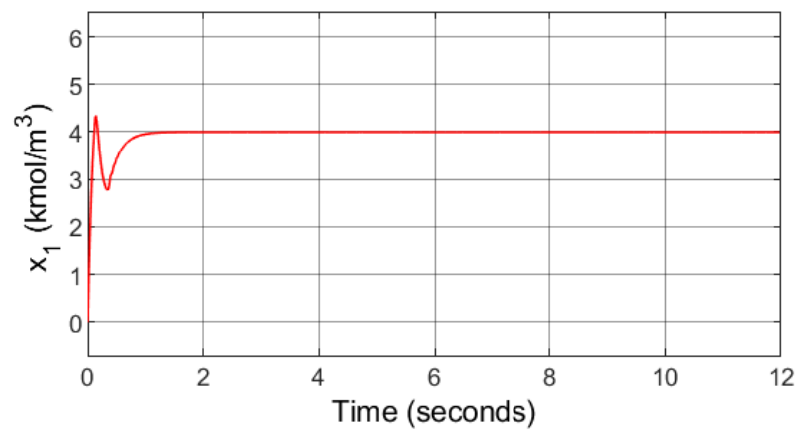


Figure 5.5: The monomer concentration

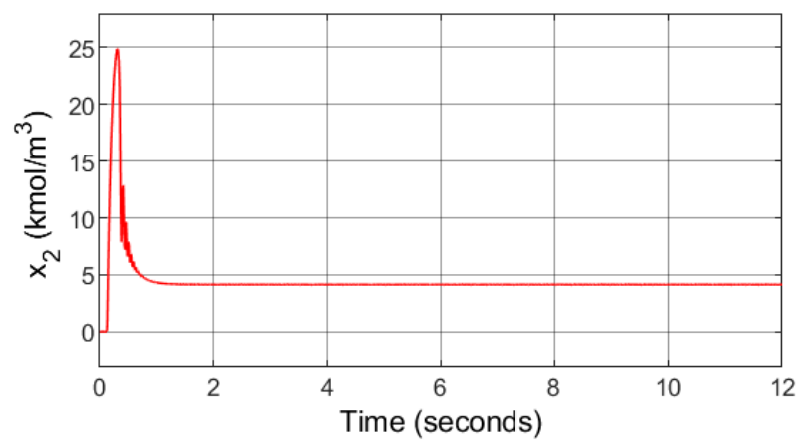


Figure 5.6: Initiator concentration

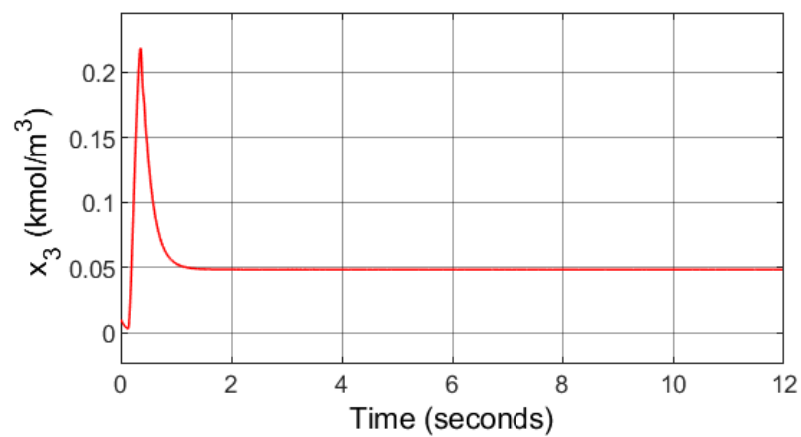


Figure 5.7: Molar concentration of death polymer chains.

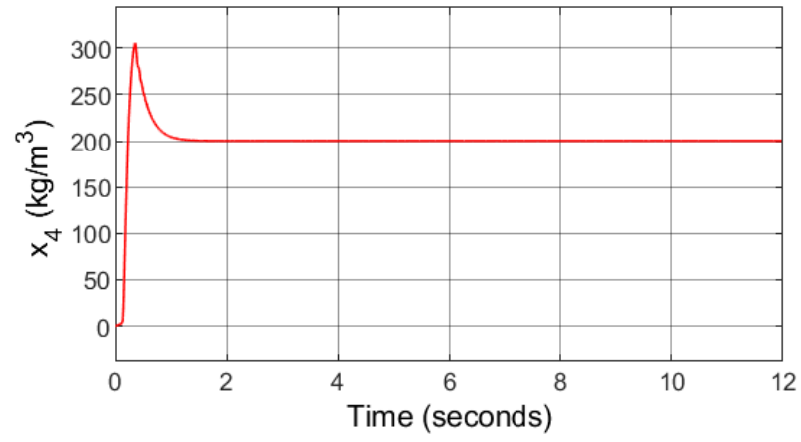


Figure 5.8: Mass concentration of death polymer chains.

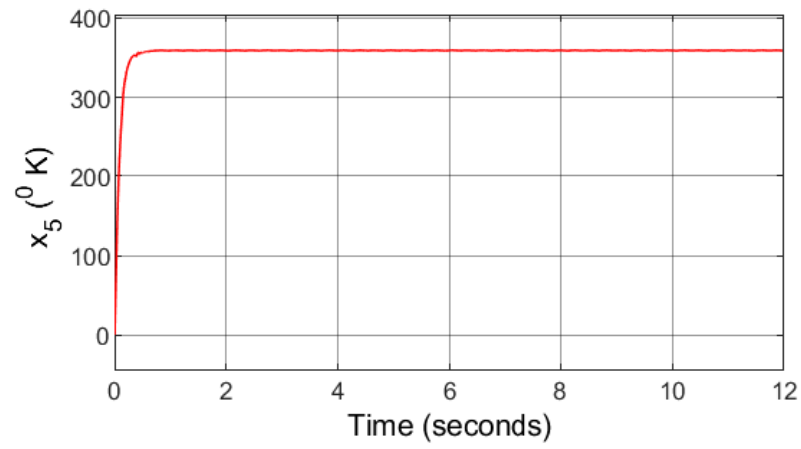


Figure 5.9: Reactor temperature.

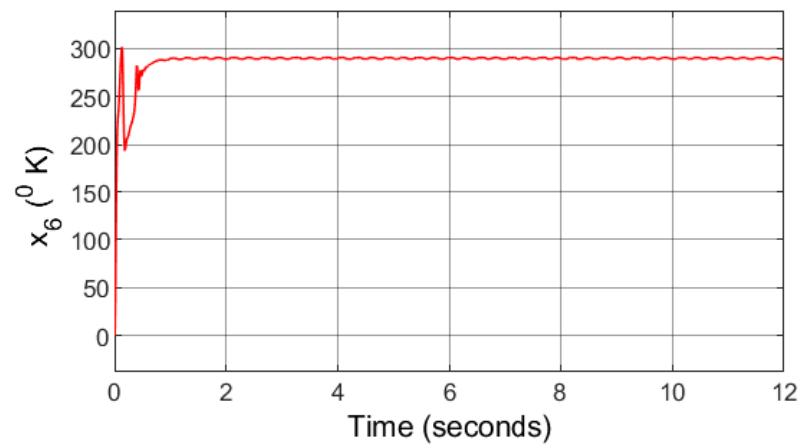


Figure 5.10: Coolant's temperature.

CHAPTER 6

NEURO-ADAPTIVE OUTPUT FEEDBACK CONTROL

6.1 Introduction

In this chapter, NNFC is developed to control the average molecular weight of the polymer ($y_1 = x_4/x_3$) and the reactor temperature ($y_2 = x_5$). The performance of the NNFC is compared with that of PID controller in order to validate its efficacy.

6.2 Output feedback control

The outputs of the system are differentiated several times until the inputs emerge. The inputs are selected to derive the outputs to track the desired trajectory in finite time. The desired trajectory vector is given by:

$$y_d = \begin{bmatrix} y_{id} & \dot{y}_{id} & \ddot{y}_{id} \end{bmatrix}^T \quad (i = 1, 2) \quad (6.1)$$

Lemma 6.1 [68] *For any real number $\varrho_1 > 0$, $\varrho_2 > 0$, $0 < m \leq 1$, if there exists a continuous positive definite function meeting the inequality,*

$$\dot{L} \leq -\varrho_1 L^m + \varrho_2 \quad (6.2)$$

then, the equilibrium point is semi-globally finite time stable.

Lemma 6.2 [69] *On the otherhand, if the following inequality is satisfied*

$$\dot{L} \leq -\varrho_1 L + \varrho L_2^n \quad (6.3)$$

with $0 < n < 1$, then, the equilibrium point is globally finite time stable.

Define the output tracking error vector as:

$$\begin{bmatrix} z_i \\ \dot{z}_i \\ \ddot{z}_i \end{bmatrix} = \begin{bmatrix} y_i - y_{id} \\ \dot{y}_i - \dot{y}_{id} \\ \ddot{y}_i - \ddot{y}_{id} \end{bmatrix}, \quad (i = 1, 2) \quad (6.4)$$

The time-derivatives of the outputs are

$$\begin{cases} \dot{y}_1 = \frac{\partial y_1}{\partial x_3} \dot{x}_3 + \frac{\partial y_1}{\partial x_4} \dot{x}_4 \\ \dot{y}_2 = \frac{\partial y_2}{\partial x_3} \dot{x}_3 \end{cases} \quad (6.5)$$

he time derivative of Eq. (6.5) yields

$$\begin{cases} \ddot{y}_1 = \frac{\partial(\dot{y}_1)}{\partial x_1} \dot{x}_1 + \frac{\partial(\dot{y}_1)}{\partial x_2} \dot{x}_2 + \frac{\partial(\dot{y}_1)}{\partial x_3} \dot{x}_3 + \frac{\partial(\dot{y}_1)}{\partial x_4} \dot{x}_4 \\ \ddot{y}_2 = \frac{\partial(\dot{y}_2)}{\partial x_1} \dot{x}_1 + \frac{\partial(\dot{y}_2)}{\partial x_2} \dot{x}_2 + \frac{\partial(\dot{y}_2)}{\partial x_5} \dot{x}_5 + \frac{\partial(\dot{y}_2)}{\partial x_6} \dot{x}_6 \end{cases} \quad (6.6)$$

The input-output dynamic equations are thus

$$\ddot{y}_1 = F_1(x) + G_1(x)u_1 + D_1 \quad (6.7)$$

$$\ddot{y}_2 = F_0(x) + G_0(x)u_1 + G_2(x)u_2 + D_2 \quad (6.8)$$

Where D_1 and D_2 are lumped disturbances terms

$$\begin{aligned} F_1(x) &= \frac{\partial(\dot{y}_1)}{\partial x_1} \left[-(k_p + k_{fm})P_0x_1 + \frac{-Fx_2}{V} \right] \\ &\quad + \frac{\partial(\dot{y}_1)}{\partial x_2} \left[-k_Ix_2 + \frac{-Fx_2}{V} \right] + \frac{\partial(\dot{y}_1)}{\partial x_3} \dot{x}_3 + \frac{\partial(\dot{y}_1)}{\partial x_4} \dot{x}_4 \\ F_0(x) &= \frac{\partial(\dot{y}_2)}{\partial x_1} \left[-(k_p + k_{fm})P_0x_1 + \frac{-Fx_2}{V} \right] \\ &\quad + \frac{\partial(\dot{y}_2)}{\partial x_2} \left[-k_Ix_2 + \frac{-Fx_2}{V} \right] + \\ &\quad \frac{\partial(\dot{y}_2)}{\partial x_5} \left[k_p \frac{(-\Delta H_p)}{\rho c_p} x_1 P_0 - \frac{UA}{\rho c_p v} (x_5 - x_6) + \frac{F(-x_5)}{V} \right] \\ &\quad + \frac{\partial(\dot{y}_2)}{\partial x_6} \left[\frac{-Fx_6}{V_w} + \frac{UA}{\rho_w c_w V_w} (x_5 - x_6) \right] \\ G_1(x) &= \frac{C_I}{V} \frac{\partial(\dot{y}_1)}{\partial x_2} \quad G_2(x) = \frac{\partial(\dot{y}_2)}{\partial x_6} \frac{T_w}{V_w}, \quad G_0(x) = \frac{\partial(\dot{y}_2)}{\partial x_2} \frac{C_I}{V}, \\ \delta_1 &= \frac{\partial(\dot{y}_1)}{\partial x_1} \frac{FC_m}{V}, \quad \delta_0 = \frac{\partial(\dot{y}_2)}{\partial x_1} \frac{FC_m}{V} + \frac{\partial(\dot{y}_2)}{\partial x_5} \frac{F(T_{in})}{V} \end{aligned}$$

$$u_1 = F_I, \quad u_2 = F_w$$

Assumption 1. The lumped disturbances are bounded by

$$|D_i| \leq \delta_i, \quad (i = 1, 2) \quad (6.9)$$

Where δ_i is the upper bound of the disturbances. The upper bound is expressed as [69]

$$\delta_i = b_{0i} + b_{1i}|z_i| + b_{2i}|\dot{z}_i| \quad (6.10)$$

Where b_{0i} , b_{1i} and b_{2i} are all positive numbers.

6.2.1 Robust control of Average molecular weight

The average molecular weight filtered error is defined as

$$\varsigma_1 = \dot{z}_1 + \lambda_1 z_1 \quad (6.11)$$

Where $\lambda_1 > 0$ is a design constant. The time derivative of ς_1 yields

$$\dot{\varsigma}_1 = F_1(x) + G_1(x)u_1 + D_1 - \ddot{y}_{1d} + \lambda_1 \dot{z}_1 \quad (6.12)$$

Setting $\dot{\varsigma}_1 = 0$, the equivalent control input is obtained as

$$u_{eq1} = \frac{1}{G_1}[-F_1 + \ddot{y}_{1d} - \lambda_1 \dot{z}_1] \quad (6.13)$$

The robust control input $u_r = G_1^{-1}(x)[-K_1\varsigma_1 - c_1 \text{sign}(\varsigma_1)]$ is added to the equivalent control input in order to achieve robust performances against disturbances, where c_1 and K_1 denote the robust gains. The proper value of c_1 is selected as [46]: $c_1 = \delta_1 + \vartheta_1$, where $\vartheta_1 > 0$. Therefore, the control law is designed as

$$\begin{aligned} u_1 = & u_{eq1} + u_{r1} \\ & G^{-1}(x)[-F_1 + \ddot{y}_{1d} - \lambda_1 \dot{z}_1 - K_1\varsigma_1 \\ & - (b_{01} + b_{11}|z_i| + b_{21}|\dot{z}_i| + \vartheta_1)\text{sign}(\varsigma_1)] \end{aligned} \quad (6.14)$$

Theorem 1. Consider the subsystem (6.7) in which the lumped disturbance satisfies the bound (6.9). If the filtered error surface is designed as (6.11) and the control input is designed as (6.12), then the tracking error converges to zero in finite time.

Proof. The following Lyapunov function candidate is chosen

$$L_1 = \frac{1}{2}\varsigma_1^2 \quad (6.15)$$

Differentiating V_1 with respect to time and substituting (6.12) gives

$$\begin{aligned} \dot{L}_1 = & \varsigma_1 \dot{\varsigma}_1 = \varsigma_1 [D_1 - K_1\varsigma_1 - (\delta_1 + \vartheta_1)\text{sign}(\varsigma_1)] \\ \leq & [|\varsigma_1 D_1| - K_1\varsigma_1^2 - (\delta_1 + \vartheta_1)|\varsigma_1|] \\ = & (|D_1| - \delta_1)|\varsigma_1| - K_1\varsigma_1^2 - \vartheta_1|\varsigma_1| \end{aligned} \quad (6.16)$$

Using (6.9), we can have

$$\begin{aligned}\dot{L}_1 &\leq -K_1\varsigma_1^2 - \vartheta_1|\varsigma_1| \\ &\leq -\sigma_1 L_1 - \sigma_2 L_1^{1/2}\end{aligned}\tag{6.17}$$

Where $\sigma_1 = 2K_1 > 0$, $\sigma_2 = \sqrt{2}\vartheta_1$. Based on Lemma 6.2, the system is finite time stable.

6.2.2 Robust control of reactor temperature

Substituting the control input, u_1 , from (6.12) into the temperature subsystem (6.8) yields

$$\ddot{y}_2 = F_2(x) + G_2(x)u_2 + D_2\tag{6.18}$$

Where

$$\begin{aligned}F_2(x) &= F_0(x) + \frac{G_0(x)}{G_1(x)}[-F_1 + \ddot{y}_{1d} - \lambda_1 \dot{z}_1 - K_1 \varsigma_1 \\ &\quad - (c_1 + \vartheta_1) \text{sign}(\varsigma_1)]\end{aligned}$$

Define the reactor temperature filtered error as

$$\varsigma_2 = \dot{z}_2 + \lambda_2 z_2\tag{6.19}$$

Where $\lambda_2 > 0$ is a design constant. The time derivative of ς_2 gives

$$\dot{\varsigma}_2 = F_2(x) + G_2(x)u_2 + D_2 - \ddot{y}_{2d} + \lambda_2 \dot{z}_2 \quad (6.20)$$

By setting $\dot{x}i_2 = 0$, the equivalent control law is computed as

$$u_{eq2} = \frac{1}{G_2}[-F_2 + \ddot{y}_{1d} - \lambda_2 \dot{z}_2] \quad (6.21)$$

In order to compensate the lumped disturbances, the robust control input is given by

$$u_{r2} = G_2^{-1}(x)[-K_2\varsigma_2 - c_2\text{sign}(\varsigma_2)] \quad (6.22)$$

Where $c_2 = \delta_2 + \vartheta_2$, $k_2 > 0$, and $\vartheta_2 > 0$ is a small constant. $u_{r2} = G_2^{-1}(x)[-K_2\varsigma_2 - c_2\text{sign}(\varsigma_2)]$ is added to the equivalent control input, where c_2 and K_2 denote the robust gains. The proper value of c_2 is selected as [46]: $c_2 = \delta_2 + \vartheta_2$, where $\vartheta_2 > 0$. Therefore, the AMW control law is designed as

$$\begin{aligned} u_2 = & u_{eq2} + u_{r2} \\ & G_2^{-1}(x)[-F_2 + \ddot{y}_{2d} - \lambda_2 \dot{z}_2 - K_2\varsigma_2 \\ & - (b_{02} + b_{12}|z_2| + b_{22}|\dot{z}_2| + \vartheta_2)\text{sign}(\varsigma_2)] \end{aligned} \quad (6.23)$$

Theorem 2. Consider the reactor temperature subsystem (6.7) in which the

lumped disturbance satisfies the bound (6.9). If the filtered error surface is designed as (6.11) and the control input is designed as (6.12), then the tracking error converge to zero in finite time.

Proof. The following Lyapunov function candidate is selected

$$L_2 = \frac{1}{2}\varsigma_2^2 \quad (6.24)$$

Differentiating V_2 with respect to time and substituting (6.12) yields

$$\begin{aligned} \dot{L}_2 &= \varsigma_2 \dot{\varsigma}_2 = \varsigma_2 [D_2 - K_2 \varsigma_2 - (\delta_2 + \vartheta_2) \text{sign}(\varsigma_2)] \\ &\leq [|D_2| |\varsigma_2| - K_2 \varsigma_2^2 - (\delta_2 + \vartheta_2) |\varsigma_2|] \\ &= (|D_2| - \delta_2) |\varsigma_2| - K_2 \varsigma_2^2 - \vartheta_2 |\varsigma_2| \end{aligned} \quad (6.25)$$

Using (6.9), we can have

$$\begin{aligned} \dot{L}_2 &\leq -K_2 \varsigma_2^2 - \vartheta_2 |\varsigma_2| \\ &\leq -\sigma_2 V_2 - \sigma_2 V_2^{1/2} \end{aligned} \quad (6.26)$$

Where $\sigma_2 = 2K_2 > 0$, $\sigma_2 = \sqrt{2}\vartheta_2$. Based on Lemma 6.2, the system is finite time stable.

Remark 1. In practical applications, it is difficult to know the exact upper bounds of the disturbances. Therefore, it is essential to estimate the upper bounds online using adaptive laws. Furthermore, due to aging and changing operating conditions, the

parameters of the chemical processes are changing continuously. However, adaptive laws cannot be used to estimate them because $F_i(x)$ and $G_i(x)$ ($i=1,2$) are nonlinear in the parameters. As such, NNs will be used to approximate them online.

6.3 Adaptive output feedback control

This section presents adaptive output feedback control in order to estimate the upper bounds, δ_i . Moreover, the nonlinear functions $F_i(x)$ and $G_i(x)$ ($i=1,2$) are approximated with NN. Hence, the adaptive control law can be expressed as

$$u_i = \hat{G}_i^{-1}(x) [-\hat{F}_i + \ddot{y}_{id} - \lambda_i \dot{z}_i - K_2 \varsigma_2 - (\hat{b}_{0i} + \hat{b}_{1i}|z_i| + \hat{b}_{2i}|\dot{z}_i| + \vartheta_i) \text{sign}(\varsigma_2)], \quad (i = 1, 2) \quad (6.27)$$

Where $\hat{F}_i$ and $\hat{G}_i$ are the estimate of F_i and G_i respectively, $\hat{b}_{0i}$, $\hat{b}_{1i}$ and $\hat{b}_{2i}$ are the estimate of b_{0i} , b_{1i} and b_{2i} respectively.

6.3.1 NN approximation

The nonlinear function $F_i(x)$ and $G_i(x)$ can be approximated by a feedforward NN in a compact set as

$$\begin{cases} F_i(X_i) = V_i^T \beta_i(X_i) + \epsilon_{fi} \\ G_i(X_i) = W_i^T \beta_i(X_i) + \epsilon_{gi} \end{cases} \quad (6.28)$$

Where

$$\beta_i(X_i) = \frac{1}{1 + e^{X_i}}, \quad (i = 1, 2)$$

$X_i \in \mathbb{R}^n$ is the NN input vector, $\beta_i(\cdot) : \mathbb{R}^n \rightarrow \mathbb{R}^L$ is a compact set activation function, $V_i, W_i \in \mathbb{R}^{L \times m}$ is the NN weight vector, $F_i(X_i), G_i(X_i) \in \mathbb{R}^m$ are the outputs, ϵ_{fi} and ϵ_{gi} are the NN approximation errors.

Assumption 2. The NN approximation errors and the weight vectors are bounded by known bounds respectively in a compact basis set.

$$\begin{cases} \|\epsilon_{fi}\| < \epsilon_{fmi}, & \|V_i\|, < V_{fi} \\ \|\epsilon_{gi}\| < \epsilon_{gmi}, & \|W_i\|, < V_{gi} \end{cases} \quad (6.29)$$

The adaptive NNs for the estimation of $F_i(X)$ and $G_i(X)$ can be written as

$$\begin{cases} \hat{F}_i(X_i) = \hat{V}_i^T \beta_i(X_i) \\ \hat{G}_i(X_i) = \hat{W}_i^T \beta_i(X_i) \end{cases} \quad (6.30)$$

and the NN estimation errors are expressed as

$$\begin{cases} \tilde{F}_i(X) = F_i(X) - \hat{F}_i(X) = \tilde{V}_i^T \beta_i(X_i) + \epsilon_{fi} \\ \tilde{G}_i(X) = G_i(X) - \hat{G}_i(X) = \tilde{W}_i^T \beta_i(X_i) + \epsilon_{gi} \end{cases} \quad (6.31)$$

Where $\tilde{V}_i = V_i - \hat{V}_i$ and $\tilde{W}_i = W_i - \hat{W}_i$. . Using (6.12), (6.9) becomes

The derivative of the filtered error surface can be rewritten as

$$\begin{aligned}\dot{\varsigma}_i &= F_i(X) + \hat{G}_i(X)u_i + [G_i(X) - \hat{G}_i(X)]u_i - \ddot{y}_{id} + \lambda_i z_i \\ &= F_i(X) + \hat{G}_i(X)u_i + \tilde{G}_i(X)u_i - \ddot{y}_{id} + \lambda_i z_i, \quad (i = 1, 2)\end{aligned}\quad (6.32)$$

Substituting (6.27) into (6.32) gives

$$\begin{aligned}\dot{\varsigma}_i &= \tilde{F}_i(X) + \tilde{G}_i(X)u_i - K_i \varsigma_i + D_i - (\hat{b}_{0i} + \hat{b}_{1i}|z_i| + \hat{b}_{2i}|\dot{z}_i| + \vartheta_i) \text{sign}(\varsigma_i)] \\ &= \tilde{V}_i^T \beta_i(X_i) + \epsilon_{fi} + [\tilde{W}_i^T \beta_i(X_i) + \epsilon_{gi}]u_i - K_i \varsigma_i \\ &\quad + D_i - (\hat{b}_{0i} + \hat{b}_{1i}|z_i| + \hat{b}_{2i}|\dot{z}_i| + \vartheta_i) \text{sign}(\varsigma_i)], \quad (i = 1, 2)\end{aligned}\quad (6.33)$$

Theorem 3. Consider system (6.8), the control input (6.12), and the filtered error surfaces (6.19) and (6.11). If the adaptation laws are designed as

$$\left\{ \begin{aligned}\dot{\hat{V}}_i &= \gamma_{1i}[\varsigma_i \beta_i(X_i) - \kappa \hat{V}_i] \\ \dot{\hat{W}}_i &= \gamma_{2i}[\varsigma_i \beta_i(X_i)u_i - \kappa \hat{W}_i] \\ \dot{\hat{b}}_{0i} &= \alpha_{0i}[\varsigma_i - \kappa \hat{b}_{0i}] \\ \dot{\hat{b}}_{1i} &= \alpha_{1i}[\varsigma_i |z_i| - \kappa \hat{b}_{1i}] \\ \dot{\hat{b}}_{2i} &= \alpha_{2i}[\varsigma_i |\dot{z}_i| - \kappa \hat{b}_{2i}]\end{aligned} \right. \quad (6.34)$$

with $\gamma_{1i} = \gamma_{1i}^T > 0$, $\gamma_{2i} = \gamma_{2i}^T > 0$ and $\kappa > 0$ is a small constant. Then, the NN weight estimation errors $\tilde{V}_i$ & $\tilde{W}_i$, and tracking error z_i are ultimately uniformly bounded in a small compact set in the neighborhood of the origin.

Proof. Consider the following Lyapunov function

$$\begin{aligned}
L_i = & \frac{\varsigma_i^2}{2} + \frac{\tilde{b}_{0i}^2}{2\alpha_{0i}} + \frac{\tilde{b}_{1i}^2}{2\alpha_{1i}} + \frac{\tilde{b}_{2i}^2}{2\alpha_{2i}} \\
& + \tilde{V}_i^T \tilde{V}_i + \frac{1}{2\gamma_{2i}} \tilde{W}_i^T \tilde{W}_i
\end{aligned} \tag{6.35}$$

Differentiating V_i with respect to time gives

$$\begin{aligned}
\dot{L}_i = & \varsigma_i \dot{\varsigma}_i - \frac{\tilde{b}_{0i} \dot{\tilde{b}}_{0i}}{\alpha_{0i}} - \frac{\tilde{b}_{1i} \dot{\tilde{b}}_{1i}}{\alpha_{1i}} - \frac{\tilde{b}_{2i} \dot{\tilde{b}}_{2i}}{\alpha_{2i}} \\
& - \frac{\tilde{V}_i^T \dot{\tilde{V}}_i}{\gamma_{1i}} - \frac{\tilde{W}_i^T \dot{\tilde{W}}_i}{\gamma_{2i}}
\end{aligned} \tag{6.36}$$

Using (6.33), we have

$$\begin{aligned}
\dot{L}_i \leq & -K_i \varsigma_i^2 + [\varsigma_i D_i - (b_{0i} + b_{1i}|z_i| + b_{2i}|\dot{z}_i|)|\varsigma_i|] \\
& - \vartheta_i |\varsigma_2| + \tilde{b}_{0i} \left[\varsigma_i - \frac{\dot{\tilde{b}}_{0i}}{\alpha_{0i}} \right] + \tilde{b}_{1i} \left[\varsigma_i |z_i| - \frac{\dot{\tilde{b}}_{1i}}{\alpha_{1i}} \right] \\
& + \tilde{b}_{2i} \left[\varsigma_i |\dot{z}_i| - \frac{\dot{\tilde{b}}_{2i}}{\alpha_{2i}} \right] + \tilde{V}_i^T \left[\varsigma_i \beta_i(X_i) - \frac{\dot{\tilde{V}}_i}{\gamma_{1i}} \right] \\
& + \tilde{W}_i^T \left[\varsigma_i \beta_i(X_i) - \frac{\dot{\tilde{W}}_i}{\gamma_{2i}} \right]
\end{aligned} \tag{6.37}$$

From (6.9) and the adaptive laws (6.34), (6.37) becomes

$$\begin{aligned}
\dot{L}_i \leq & -K_i \varsigma_i^2 - \vartheta_i |\varsigma_2| + \kappa \tilde{b}_{0i} \hat{b}_{0i} + \kappa \tilde{b}_{1i} \hat{b}_{1i} + \kappa \tilde{b}_{2i} \hat{b}_{2i} \\
& + \kappa \tilde{V}_i^T \hat{V}_i + \kappa \tilde{W}_i^T \hat{W}_i
\end{aligned} \tag{6.38}$$

Based on the following Young's inequalities,

$$\left\{ \begin{array}{l} \tilde{b}_{0i}\hat{b}_{0i} = \tilde{b}_{0i}[b_{0i} - \tilde{b}_{0i}] \leq \frac{b_{0i}^2}{2} - \frac{\tilde{b}_{0i}^2}{2} \\ \tilde{b}_{1i}\hat{b}_{1i} \leq \frac{b_{1i}^2}{2} - \frac{\tilde{b}_{1i}^2}{2}, \quad \tilde{b}_{2i}\hat{b}_{2i} \leq \frac{b_{2i}^2}{2} - \frac{\tilde{b}_{2i}^2}{2} \\ \tilde{V}_i^T \hat{V}_i \leq \frac{V_i^2}{2} - \frac{\tilde{V}_i^2}{2}, \quad \tilde{W}_i^T \hat{W}_i \leq \frac{W_i^2}{2} - \frac{\tilde{W}_i^2}{2} \\ \vartheta_i |\varsigma_i| \leq \frac{\vartheta_i^2}{2} + \frac{|\varsigma_i|^2}{2} \end{array} \right. \quad (6.39)$$

Equation (6.38) becomes

$$\begin{aligned} \dot{L}_i &\leq - (K_i - 1/2)\varsigma_i^2 - \frac{\tilde{b}_{0i}^2}{2} - \frac{\tilde{b}_{1i}^2}{2} - \frac{\tilde{b}_{2i}^2}{2} - \frac{\tilde{V}_i^2}{2} - \frac{\tilde{W}_i^2}{2} \\ &\quad + \frac{b_{0i}^2}{2} + \frac{b_{1i}^2}{2} + \frac{b_{2i}^2}{2} + \frac{V_i^2}{2} + \frac{W_i^2}{2} - \frac{\vartheta_i^2}{2} \\ &\leq - \varrho_{1i} V_i + \varrho_{2i} \end{aligned} \quad (6.40)$$

Where $\varrho_{1i} = \min\{(K_i - 1/2), \alpha_{0i}, \alpha_{1i}, \alpha_{2i}, \gamma_{1i}, \gamma_{2i}\}$, $\varrho_{2i} = \frac{b_{0i}^2}{2} + \frac{b_{1i}^2}{2} + \frac{b_{2i}^2}{2} + \frac{V_i^2}{2} + \frac{W_i^2}{2} - \frac{\vartheta_i^2}{2}$

Integrating (6.40) gives

$$L_i(t) \leq L_i(0)e^{-\varrho_{1i}t} + \frac{\varrho_{2i}}{\varrho_{1i}}(1 - e^{-\varrho_{1i}t}) \leq L_i(0) + \frac{\varrho_{2i}}{\varrho_{1i}} \quad (6.41)$$

From the definition of V_i , we obtain that

$$\zeta_i^2 \leq 2 \left[L_i(0) + \frac{\varrho_{2i}}{\varrho_{1i}} \right] \quad (6.42)$$

Therefore, according to Lemma 6.1 the errors $\tilde{V}_i$, $\tilde{W}_i$ and $\tilde{z}_i$ will converge to a compact set $\zeta_c = \{\zeta | \zeta^2 \leq V_i(0) + \frac{\varrho_{2i}}{\varrho_{1i}}\}$ and thus the closed loop system is uniformly

ultimately bounded.

6.4 PID controller

The PID controller is designed as follows: $u_1 = K_{p1}(y_1 - y_{1d}) + K_{d1}(\dot{y}_1 - \dot{y}_{1d}) + K_{i1} \int (y_1 - y_{1d})dt$, $u_2 = K_{p2}(y_2 - y_{2d}) + K_{d2}(\dot{y}_2 - \dot{y}_{2d}) + K_{i2} \int (y_2 - y_{2d})dt$.

6.5 Simulation results and discussions

The NNFC tuning parameters are $\lambda_1 = 3.5$, $K_1 = 20$, $\lambda_2 = 30$, $K_2 = 20$ and the desired outputs are $y_{1d} = 3 \times 10^4 kg/kmol$, $y_{2d} = 325^0K$. The NN parameters are $\gamma_{11} = \gamma_{12} = 0.0001$, $\gamma_{21} = 0.008$, $\gamma_{22} = 0.001$, $\kappa = 0.0001$, the number of nodes of the hidden layer $L = 10$, and the input vector $X_i = [1, z_i, \dot{z}_i]$. The PID parameters are $K_{p1} = 260$, $K_{i1} = 100$, $K_{d1} = 25$, $K_{p2} = 800$, $K_{i2} = 125$, $K_{d2} = 60$.

The simulation results are shown in Figs. 6.1-6.9. The outputs under NNFC settles and follows the desired trajectories faster than the PID as shown in Fig. 6.1. The tracking errors converge to zero at faster rate under NNFC than PID as presented in Fig. 6.2. The control inputs under NNFC have no overshoots as shown in Fig. 6.3. The states of the process are shown in Figs. 6.4-6.9

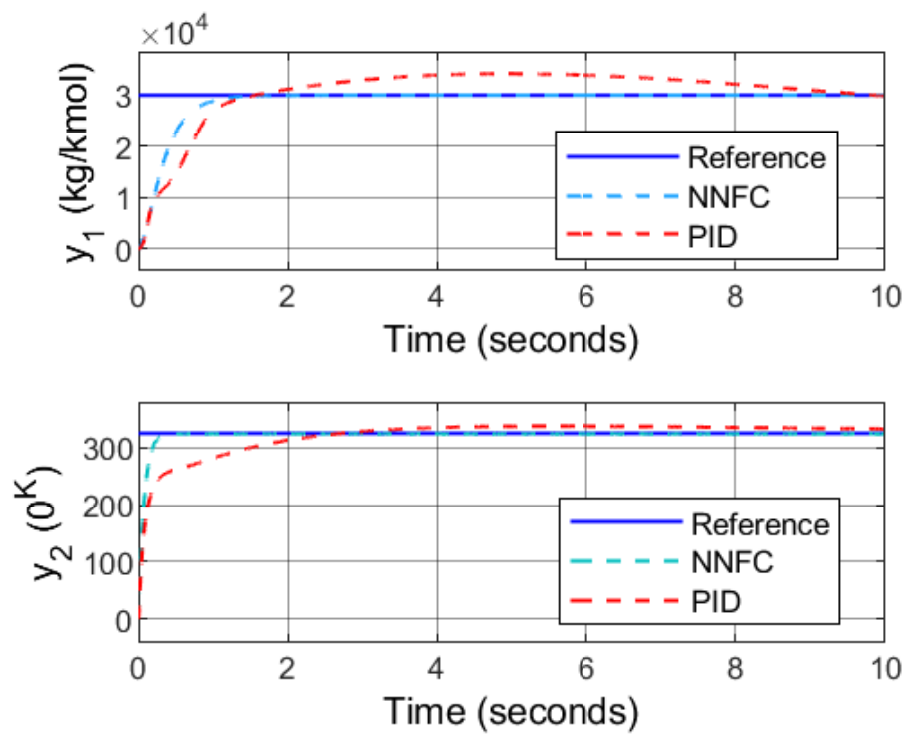


Figure 6.1: AMW (above)
and reactor temperature (below)

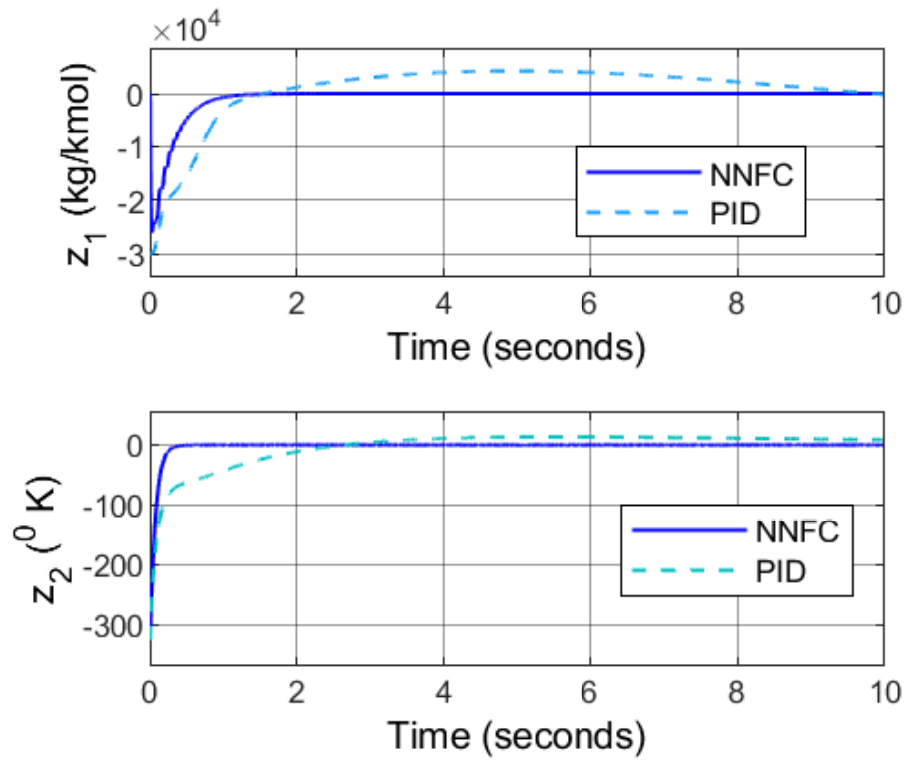


Figure 6.2: Average molecular weight tracking error (top) and the reactor temperature tracking error (below)

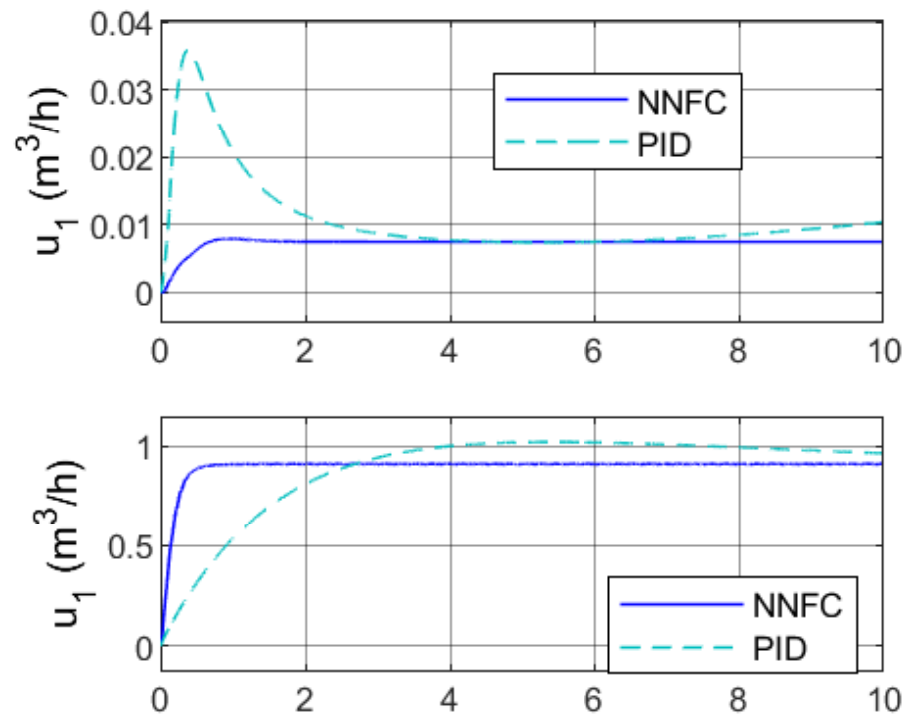


Figure 6.3: The initiator flow rate (above)
and the coolant flow rate (below)

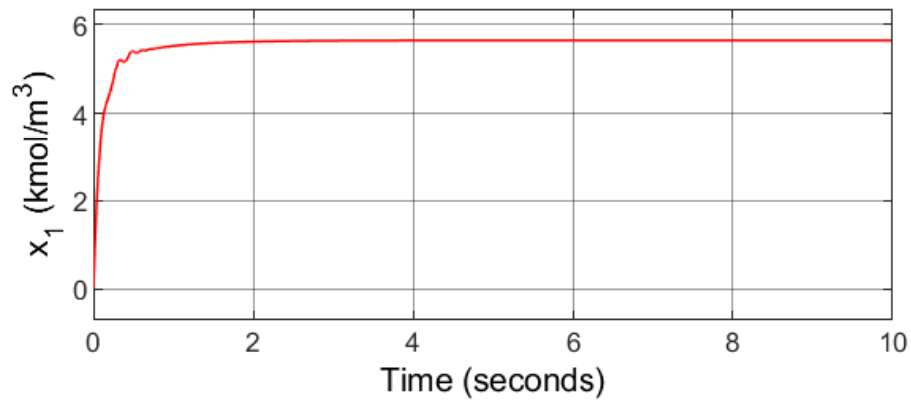


Figure 6.4: The monomer concentration

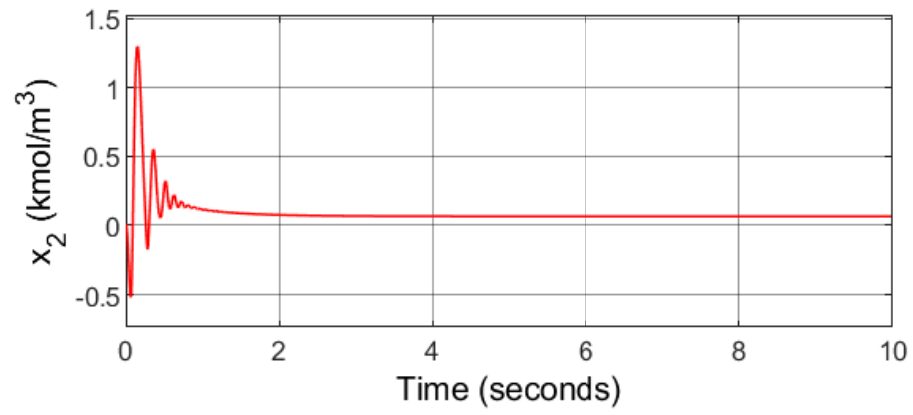


Figure 6.5: Initiator concentration

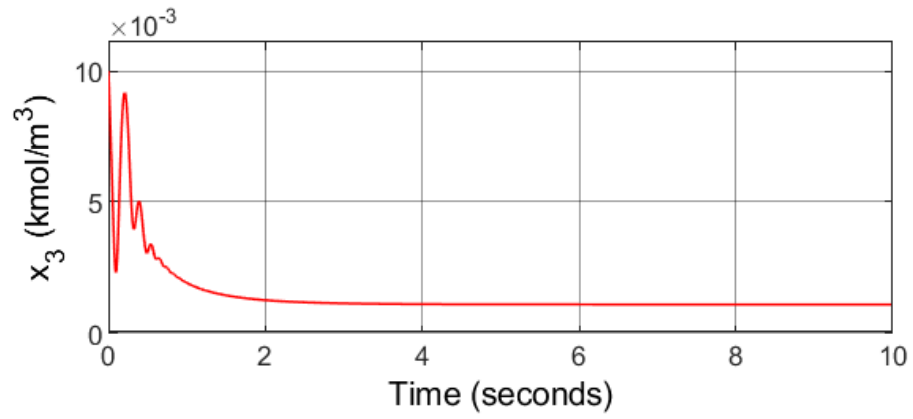


Figure 6.6: Molar concentration of death polymer chains.

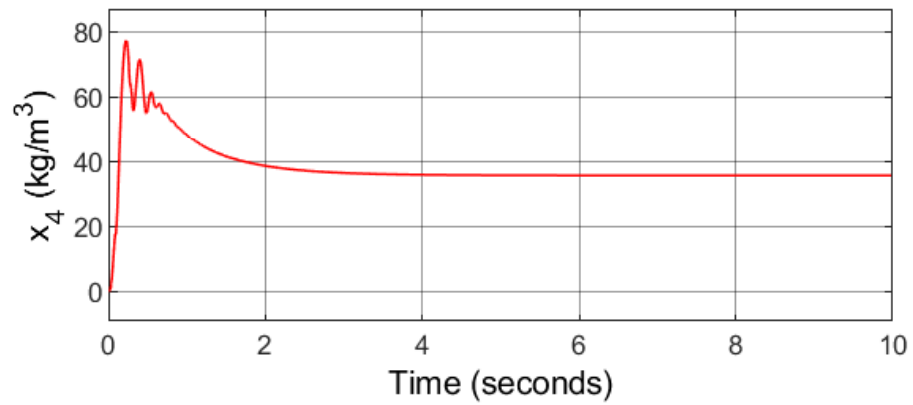


Figure 6.7: Mass concentration of death polymer chains.

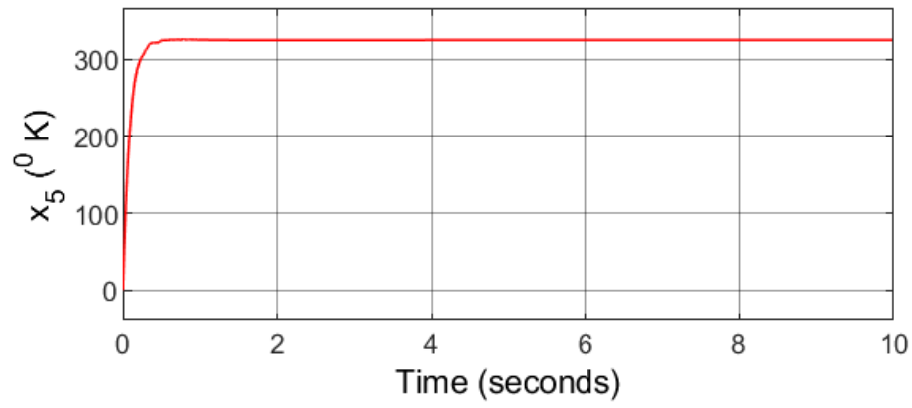


Figure 6.8: Reactor temperature.

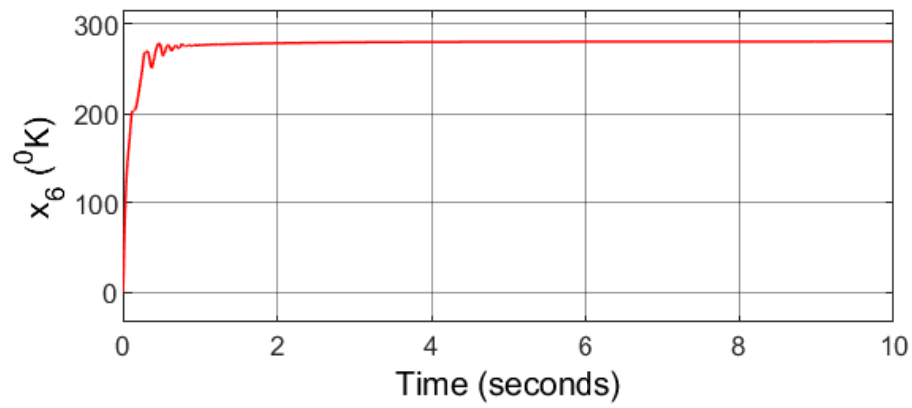


Figure 6.9: Coolant's temperature.

CHAPTER 7

CONCLUSIONS

In this work, control methods have been successfully implemented for the polymerization reactor under different scenarios. The dynamic system of the polymerization reactor is strongly coupled nonlinear system and thus the control design is challenging. A, NBFSMC was designed to control the reactor temperature and average molecular weight of the polymer in the presence of unknown input deadzone. In addition, A NNSMC was designed to control the reactor temperature and the monomer concentration in the presence of unknown disturbances. Furthermore, a finite time based NNFC was designed to control the reactor temperature and average molecular weight of the polymer in the presence of unknown disturbances. Simulations were carried out in MATLAB/SIMULINK and excellent results were obtained.

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