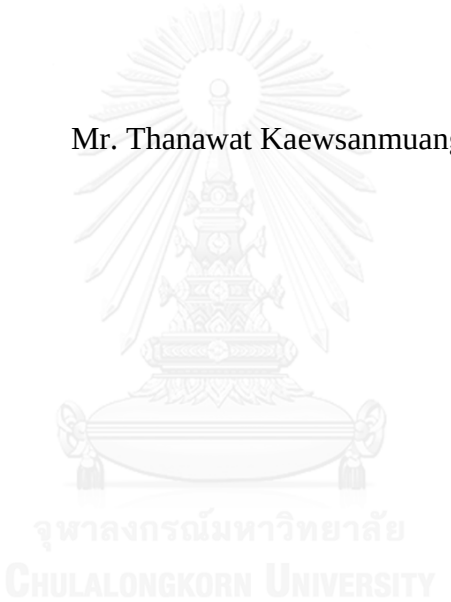
ตัวประมาณค่าไฮบริดจ์ระหว่างตัวสังเกตค่าแบบเลื่อนและตัวประมาณค่าโครงข่ายประสาทเทียมสำหรับกระบวนการเกิดพอลิเมอร์ของเอทิลีนในวัฏภาคแก๊ส

นายธนวัฒน์ แก้วแสนเมือง

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต
สาขาวิชาวิศวกรรมเคมี ภาควิชาวิศวกรรมเคมี
คณะวิศวกรรมศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย
ปีการศึกษา 2559

HYBRID ESTIMATION BETWEEN SLIDING MODE OBSERVER AND NEURAL NETWORKS ESTIMATOR FOR GAS-PHASE ETHYLENE POLYMERIZATION PROCESS

Mr. Thanawat Kaewsanmuang



A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering Program in Chemical Engineering
Department of Chemical Engineering
Faculty of Engineering
Chulalongkorn University
Academic Year 2016

Thesis Title	HYBRID ESTIMATION BETWEEN SLIDING MODE OBSERVER ANDNEURAL NETWORKS ESTIMATOR FOR GAS-PHASE ETHYLENE POLYMERIZATION PROCESS
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Field of Study	Chemical Engineering
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ธนวัฒน์ แก้วแสนเมือง : ตัวประมาณค่าไฮบริดจ์ระหว่างตัวสังเกตค่าแบบเลื่อนและตัวประมาณค่าโครงข่ายประสาทเทียมสำหรับกระบวนการเกิดพอลิเมอร์ของเอทิลีนในวัฏภาคแก๊ส (HYBRID ESTIMATION BETWEEN SLIDING MODE OBSERVER ANDNEURAL NETWORKS ESTIMATOR FOR GAS-PHASE ETHYLENE POLYMERIZATION PROCESS) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: ศ. ดร. ไพศาล กิตติศุภกร, 63 หน้า.

การประมานค่าความเข้มข้นของเอทิลีนของกระบวนการเกิดพอลิเมอร์ของเอทิลีนในวัฏภาคแก๊สเป็นที่ทราบกันว่าเป็นงานยาก เนื่องจากปฏิกิริยามีความซ้อนและไม่เป็นเชิงเส้นสูง นอกจากนี้ กระบวนการนี้ยังดำเนินการในช่วงอุณหภูมิแคบ ดังนั้น มันจึงมีแนวโน้มที่จะมีพฤติกรรมที่ไม่มีเสถียรภาพและควบคุมไม่อยู่ได้ง่าย ในงานวิจัยที่ผ่านมา การใช้ตัวประมานค่าได้ผลลัพธ์ที่ยังไม่เป็นที่น่าพึงพอใจ ดังนั้น วิถีทางไฮบริดจ์คือวิธีการแก้ปัญหาที่ดีที่สุด ตัวประมาณค่าไฮบริดจ์คือการรวมกันของสองตัวประมาณค่าเพื่อเพิ่มสมรรถนะของตัวประมาณค่าและเอาชนะข้อจำกัดของพวกมัน งานวิจัยนี้ได้นำเสนอตัวประมาณค่าไฮบริดจ์ซึ่งรวมกันระหว่างตัวสังเกตค่าแบบเลื่อน (เอสเอ็มโอ) และตัวประมาณค่าโครงข่ายประสาทเทียม (เอ็นเอ็น) เพื่อประมาณค่าความเข้มข้นของเอทิลีน เอสเอ็มโอถูกจัดเตรียมเพื่อประมาณค่าของตัวแปรสเตททั้งหมดในช่วงต้น แต่อย่างไรก็ตาม มันยังมีความแตกต่างของการประมาณค่าระหว่างตัวแปรสเตทกับค่าที่แท้จริง จากนั้นตัวประมาณค่าเอ็นเอ็นถูกใช้เพื่อประมาณค่าความเข้มข้นของเอทิลีนอีกครั้งเพื่อลดค่าความแตกต่างของเอสเอ็มโอ สมรรถนะของประมาณค่าไฮบริดจ์เอสเอ็มโอ-เอ็นเอ็นถูกเปรียบเทียบกับเอสเอ็มโอและตัวประมาณค่าเอ็นเอ็นสภาวะปกติ สภาวะนอยส์และสภาวะตัวแปรรบกวน ผลของการจำลองแสดงให้เห็นว่า ประมาณค่าไฮบริดจ์เอสเอ็มโอ-เอ็นเอ็นคือคือวิถีทางที่ดีที่สุดในการประมาณค่าความเข้มข้นของเอทิลีนและประมาณค่าได้แม่นยำและยังมีความสามารถในการจัดการนอยส์ได้เมื่อเทียบกับตัวประมาณค่าตัวเดียว

ภาควิชา วิศวกรรมเคมี ลายมือชื่อนิสิต .....

สาขาวิชา วิศวกรรมเคมี ลายมือชื่อ อ.ที่ปรึกษาหลัก .....

ปีการศึกษา 2559

5770422721 : MAJOR CHEMICAL ENGINEERING
KEYWORDS: HYBRID ESTIMATOR / ETHYLENE POLYMERIZATION / NEURAL NETWORK / SLIDING MODE OBSERVER

THANAWAT KAEWSANMUANG: HYBRID ESTIMATION BETWEEN SLIDING MODE OBSERVER ANDNEURAL NETWORKS ESTIMATOR FOR GAS-PHASE ETHYLENE POLYMERIZATION PROCESS. ADVISOR: PROF. DR. PAISAN KITTISUPAKORN, Ph.D., 63 pp.

Estimation of an ethylene concentration of gas-phase ethylene polymerization process has been known to be a difficult task because of the complex and high nonlinearity of the reactions. Besides, this process operates in a narrow temperature range, so it is to be prone to unstable behavior and runaway easily. In the past research, estimator usage produced unsatisfactory results, therefore hybrid approached is the best solution. Hybrid estimator is combination of two estimators to enhance the estimator's performance and overcoming their limitations. This research work proposes a hybrid estimator which combined between sliding mode observer (SMO) and neural network (NN) estimator to estimate the ethylene concentration. Initially, the SMO is provided to estimate of all state variables. However, it has usually been prone to the error of the estimation between state variables and actual data. Then, the NN estimator is used to provide the estimates the ethylene concentration again for reducing the error value of SMO. Performance of the SMO-NN hybrid estimator has been compared with the SMO and NN estimator in normal, noise and various disturbance conditions. Simulation results have shown the SMO-NN hybrid estimator is the best approached in estimating the ethylene concentration and provide good accuracy and able to handle noise compared with single estimator.

Department: Chemical Engineering Student's Signature .....
Field of Study: Chemical Engineering Advisor's Signature .....
Academic Year: 2016

ACKNOWLEDGEMENTS

I would first like to thank and express my gratitude to my thesis advisor, Professor Dr. Paisan Kittisupakorn, for his encouragement, supervision, advice, inspiration and helpful suggestions throughout the course of this Master Degree study. Without the support from him, this thesis would have never been completed. Furthermore, I would also like to thank Professor Mohamed Azlan Hussain for his time to discuss an estimator and useful comments on this thesis.

I would like to thank to all my friends, colleagues in the Control and Systems Engineering Research Laboratory and staffs in the Department of Chemical Engineering, Chulalongkorn University for their friendship and assistance over the years.

Financial support to this work under The Institutional Research Grant (The Thailand Research Fund), IRG 5780014, and Chulalongkorn University, Contract No. RES_57_411_21_076.

Finally. I would like to thank my family for their love, encouragement and financial supported me. Without their support, my research work would not have finished.

CONTENTS

Page

LIST OF TABLES

Page

LIST OF FIGURES

Page

Chapter 1

Introduction

1.1 Importance and reasons

The state feedback law is often based on the assumptions that all states are available for online measurement. Nonetheless, in practice, some of them may not be measurable due to lack of measurement or the high price of sensor devices. Therefore, measuring the states is not only difficulty but also the high cost of installation of these devices. Hence, devices known as an estimator have been developed to reconstruct the state vector for estimate the states or variables.

Estimators are applied to several chemical processes for estimating variables such as growth rate and kinetic coefficient in biochemical process (Zhang and Guay 2002), composition in batch distillation column (Jana 2010) and temperature in heat exchanger (Bagui, Abdelghani-Idrissi et al. 2004). However, estimators are still restrictions and for overcome their limitations, researchers have also developed estimators called “hybrid estimators” which are combinations of various estimators. In order to overcome the limitations of the single estimator, the hybrid estimator is used in this work. In addition, it can improve the single estimator inerasably.

The gas-phase ethylene polymerization reactor using catalyst is a high-complex systems, phenomena in reactor namely the various heat and mass transfer mechanisms, the kinetics of heterogeneous polymerization and flow characteristics of solids and gas is combined in a manner of realistic. Reaction which occurring in the reactor is highly exothermic reactions, unusual steady-state is cause of strong

interaction in this process. Thus, in order to obtain accuracy state or variables for control law, it is very necessary using the hybrid estimator for estimating states in this high complex system.

Accordingly, the purpose of this work is to design the hybrid estimator which are combined between sliding mode observer (SMO) – simple estimator designed is based on the Luenberger observer methodology with neural network (NN) for estimating the ethylene concentration in this system by using MATLAB software.

1.2 Objective

This work aims to design the hybrid estimator to estimate the ethylene concentration for the gas-phase ethylene polymerization process and compare effectiveness of estimation between hybrid estimator and single estimator.

1.3 Scopes of this work

i. The ethylene polymerization process well-mixed model proposed by McAuley, Macdonald, and McLellan is applied.

ii. Modeling and parameters used in this work are validated against plant data.

iii. Modeling of the process is performed by MATLAB.

iv. Effect of operating parameters (the reactor temperature, T and the molar flow rates of ethylene, F_{M1}) on dynamics behavior process are investigated.

v. Comparison of effectiveness of estimator between hybrid estimator and single estimator (Sliding mode observer, SMO and Neural network estimator, NN) are investigated.

Chapter 2

Literature reviews

In recent year, hybrid estimator has been a growing interest in the use for estimating unmeasured parameters and variables. Literature reviews regarding design of hybrid observer are presented in this chapter. The reviews consist of two parts. The first part introduces the single estimator which applied to polymerization process. The second part presents hybrid estimator that is published various papers.

2.1 Estimator

The estimator is used for estimating the uncertainty and unknow parameters in the polymerization process. The estimators such as an extend Kalman filter (EKF), an extend Luenberger observer (ELO) and a high-gain observer are normally applied in this process. These estimators have been reviewed in many literatures as followings.

McAuley and MacGregor (1991) presented a methodology for density prediction and on-line melt index in a reactor of fluidized bed polyethylene by using extend Kalman Filter (EKF). When the laboratory results analyze enhance obtainable, a recursive estimation error method will update adjusted parameters. The result presented that estimation of density and melt index are able of effectively by using this technique.

Appelhaus and Engell (1996) reported about the implementation of an observer which is an extend Kalman Filter (EKF) in a pilot plant reactor based on a model of polymerization. The result shows that two important concentrations in the polymer melts, specific surface and the product of mass transfer coefficient in a

polyethylene terephthalate (PET) reactor can be able to determine by the observer. The new possibility for improved process control is offers by the latter parameter knowledge.

Gentric et al. (1999) discussed the determination of optimal the temperature policy of α-methylstyrene and styrene in a reactor of batch emulsion polymerization. In addition, estimation the non-measured state variables which are number of particles per unit volume and monomer concentration are used by an extended Kalman filter. The result of experimental for this complex system presented that estimations is excellent. The observer tracked a good temperature and the control and the estimation is well.

Yang et. al (1999) shown that three different modeling of the neural network which applying in a reactor of semi-batch polymerization. Initiator and monomer concentration are estimated by concentration of initiator in feed, feed temperature and temperature of reactor. The simulation results shown that estimation difficult-to-measure polymer variables with acceptable accuracy for semi-batch reactor is proposed by the multi-stage approach proposed.

Pico et al. (2009) reported the estimation of substrate concentration and specific growth rate in fermentation process from biomass measurements. Exactly, Lyapunov stability theory is used to demonstrate finite-time convergence by sliding-mode observers (SMO). The convergence rate of the real substrate concentration is increased by observer in this condition of substrate estimation.

Hajatipour and Farrokhi (2010) indicated that observer uses the sliding-mode observer (SMO) as the high gain property for get the estimated states to the system fast convergence. Furthermore, for maintaining good estimation of the states and to

introduce to make the proposed observer less sensitive to measurement noises, the Variable Relay-Equivalent Gain technique is applied to this work.

Another work of Kuroda and Kim (2002), they applied NN estimator to modeling the behavior of temperature caused by exothermic reactions in a polymerization process. In batch emulsion polymerization, there may occur unexpected thermal reactive runaway. Therefore, it is difficult to control the behavior of the system in order to keep uniform fine product quality in each batch job. The NN is applied in the batch polymerization process for estimating the energy balance. The results shown that the temperature changes caused by exothermic reactions could be easily estimated and predicted by such neural network in the complicated polymerization processes. However, the single estimator has the unsatisfied results about the accuracy and the robustness when using in this process. Thus, the hybrid estimator that combined two different estimators is applied for solving the problems.

2.2 Hybrid estimator

In recent year, the hybrid estimator that consisted of two or more estimators becomes a popular estimator in many industries owing to it has the higher accuracy and robustness than the single estimator. The hybrid estimator is studied and reported in the following literatures.

Ng and Hussian (2004) presented hybrid neural network which are combined between neural network and first principle model (FPM). They developed two various hybrid estimator which are applied for estimating the overall heat transfer coefficient and the rate of polymerization in a reactor of semi-batch polymerization. The simulation shown that hybrid estimator can estimate accurately and fast convergence rate. In some of the conditions, the simulation result has been exposed that the HNN is more easier to apply and accurate than the extend Kalman filter.

Aguilar-Lopez and Maya-Yescas (2005) proposed a hybrid estimator in a batch stirred polymerization reactor. The hybrid estimator including a sliding mode observer and proportional-type contribution for the measurement of error. In this process, the hybrid estimator is provided for estimating monomer concentration, polydispersity, filtering of temperature and average molecular weight. The SMO offers model uncertainties and robustness in contrast to measurements noisy. They compared the hybrid estimator through simulation of numerical in order to a classic proportional observer and the hybrid estimator presents better performance in contrast to noisy measurements and non-modelled dynamics.

Hulhoven et. al (2006) designed hybrid observer combining Luenberger observer and asymptotic observer. They used this hybrid observer for estimating biomass concentration in fed-batch bacteria fermentation system. An adjustable rate

of convergence is accurate in the process model by the Luenberger observer. Whereas, for avoid using the kinetic model, they used a state transformation from the asymptotic observer but the process operating conditions define the convergence rate. Hence, the hybrid observer is proposed, which builds two state estimation algorithms. The results shown that developed hybrid observer can evolves between the asymptotic and exponential observer and in the process model is evaluated a level of confidence.

Sheibat-Othman et. al (2008) presented nonlinear observers which is an apply in polymerization reactor. The termination rate coefficient is estimated by a high gain continuous-discrete nonlinear observer and the radical concentrations is observed by the adaptive observer. A function of the polymer concentration investigates by a slightly decreasing profile. Besides, it is remained by the estimation strategy. As the result, the variation of k_t with the concentration of polymer can estimate and derive by this model.

Chapter 3

Theory

3.1 Ethylene polymerization process

3.1.1 Process description

Polymer in this world which is the most popular is polyethylene. The Ziegler-Natta catalysts with the gas-phase ethylene polymerization process produced a large proportion of polyethylene. The gas-phase polyethylene production has more advantage when compared with the other method because it does not use solvent in the process. Thus, this process must not produce and recover the solvent. In addition, the gas-phases ethylene polymerization process can operate at low temperature. So, this process saves the energy. However, it should be careful about the zone of the reaction. This process must keep the reactant below the melting point for protect agglomeration and particle melting as well as it must keep above the dew point for avoid condensation. The model of McAuley et al. (1990) is developed based on the well mix model for applying in the polymerization of the polyethylene. In Figure 3.1, producing of the polyethylene is explained. Major component namely the monomer (ethylene), co-monomer (butene), hydrogen (H_2) and nitrogen (N_2) is used as feed gas which is combined with the recycle gas before enter to the reactor.

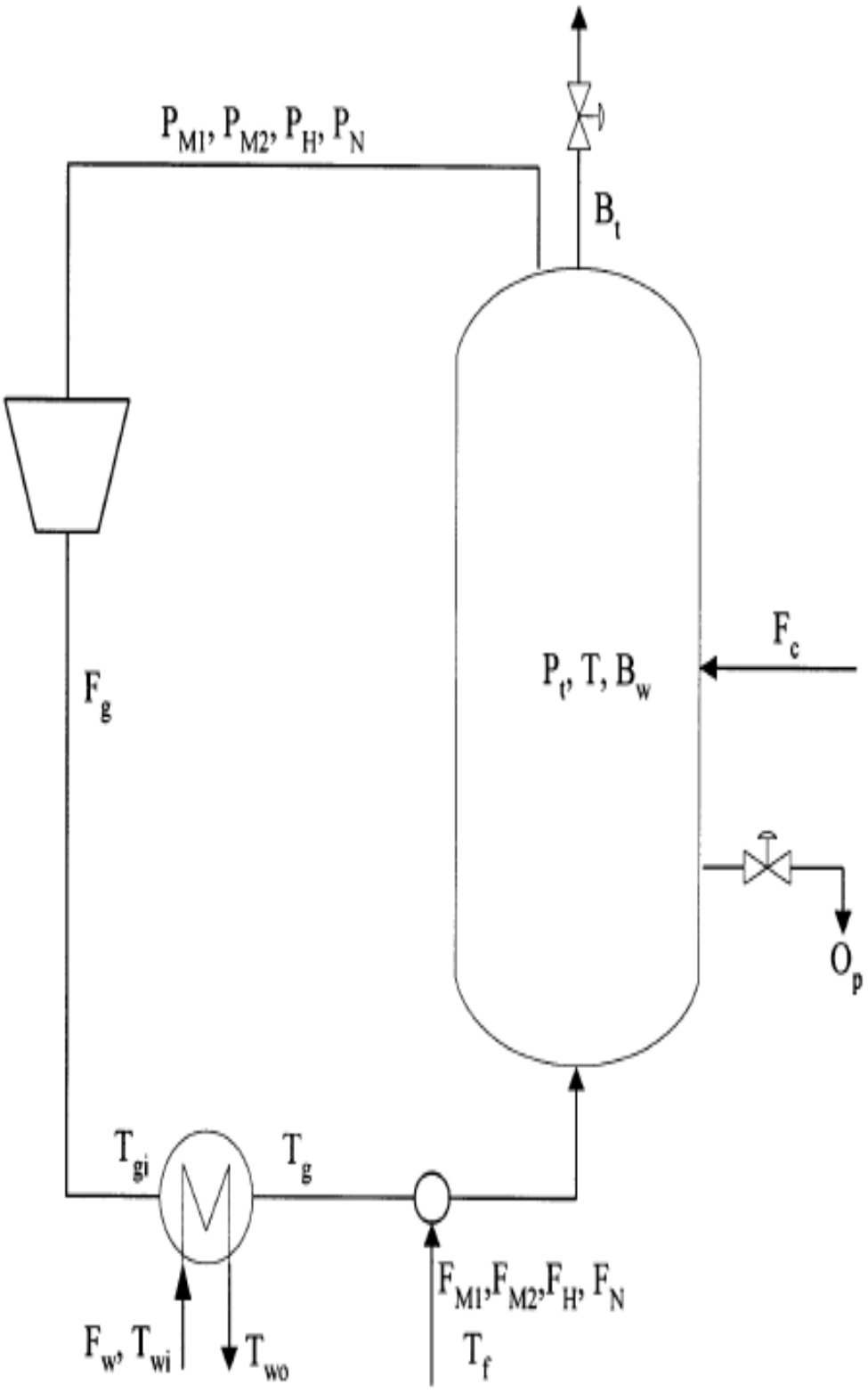


Figure 3. 1 Schematic of the polyethylene reactor.

The ethylene polymerization process has the major assumption as follows:

1. All of temperature and gases concentration is assumed that well mix model.

2. A pseudo-homogenous single-phase is used in this model. Hydrodynamic characteristics of the reactor used describe the properties of emulsion phase and the bubble phase.

3. We neglect mass and heat transfer which is generate between the emulsion gas and the solid particle as well as mass and heat transfer which is generate by the emulsion gas and the bubble gas.

4. In the reactor, we used catalyst which entries unceasingly.

5. Particle size which used in this model is assumed that their have constant mean size.

6. Reaction generate immediately and gas recycle return to the reactor instantly.

3.1.2 Process model for parameter estimations

M_1 as ethylene, M_2 as butene, H as hydrogen and N as nitrogen are placed in the mole balance of the process as follow:

$$V_g \frac{dC_{M1}}{dt} = F_{M1} - x_{M1}B_t - R_{M1} \quad (1)$$

$$V_g \frac{dC_{M2}}{dt} = F_{M2} - x_{M2}B_t - R_{M2} \quad (2)$$

$$V_g \frac{dC_H}{dt} = F_H - x_H B_t - R_H \quad (3)$$

$$V_g \frac{dC_N}{dt} = F_N - x_N B_t \quad (4)$$

With $R_{M1} = C_{M1} Y_c k_{p1} e^{-(E/R)(1/T - 1/T_{ref})}$ (5)

$$R_{M2} = C_{M2} Y_c k_{p2} e^{-(E/R)(1/T - 1/T_{ref})} \quad (6)$$

Here V_g is the reactor volume, C_{M1}, C_{M2}, C_H, C_N are the concentration of ethylene, butene, hydrogen and nitrogen. F_{M1}, F_{M2}, F_H, F_N are the molar flow rates of ethylene, butene, hydrogen and nitrogen. x_{M1}, x_{M2}, x_H, x_N are the mole fraction of ethylene, butene, hydrogen and nitrogen. B_t is the bleed flow rate and R_{M1}, R_{M2}, R are the gases constant. R_{M1} depends on the ethylene propagation rate constant (denoted by k_{p1}), R_{M2} depends on the butene propagation rate k_{p2}) and R is the ideal gas constant. Y_c is the number of mole at catalyst site, E is the activation energy for propagation, T and T_{ref} are the reactor and reference temperature, respectively.

Number of moles at the catalyst site is described by:

$$\frac{dY_c}{dt} = F_c a_c - k_d Y_c - O_p Y_c / B_w \quad (7)$$

With $O_p = M_{w1}(R_{M1}) + M_{w2}(R_{M2})$ (8)

Where F_c is the catalyst flow rate, a_c is the active site concentration, k_d is the deactivation rate constant, O_p is the polymer outlet rate, B_w is the mass of polymer and M_{w1}, M_{w2} are the molecular weight of ethylene and butane, respectively.

Reactor temperature and recycle stream temperature are given as follows:

$$(M_r Cp_r + B_w Cp_p)\frac{dT}{dt} = HF + HG - HR - HT - HP \quad (9)$$

$$M_g Cp_g \frac{dT_g}{dt} = F_g Cp_g (T_{gi} - T_g) + F_w Cp_w (T_{wi} - T_{wo}) \quad (10)$$

where $HF = (F_{M1} Cp_{M1} + F_{M2} Cp_{M2} + F_H Cp_H + F_N Cp_N)(T_f - T_{ref})$ (11)

$$HG = F_g Cp_g (T_g - T_{ref}) \quad (12)$$

$$HT = (F_g + B_T) Cp_g (T - T_{ref}) \quad (13)$$

$$HP = O_p Cp_p (T - T_{ref}) \quad (14)$$

$$HR = M_{w1} R_{M1} \Delta H_R \quad (15)$$

The total pressure of the reactor is given by:

$$P_t = (C_{M1} + C_{M2} + C_H + C_N) RT \quad (16)$$

The relation of cooling water with the temperature is given by:

$$F_w Cp_w (T_{wi} - T_{wo}) = 0.5UA[(T_{wo} + T_{wi}) - (T_{gi} + T_g)] \quad (17)$$

Here HF, HG, HT, HP are the sensible heat of fresh feed, recycle gas, reactor and product respectively while HR is the enthalpy generated from the polymerization, $M_r Cp_r$ is the thermal capacitance of the reaction vessel, M_g is water hold up in heat exchanger. $Cp_{M1}, Cp_{M2}, Cp_H, Cp_N$ are the heat capacity of ethylene, butene, hydrogen and nitrogen respectively. Cp_p is the heat capacity of polymer whereas Cp_g and Cp_w are the heat capacity of recycle gas and water. Besides that, F_w, F_g are the cooling water and recycle flow rate accordingly, T_{wi}, T_{wo} are the cooling water temperature (before and after cooling) while T_{gi}, T_g are the recycle temperatures (before and after cooling). UA is the overall heat transfer coefficient, ΔH is the heat of reaction and P_t is the total pressure.

The polyethylene process model which is developed by McAuley et al. (1995) can calculate by Eqs.(1)–(17). This model is slightly changed to calculate heat removal. The external heat exchanger is used for remove which generated by reaction. The well-mix model is assumed to this system. We used ideal gas law for calculating the partial pressure of the substrate.

3.2 Sliding mode observer (SMO)

Unique properties are contained in the Sliding mode observers. The sliding mode observers can use the error the estimated value and the measured from the plant to build sliding motion.

The problem of state estimation for the nonlinear system

$$\dot{x} = f(x) + B(x)u, \tag{18}$$

where $x \epsilon R^n$, by output vector measurements

$$y = g(x) \epsilon R^m \tag{19}$$

has been considered. For exactly known smooth nonlinearities f and g and if $B = 0$, the method of global linearization by using nonlinear state transformation permits to obtain a system in the new variables $z \epsilon R^n$ which is linear with respect to z and has in the right-hand side nonlinear function only of the measurements y. After that, the standard linear pole-placement technique can provide for designing observer.

For successful application of the technique the nonlinear transformation must be determined. The essential and necessary conditions of existence for this transformation were given by Krener and Respondek (1985). These conditions are more restrictive considerably than the observability condition of the system 18, 19. On other hand, the problem of integration of a corresponding partial differential equation for obtaining this transformation makes sometimes this method difficult to implement in practical situations.

Observers based on sliding mode approach first were developed for linear case.

$$\dot{x} = Ax + Bu, \tag{20}$$

$$y = Cx. \tag{21}$$

By structure they are very similar to the standard full order observers with replacement of the linear innovative term by a discontinuous function:

$$\dot{\hat{x}} = A\hat{x} + Bu + Lsign(y - C\hat{x}), \tag{22}$$

where L is the observer gain and $sign$ is understood componentwise for vector argument $z = col(z_1, \dots, z_n)$ and $sgn(z) = col(sgn(z_1), \dots, sgn(z_n))$ (23)

3.3 Artificial neural networks (ANNs)

Artificial Neural Networks (ANNs) are the tools which using computational. Artificial Neural Networks can be able to calculate or solve the system which has more nonlinear. In addition, it uses data in the historical as knowledge for generate structure to build model (Hecht-Nielsen 1990).

3.3.1 A biological neuron

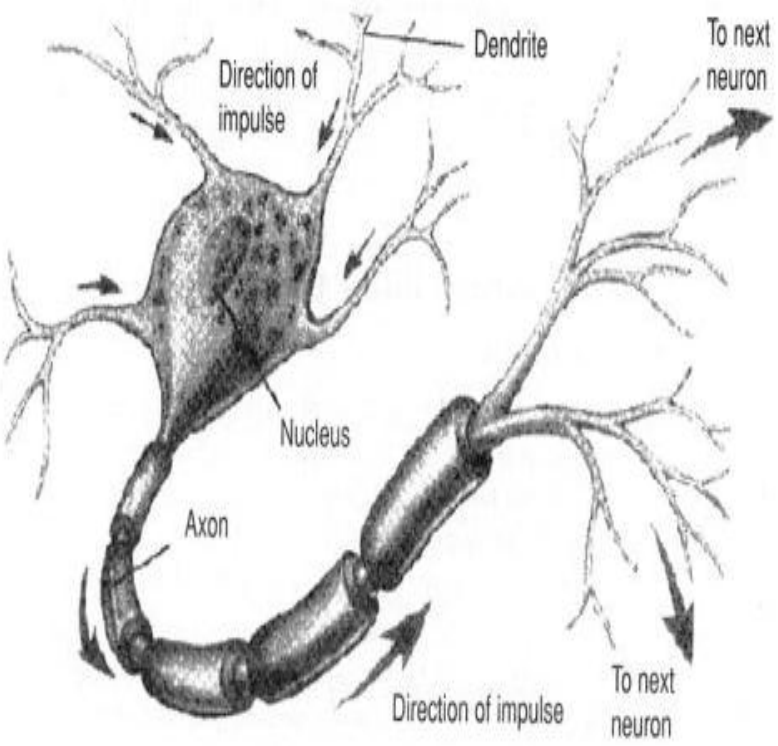


Figure 3. 2 A biological neuron

The neuron within the brain have various type, but it has same component as four basics. The four basics component including axon, synapses, dendrite and soma

Soma: The soma or cell body is the body of neuron. Within the soma including biochemical and nucleus.

Dendrite: Shape of dendrite like hair and it has many branches. Duty of dendrite receive data or signal from external or the other neuron.

Axon: Duty of axon is decision and transfer data or signal along body to the synapse. Shape of axon is tubular and long.

Synapse: The tail of the neuron has the branch like dendrite. When two neurons connected together, point of connection is called synapse. The first neuron transfer

signal trough axon and then it sent signal to the next neuron. After that, dendrite of another will received input and evaluate.

3.3.2 An artificial neural

A biological neuron was mimic four functions by the artificial neural network. An artificial neuron is demonstrated in Figure 3.3.

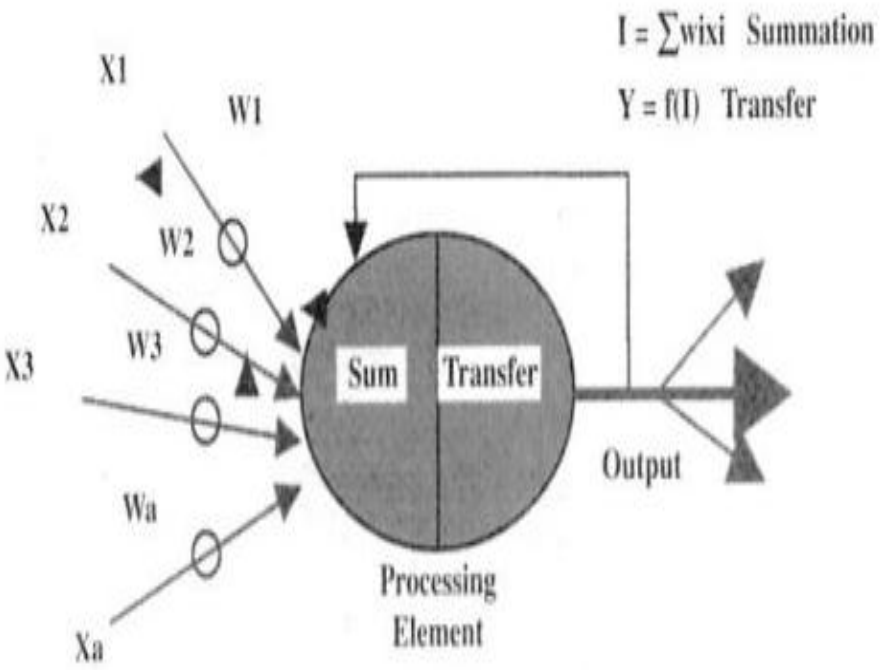


Figure 3. 3 A basic artificial neuron.

In Figure 3.3, the mathematical symbol, $x(a)$ is presented to the various inputs of the network. The connection weight multiplied by each of these inputs. $w(a)$ is represented the weights. Before feed to the transfer function, these data were sum of product in order to build result and then there will be sent to output. An artificial neuron includes seven major components. The input layer, the hidden layer and the output layer is used in the neural network.

Component 1. Weighting Factors: A neuron received many contemporary inputs. Each input has its own connected weight, which gives the input the impact that it needs on the processing element's summation function. Some inputs are structured more important than others to have a superior effect on the processing element as they combine to produce a neural response. Weights were modified that determine the intensity of the input signal as registered by the artificial neuron.

Component 2. Summation Function: In the previous component, sum of products in weights is complex less than the summation function. Before the signal data is sent to the transfer function, the weighting coefficients and the input will be merged. The maximum, minimum, the majority is selected by the summation function.

Component 3. Transfer Function: The next step of transfer data is transfer function. When we receive results transforms form the summation function, and then signal will sent via the transfer function. The transfer function will compare value that receive from the summation function with threshold in order to regulate the output. The processing element will create signal, if result of summation function has larger than the threshold. On the other hand, the processing element will ignore if result of summation function has below than the threshold value.

Component 4. Limiting and Scaling: This procedure is attach from the activation function. Because, data or information have various of data then we must ensure that data scale is not lower bound or exceed an upper.

Component 5. Output: One output signal accepts each processing element which may be receive from many nodes. Output is the result which came from learning of the neural network.

Component 6. Error Function: The modification between the desired output and the current output are considered which are changed using the error function for coordinate an architecture network in most learning networks. The previous layer propagate backward by this error.

Component 7. Learning Function: The weights of the inputs in each node consistent with some neural which is calculated algorithm.

3.3.3 Artificial neural networks

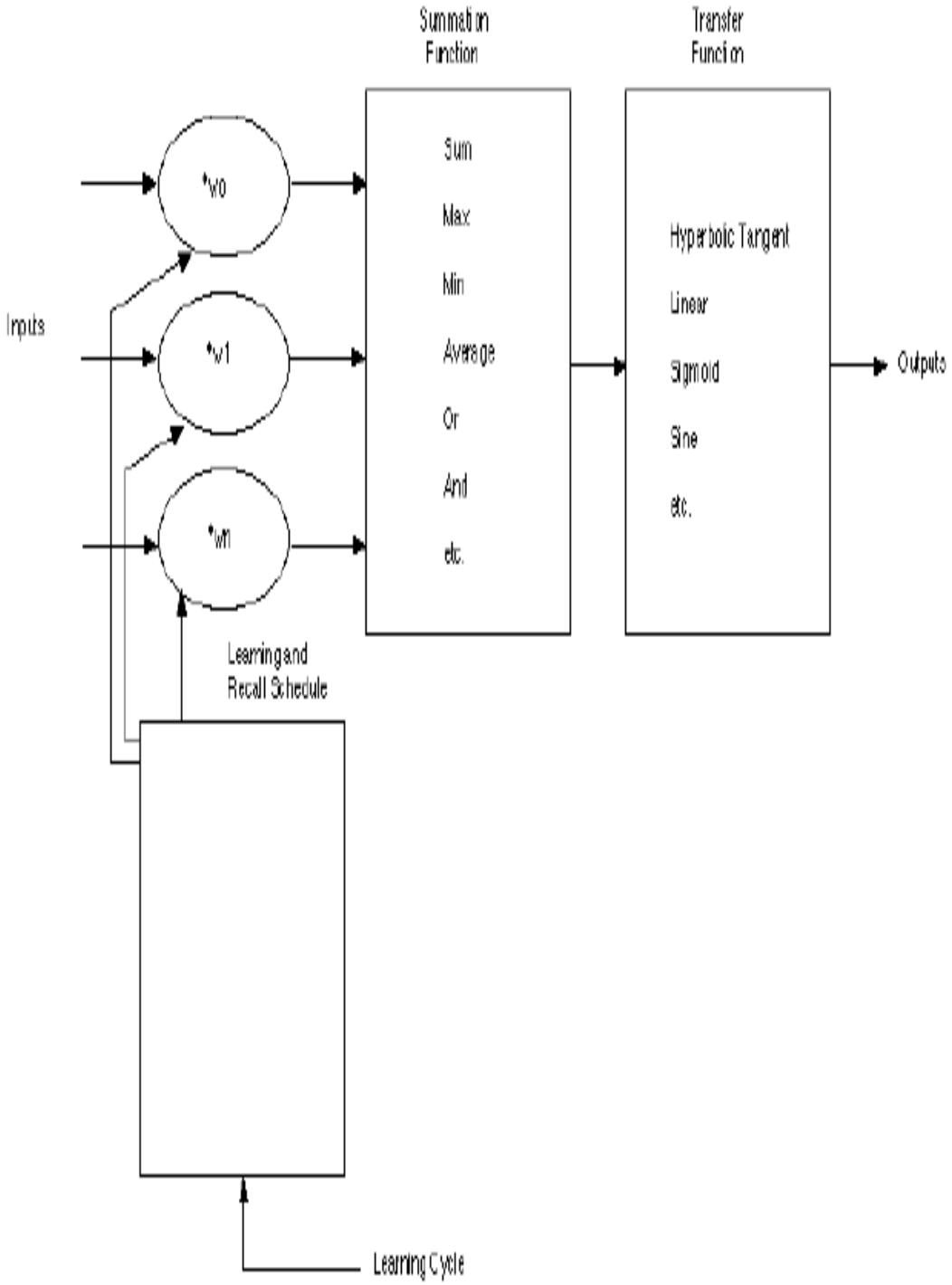


Figure 3. 4 An artificial neural network

In Figure 3.4 illustrate an artificial neural network. From the upper left, inputs go into the processing element. In the first, weighting factor is fed to the inputs. Input which is change fed to the summation function. In summation function will calculate sum of product.

The summation function in the output is sent to an activation function, that it tries this number into a real output through some algorithm. The activation function can also control its value through thresholds or scale the output. This output is sent to an outside connection or other processing elements, as uttered via the network structure.

3.3.4 Activation (Transfer) functions

The activation function of the neural network should variance as well as enable correcting error continuously. Computation of local gradient required the derivative of the activation function. The most activation function which is found in the various paper is the sigmoid function. The S-shape is contained to the sigmoid function. The sigmoid function is common form to apply in the neural network because of an increasing function. In addition, the sigmoid function is positive value which it has advantage for protect balance concerning nonlinear and linear behavior. What more, the transfer functions can also be active as shown in Figure 3.5.

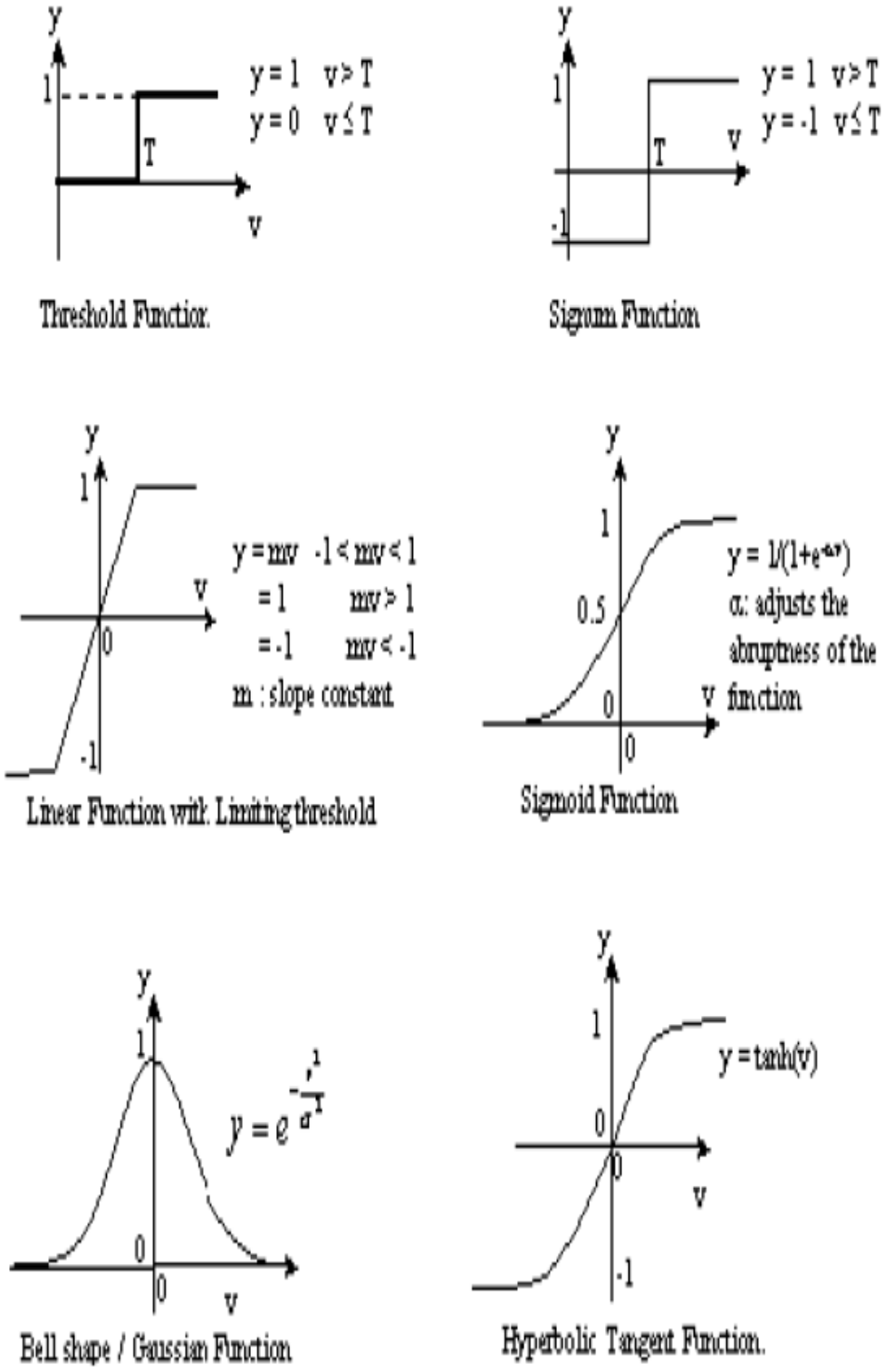


Figure 3. 5 Transfer functions with different characteristic constant values

3.3.5 Layer arrangement in a neural network

In many ways, the neurons can be grouped together. In the human mind, the grouping can generate, too. Example of system in self-organizing way, interactive or a dynamic. From microscopic components, a three-dimensional world constructs the neural network.

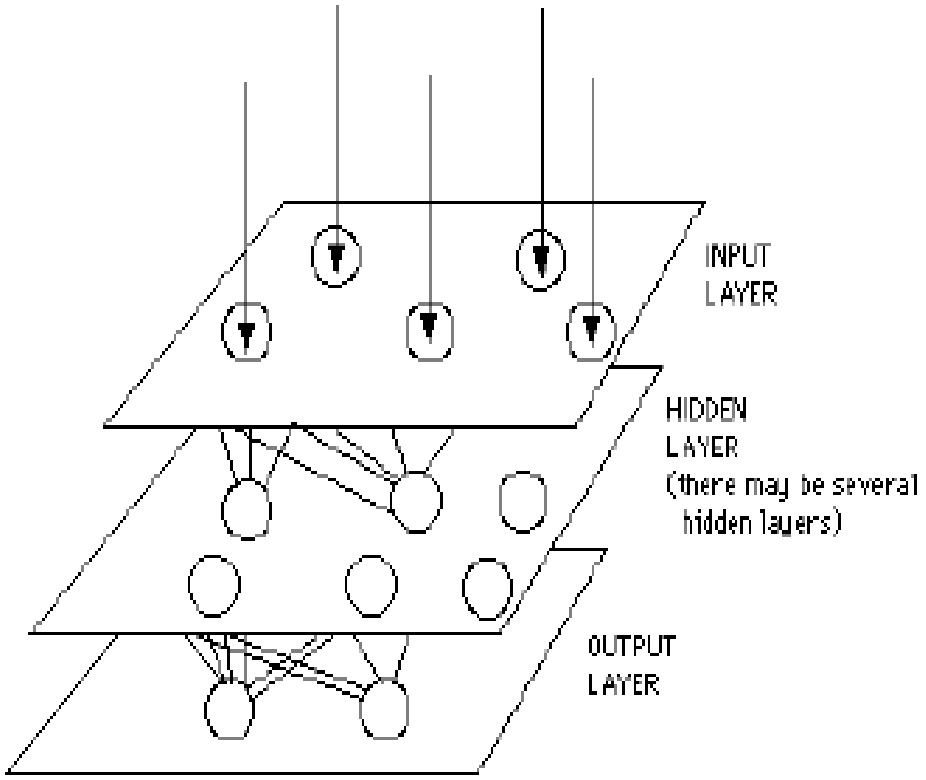


Figure 3. 6 Layer arrangement in a neural network

Essentially, a neural network is grouped into layers, the connections concerning these layers, and the activation functions or summation function that comprises a functioning neural network. Input layer, output layer and hidden layer is the least of layer which require in the most applications network. The data from electronic sensors in real-time applications or from input files is informed in the input layer. The layer of output will send information to the outside world directly, to a subordinate computer system or to another device. Many hidden layers are between input layer and output layer. In various interconnected structures are comprise in the hidden layer.

3.3.6 Types of artificial neural networks

3.3.6.1 Single layer feed forward network

In this type, the neural network contains a single layer of weights, which is connected directly to the outputs. This structure includes two layers; input layer and output layer as shown in Figure 3.7. A feed-forward type is considered in this type. The weights and the inputs is calculated by sum of the products in each node. If the value of result is above some threshold, nodes will send signal to next node. On the other hand, if result of sum product is below threshold, it will not send signal.

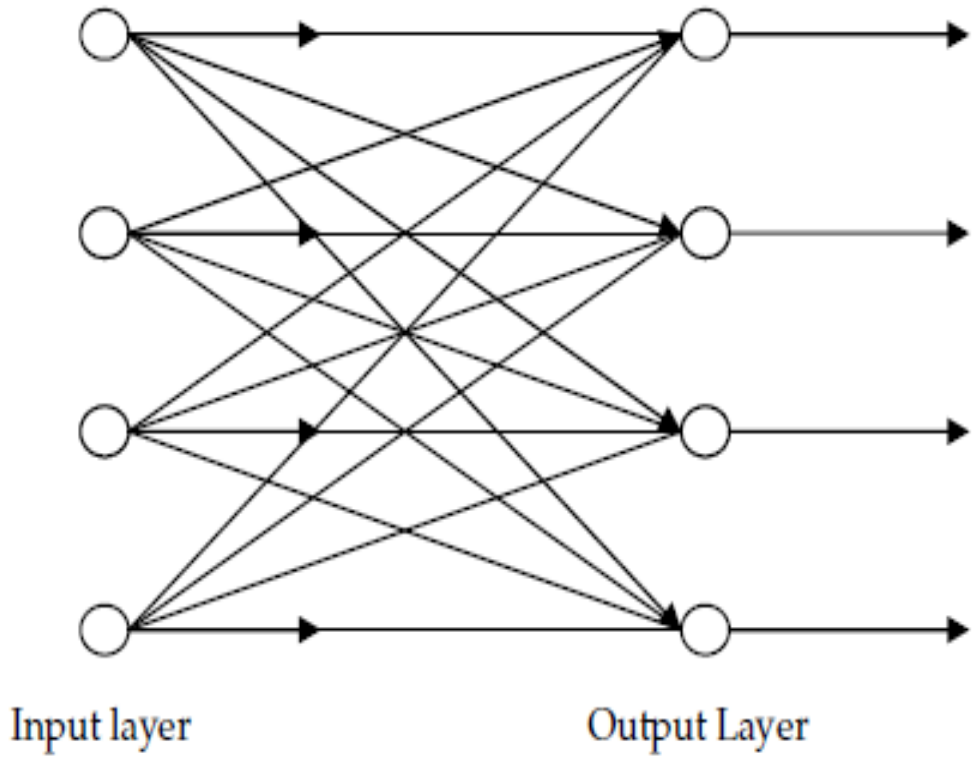


Figure 3. 7 A Single layer feedforward network

3.3.6.2 Multilayer feed forward network

Multilayer feed forward network (Figure 3.8) contains of one or more hidden layers, which are named hidden units or hidden neurons. The hidden neurons function is to relate concerning the output of network and the external input in to extract higher order statistics and some useful manner. For the input layer of neural network, input will transfer signal to the neurons or node to next layer. Node of next layer will receive signal and then sum for sending to the next node in the next layer.

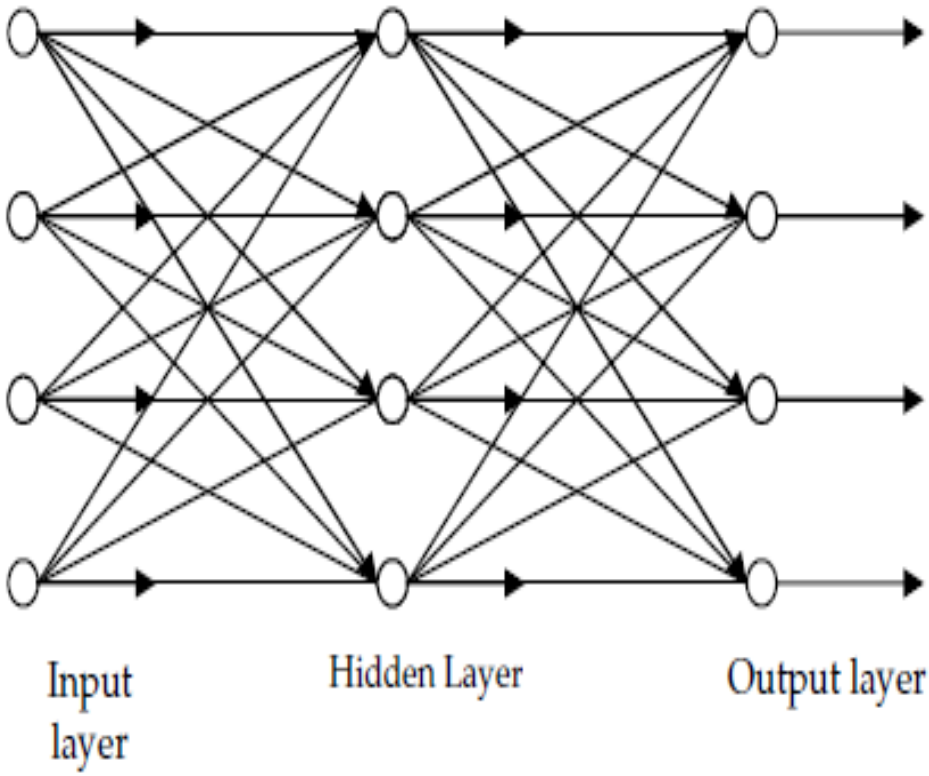


Figure 3. 8 A multilayer feed forward network

3.3.6.3 Recurrent network

In the recurrent network, the neurons output can be feedback to the neurons in the other layers or to the same neurons. Signal propagate in both backward and forward directions. Illustration of recurrent networks namely the Jordan network, the Elman network, and the Hopfield network. A dynamic memory of recurrent networks use outputs at a given instant reflect the current inputs and previous output as shown in Figure 3.9. The recurrent networks are useful in mapping dynamic change in a system.

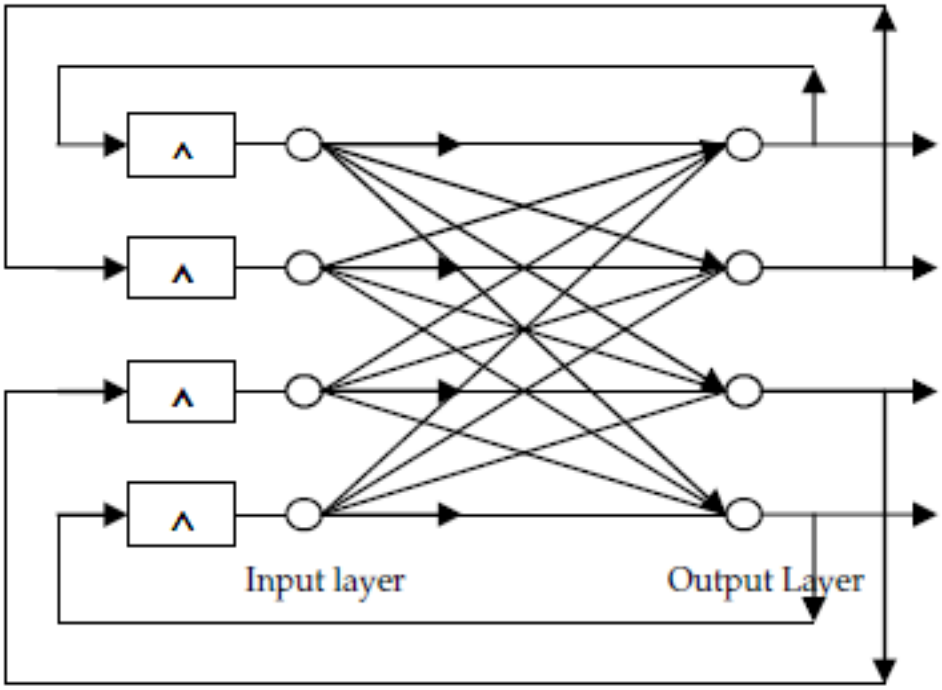


Figure 3. 9 A recurrent network

3.3.7 Training of artificial neural networks

When we obtain neural network structure which is generated appreciated structure. Next step, network will be trained. Weights are random in the initiate and then it will be train for adjusting the weight. Methods of training have two algorithm including supervised and unsupervised.

3.3.7.1 Supervised training

In supervised training, a set of training data or examples data, which has been obtained from actual process behavior are fed to the training algorithms. The network is trained to calculate the inputs which matching output correctly. The outputs of network are compared with the targets value when the network is added by the input. The training algorithms make use of the error concerning the target value and output value in order to modify the weights and biases for driving the outputs of network following to the targets value. In this technique, the trainer knows exactly the desired

output. The error between the desired output and the actual value is exploited to adjust the strengths of the connection such as weights between neurons and the training performed until it reaches the required performance. In addition, this method is used in most applications.

3.3.7.2 Unsupervised or adaptive training

In unsupervised training, only weights and biases are changed in response to inputs of network. The target outputs are not available. The clustering operations are performed by these algorithms which a finite number of classes grouped to input patterns. Most of applications which is usages such as pattern recognition. In this method, the trainer does not know the desired teaching signal. The methodology of training is similar to the supervised training method. This method is also used as the pre-processing for the supervised training method to improve training for better convergence. The hidden neurons must fide ways to organize themselves. In this method, no outputs of example are offered to the network in contrast to it can be compared to the predicted performance for a given input vector.

3.3.8 Training algorithms

Since in this study, I am nervous about the feed forward neural network, that uses the method of supervised training, I will describe the training algorithm involved for training the feedforward only in the next section.

3.3.8.1 The data rule

For train a single layer network, one of the original supervised learning method used is the data rule. In this method, the inputs offered to the outputs and the

network are calculated. These outputs value are compared with the targets values and difference between them is calculated to give the error, ε , i.e.

$$\varepsilon = target - output \tag{24}$$

The modification of the weights is proportional to the past calculated error, the input and a learning coefficient as given below,

$$\Delta i = \mu \varepsilon x_i \tag{25}$$

$$w_i(k+1) = w_i(k) + \Delta i \tag{26}$$

where x_i is the inputs before the weight is moderated and μ is the learning coefficient with value selected randomly. In order to obtain better convergence during training, the learning rate coefficient is normally set between the values of 0 to 1. The drawback of this rule is that the output of the network must be known for calculate and adjust the weights. As a consequence of this, the delta rule is only applicable efficiently for a single layer network. As for the multilayer network, the backpropagation method is presented and will be define in the next section.

3.3.8.2 The backpropagation method

The objective of this training method is in order to train the weights of a multilayer network for obtain the required and the targeted outputs corresponding to a given set of inputs to the network. The methodology of the conventional backpropagation method is mentioned below by highlighting the important steps:

1. Weight and biases are initialized with values between -1 and 1 randomly.

2. Inputs are summed and propagated to the hidden layer for a node j as:

$$net_j = \sum_{i=1}^{Ni} w_{ji} O_i^1 + \theta_j \tag{27}$$

3. Output from node j is given by

$$O_j^2 = f(net_j) \quad (28)$$

where f is the transfer function or activation used in the hidden nodes

4. Hidden layer output is propagated to node k at the output layer given as:

$$net_k = \sum_{j=1}^{Nj} w_{kj} O_j^2 + \theta_k \quad (29)$$

5. Output from the node k is:

$$O_k^3 = f(net_k) \quad (30)$$

6. Error is solves at the layer as:

$$e = \sum_{k=1}^{Nk} (t_k - O_k^3)^2 \quad (31)$$

7. Weights are adjusted along the negative gradient descent of the error, e as:

$$\Delta w_{kj} = -\mu \frac{\partial e}{\partial w_{kj}} \quad (32)$$

where μ is the learning rate applied in the training.

8. Weights in the hidden layers and output layer are then adjusted by equations follow:

$$\Delta w_{ji} = \mu O_j^2 (1 - O_j^2) O_i^1 \sum_{k=1}^{Nk} \delta_k^3 w_{kj} \quad (33)$$

and $$\Delta w_{kj} = \mu (t_k - O_k^3) O_k^3 (1 - O_k^3) O_j^2 \quad (34)$$

9. The momentum term is then enhanced to the eq.(34) for facilitate convergence and to avoid local minima to occur:

$$\Delta w(t) = \Delta w(t) + \alpha w(t-1) \quad (35)$$

where α is the momentum term.

In training of multilayered neural networks, the backpropagation algorithm is verified to be extremely effective. Filtering of errors is used in the system and applied to modify the connection concerning the layers in a supervised learning

approach, thus improving performance. Another method of training which gives faster convergence is the Levenberg-Marquardt method as explained in the next section.

3.3.8.3 Levenberg-Marquardt method

Levenberg-Marquardt method is a nonlinear least square optimization algorithm based on Newton's method. In order to minimize a function $R(x)$ with respect to the parameter vector x, therefore Newton's method would be:

$$\Delta x = -[\nabla^2 R(x)]^{-1} \nabla R(x) \tag{36}$$

where $\nabla^2 R(x)$ is the Hessian matrix and $\nabla R(x)$ is the gradient. Suppose that $R(x)$ is a sum of squares function,

$$R(x) = \sum_{i=1}^{N} e_i^2(x) \tag{37}$$

then it can show that

$$\nabla R(x) = J^T(x) e(x) \tag{38}$$

$$\nabla^2 R(x) = J^T(x) J(x) + S(x) \tag{39}$$

where $J(x)$ is the Jacobian matrix and

$$P(x) = \sum_{i=1}^{N} e_i(x) \nabla^2 e_i(x) \tag{40}$$

For the Gauss-Newton method, it is assumed that $P(x) \approx 0$, and the weight updates in eq.(36) becomes,

$$\Delta x = [J^T(x) J(x)]^{-1} J^T(x) e(x) \tag{41}$$

The Levenberg-Marquardt modification to the Gauss-Newton method is,

$$\Delta x = [J^T(x) J(x) + \vartheta I]^{-1} J^T(x) e(x) \tag{42}$$

The parameter ϑ is the multiplied by some factor β whenever a step would result in an increased $R(x)$. When a step reduces $R(x)$, ϑ is divided by β. Remark that when ϑ is great, the system converts steepest descent with step $1/\vartheta$, while for smaller ϑ, the algorithm becomes Gauss-Newton. The Levenberg-Marquardt method is interpolated concerning the truncated Taylor-series and the approaches based on the maximum neighborhood gives an adequate representation of the nonlinear model. This technique is located that it has beneficial when compared with the other algorithm. In this work, the neural network model is trained by using this method.

Chapter 4

Simulation

The method of the process simulation is shown in this chapter that consist of three parts. The first part represents dynamic model of ethylene polymerization process that the nonlinear equation model is solved. The second part introduce the estimator which is applied in this process namely sliding mode observer (SMO) and neural network (NN). Ultimately, the hybrid estimator that combines between SMO and NN is designed. The simulation of the ethylene polymerization process is solved by using MATLAB software.

4.1 Dynamic model of ethylene polymerization process

The process model that was improved by McAuley, McDonald and Mclellan is applied in this work. Kinetic parameters were validated compared to plant data that cause of selecting this model. The description on the parameters and various states of the process model is described in the previous chapter. The nonlinear differential equations can presente in state space vector equation of the form

$$\frac{dx(t)}{dt} = f(x(t), u(t), D(t), \emptyset) \tag{43}$$

$$y = g(x(t), \emptyset) \tag{44}$$

where x is a vector of state variables, which variable as C_{M2} (butene concentration), C_{M1} (ethylene concentration), C_N (nitrogen concentration), C_H (Hydrogen concentration), Y_c (Number of moles at the catalyst site), T_g (recycle stream temperature) and T (reactor temperature)

u is a vector of input variables that are the process inputs namely F_{M2} (molar flow rates of bulene), F_{M1} (molar flow rates of ethylene), F_N (molar flow rates of nitrogen), F_H (molar flow rates of hydrogen), F_g (recycle flow rate), F_w (cooling water flow rate), and F_c (catalyst flow rate) and T_f (feed temperature)

D is a vector of measurable disturbance variables

y is a vector of measured output (reactor temperature, T)

$\emptyset$ is the system constant parameters

The model of ethylene polymerization process is simulated in the MATLAB program with values of the steady state operating condition and process parameters that is shown in Table 4.1 and Table 4.2.

Table 4. 1 Steady state operating condition

C_{M1}	297.06 mol/m^3	Y_c	5.849	mole
C_{M2}	116.17 mol/m^3	T	355.85	K
C_H	105.78 mol/m^3	B_t	10.39	mole/s
C_N	166.23 mol/m^3	F_w	3.11x10^4	mole/s
F_{M1}	131.13 mol/s	T_g	324.7	K
F_{M2}	3.5100 mol/s	T_{wo}	308	K
F_H	1.6000 mol/s	T_{wi}	293	K
F_N	2.5200 mol/s	F_c	2	kg/h

Table 4. 2 Process parameters

B_w	70x10^7	g	k_{p1}	85	L/mole s
C_p	0.85	cal/g K	k_{p2}	3	L/mole s
E	9000	cal/mole	T_f	293	K
V_g	500	m^3	ΔP	3	atm
T_{ref}	360	K	a_c	0.548	mole/kg
ΔH	-894	cal/g	Cp_{M1}	11 K	cal/mole
k_d	0	1/s	Cp_{M1}	24 K	cal/mole
$M_r Cp_r$	1400	kcal/K	Cp_H	7.7 K	cal/mole
F_g	8500	mole/s	Cp_N	6.9 K	cal/mole
UA	1.263x10^5	cal/s K	Cp_w	18 K	cal/mole

4.2 Estimator

4.2.1 Design of SMO

The sliding mode observer drive estimated states to hypersurface by using nonlinear high-gain feedback. The hypersurface is no discrepancy concerning the measured value and the estimated value. A scaled switching function such as the signum (i.e., sgn) of the estimated is used in the observer for the nonlinear gain. Hence, due to this high-gain feedback, the vector field of the observer has a crease in it so that observer trajectories slide along a curve where the estimated output matches the measured output exactly. When process is check observability, so the observer can drive process to the actual value. In this work, the SMO is used to estimate ethylene concentration of the ethylene polymerization process by measured reactor temperature. The structure of SMO illustrates in Figure 4.1.

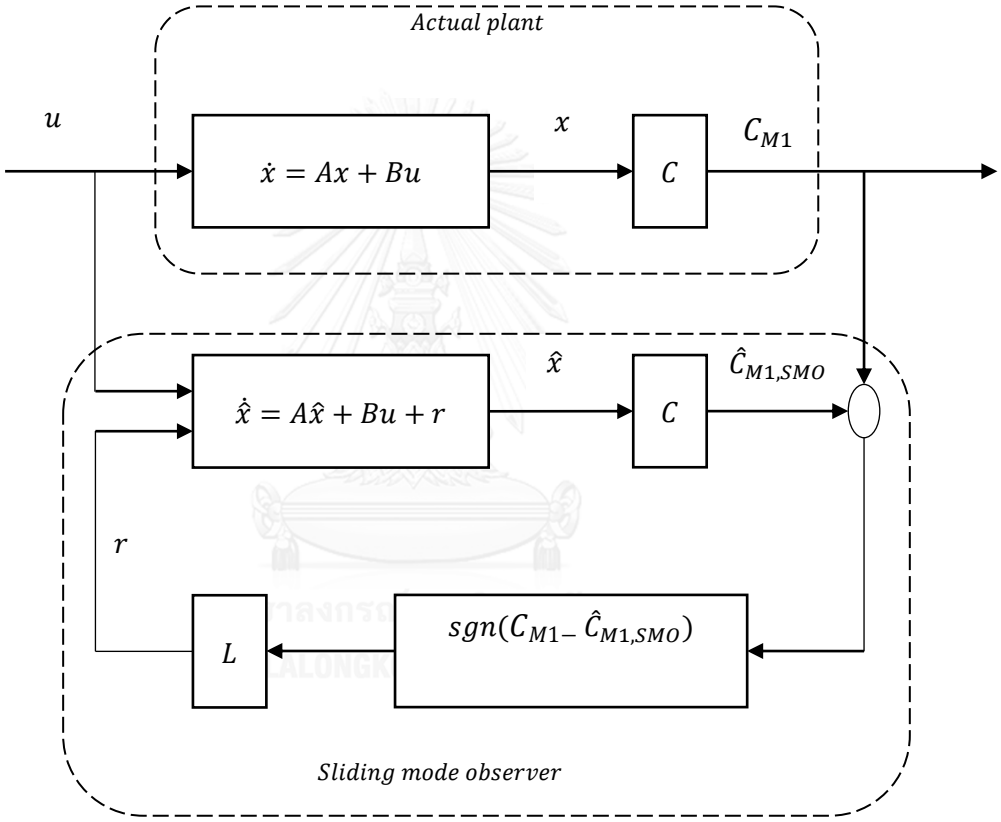


Figure 4. 1 The schematic diagram of SMO design

A class of nonlinear systems can construct by the sliding mode observer. The original variable estimate $\hat{x}$ can write by this observer follow as:

$$\dot{\hat{x}} = A\hat{x} + Bu + Lsign(y - \hat{y}) \tag{45}$$

with $L = place(A, C, m)$ (46)

where $\dot{\hat{x}}$ is the estimated value

$\hat{y}$ is the output yields the estimated state vector $\hat{x}$

y is the measurement vector from nonlinear model, which variable as T

$sign$ is understood componentwise for vector argument $z = col(z_1, \dots, z_n)$ and $sgn(z) = col(sgn(z_1), \dots, sgn(z_n))$

L is the observer gain which is solved by the pole position using the equation shown in eq.(46)

A is 7Nx7N Jacobians matrix which is calculated by

$$A = \frac{\partial f}{\partial x} = \begin{matrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{matrix}$$

C is Nx7N Jacobians matrix as [0 0 0 0 0 1 0]

m is the chosen position for the error dynamics that is characteristics equation.

4.2.2 Design of NN

In this section, the neural network estimator is trained to estimate the ethylene concentration. Data for training the neural network in the simulation work are obtained by solving the ordinary differential equations (ODEs) that govern the ethylene polymerization process as discussed in the previous chapter. Equation (1), (2), (3), (4), (7) and (9) in chapter III are solved to obtain process states according to changes in the manipulated variable such as coolant temperature, T_w. Two data sets have been prepared for training the neural network model and one is used for cross validation purposes in order to test the validity of the trained neural network. The system identification is improved by training procedure which is trained switch between two training data set. Figure 4.2, 4.3 and 4.4 show the first, second training and the cross validation data sets respectively.

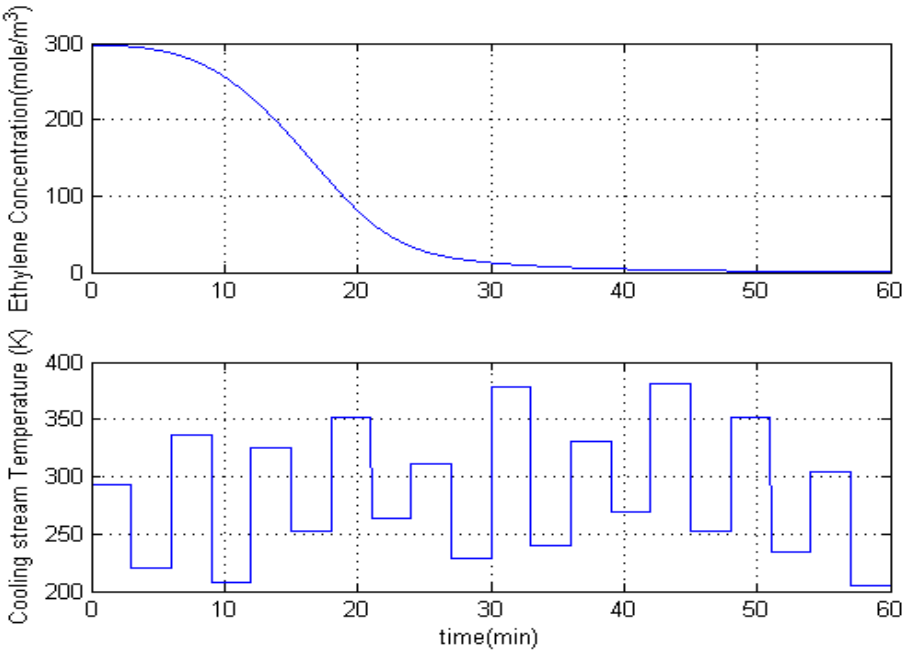


Figure 4. 2 First training data set for NN

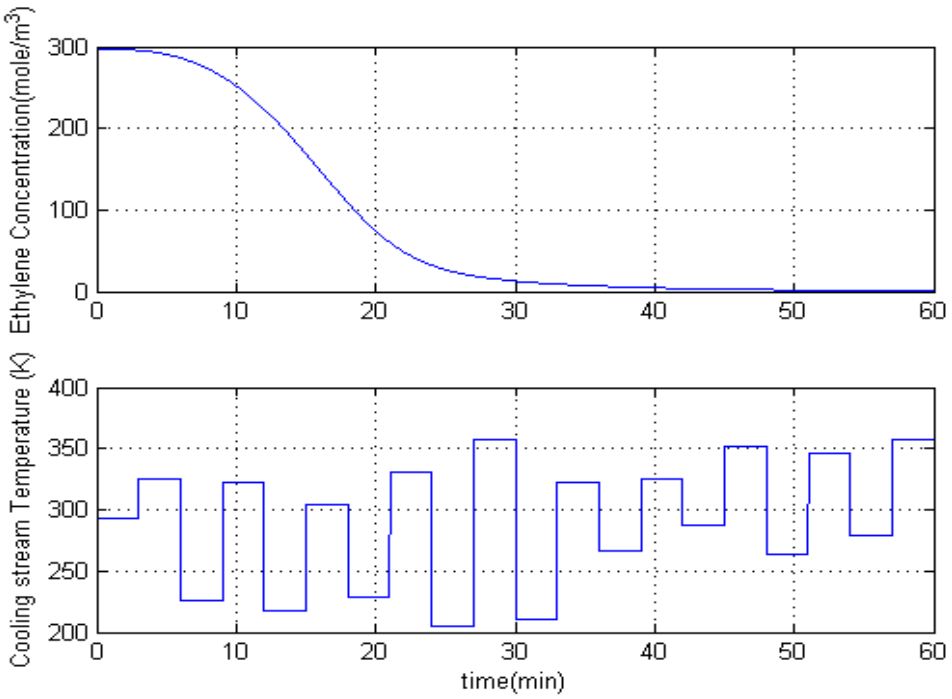


Figure 4. 3 Second training data set for NN

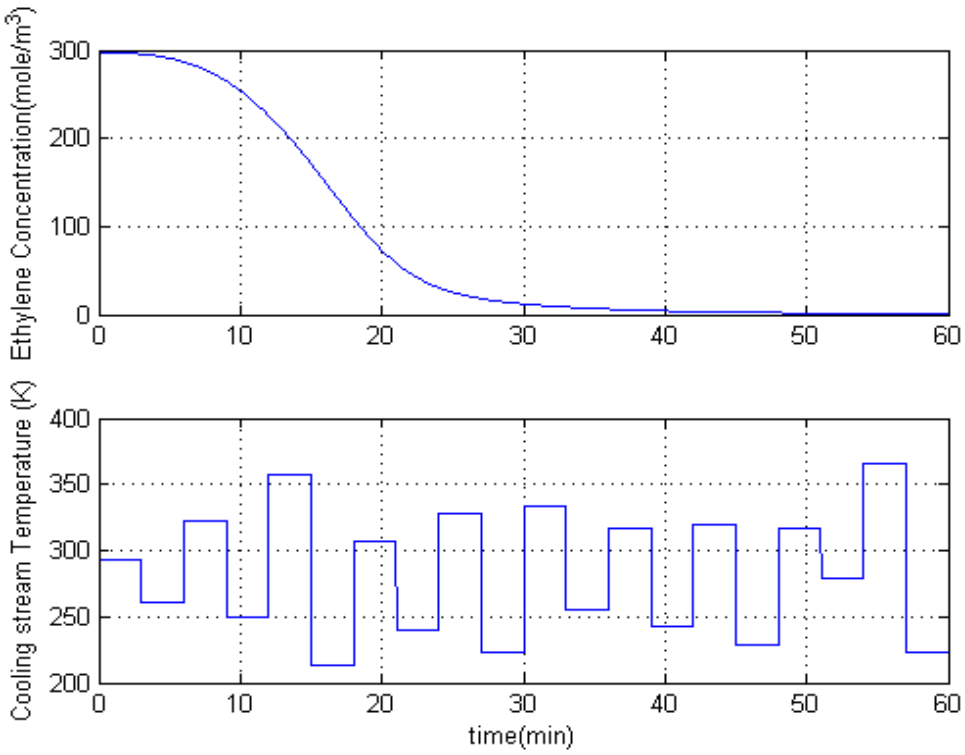


Figure 4. 4 Cross validation data set for NN

The inputs of the neural network model are reactor temperature (T) and recycle stream temperature(T_g). The desired network output is assigned to be the ethylene concentration, C_{M1}. During training, the weights each input are modified for obtain value with corresponding the target value. Performance index is represented of the model by using training technique. Primarily, weights and bias is random thus training algorithm is used in order to obtain the weights and bias appreciatory. Performance index will update and develop whereas the weights are adjusted throughout training. When error frequency is minor or achieves its desired value, the training procedure will finish. Mean squared-error (MSE) is used to the performance index.

The training data two sets is switched for training until the neural network obtain the MSE value satisfy. For obtain the feed forward neural network model, the hidden nodes number play vary significant role in the network performance. Try and error method is use in selection of the hidden node. The correct number of hidden nodes is chosen when neural network obtain the minimum-trained error. Another data set is used to validate neural network model which is excluding the two training data sets.

Table 4. 3 The components of neural network models

Parameters	Description
Network	Feed forward neural network
Performance function	MSE
Training algorithm	Levenberg-Marquardt
Epochs	300
Node in hidden layer	5
Activation function	Sigmoid function
Node in hidden layer	1
Activation function	Linear function

In this study, the forward model for the ethylene polymerization process is a two-layered feedforward neural network consisting of 4 input nodes, 5 hidden nodes and 1 output node as shown Figure 4.5. The input of this model are temperature of reactor and temperature of the recycle stream. These inputs are chosen because they are online measured in the plant. The sigmoid transfer function is applied in the hidden nodes and in the output node used linear transfer function. The network is trained using the Levenberg-Marquardt backpropagation algorithm until it satisfies or less than performance with criteria of mean square error (MSE) of 0.0001. The error which is between the actual desired values and the output from the network training was defined. The details of component of NN estimator as shown in Table 4.3.

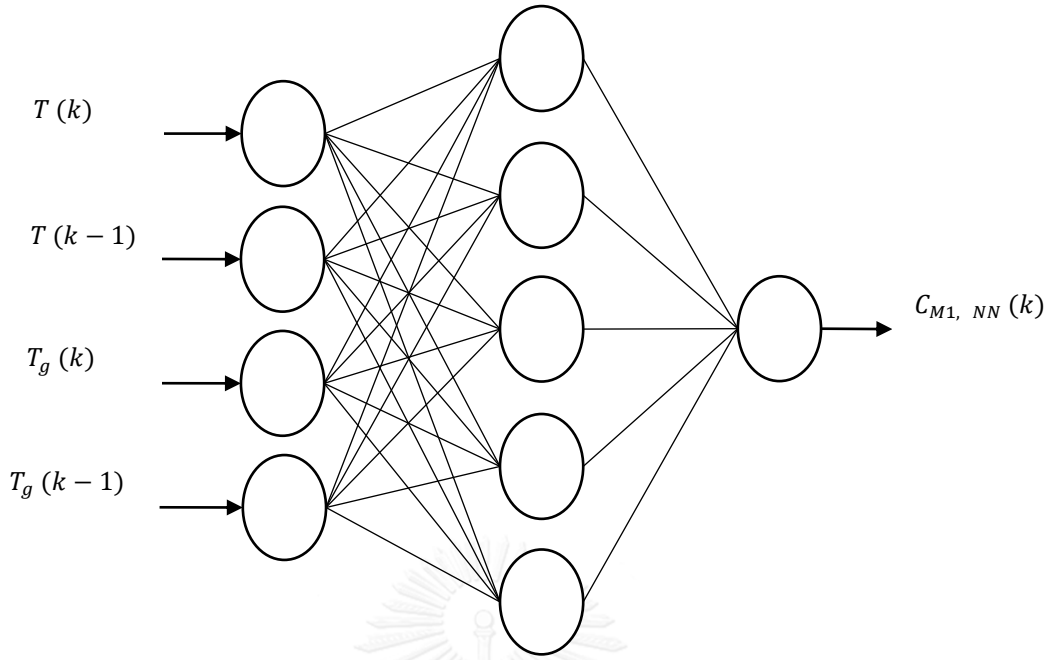


Figure 4. 5 The structure of NN in the NN estimator

In this work, an algebraic equation can be presented on the neural network output. The output of the neural network can solve by the general equation as shown in eq.(47).

$$O = f^2(w^{2,1}f^1(w^{1,1}p + b^1) + b^2) \tag{47}$$

where O is outputs from the neural network

p is inputs to the neural network

f^1 is activation function at layer1 (input layer)

f^2 is activation function at layer2 (hidden layer)

$w^{1,1}$ is weight at layer 1 (input layer)

$w^{2,1}$ is weight at layer 2 (hidden layer)

b^1 is bias value at layer 1 (input layer)

b^2 is bias value at layer 2 (hidden layer)

4.3 Hybrid estimator

In this research, I design the hybrid estimator that merges between the sliding mode observer (SMO) and neural network (NN) for estimating the ethylene concentration. The hybrid estimator, SMO-NN, is developed from SMO combined with NN. The first step, the SMO is used to estimate state variable of the. I used the SMO firstly since the SMO recommends to stable estimation and fast convergence whereas it can create the signal or sliding motion on the output error and the measured error. And then, the $\hat{C}_{M1,SMO}, T$ and T_g are sent to the NN for estimating the ethylene concentration again. The structure of SMO-NN hybrid estimator is shown in Figure 4.6.

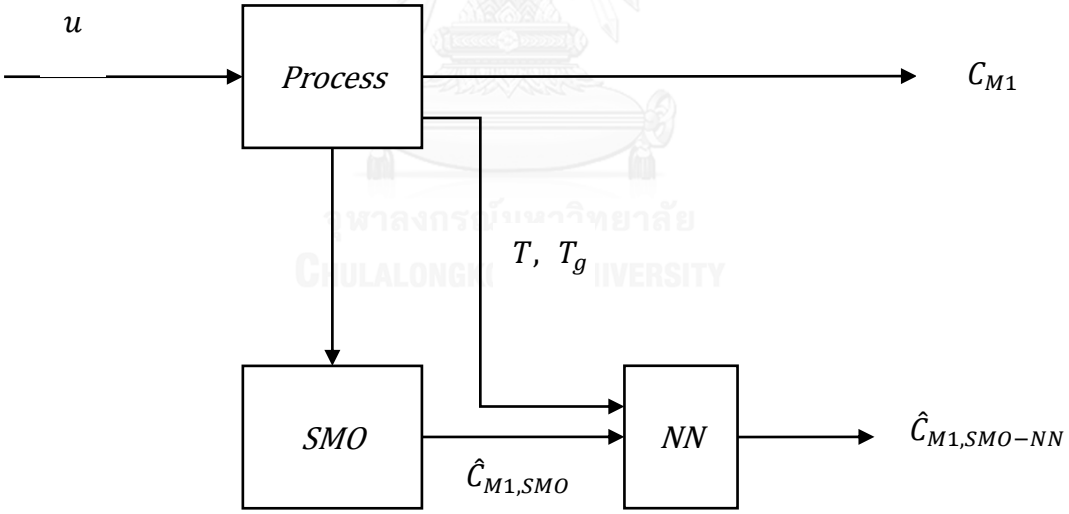


Figure 4. 6 The structure of SMO-NN hybrid estimator.

For SMO in this structure, the SMO used applied to estimate the state variable which is the ethylene concentration. The SMO structure represents in the previous section. After that, NN inputs are selected as the value of estimated state variables from the SMO that including $\hat{C}_{M1,SMO}, T$ and T_g for estimating ethylene concentration

again. In this structure, $\hat{C}_{M1,SMO}$ estimated by the SMO is added to input of neural network for increasing accuracy. In the NN estimator, $\hat{C}_{M1,SMO}$ does not chosen to input because it cannot online measured but $\hat{C}_{M1,SMO}$ can use to input of the hybrid estimator due to estimating by the SMO. The optimal NN estimator consists of 6 nodes of input layer, 4 nodes of a hidden layer and a node of output layer (6-4-1 configuration). The optimal NN is used to estimate the ethylene concentration which is the output of the SMO-NN hybrid estimator from the estimated state variables of SMO. The topology of NN has exposed in Figure 4.7. The details component of hybrid neural network as shown in Table 4.4.

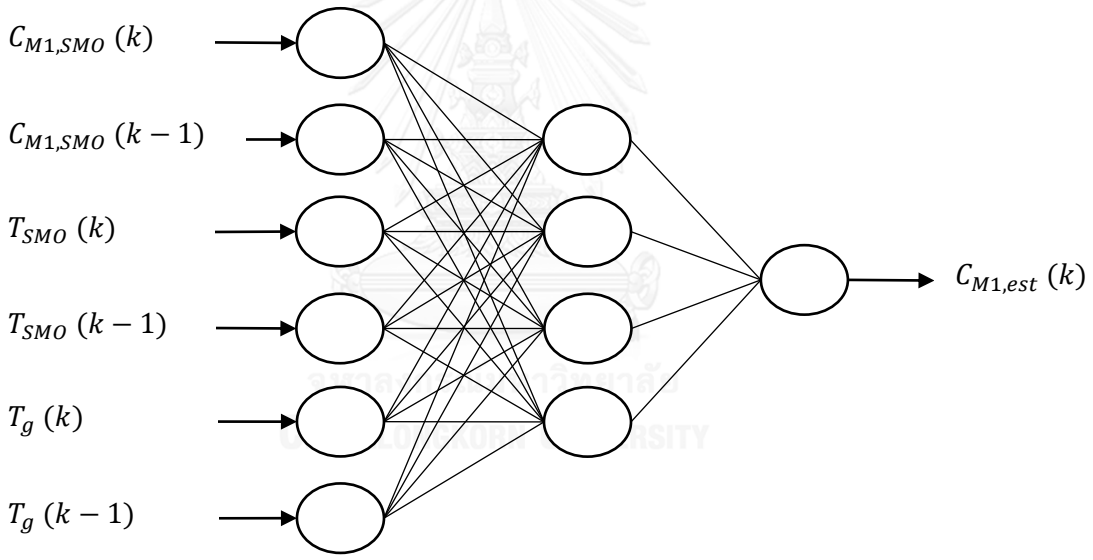


Figure 4. 7 The structure of NN in the SMO-NN hybrid estimator

Data for training the NN in the SMO-NN hybrid estimator are obtained by solving the ordinary differential equations (ODEs) and the SMO. The training method of the NN estimator is same as the NN estimator of the SMO-NN hybrid estimator. The two training sets data and the cross validation data sets of the networks show in Figure 4.8, 4.9 and 4.10 respectively. The details of component of NN hybrid estimator as shown in Table 4.2.

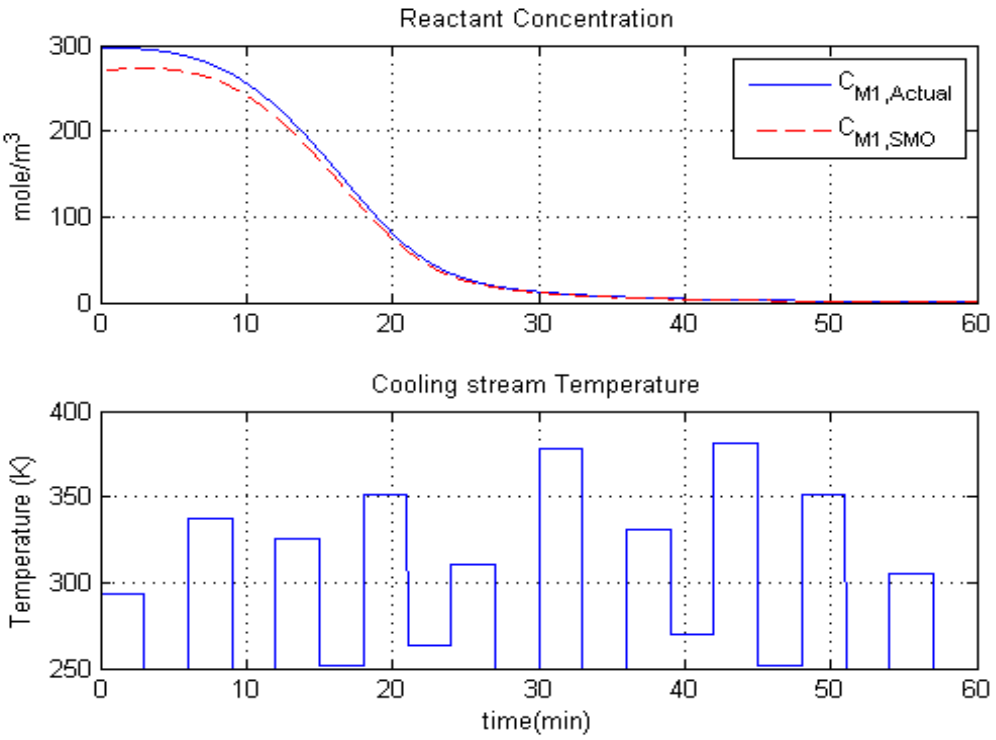


Figure 4. 8 First training data set for SMO-NN

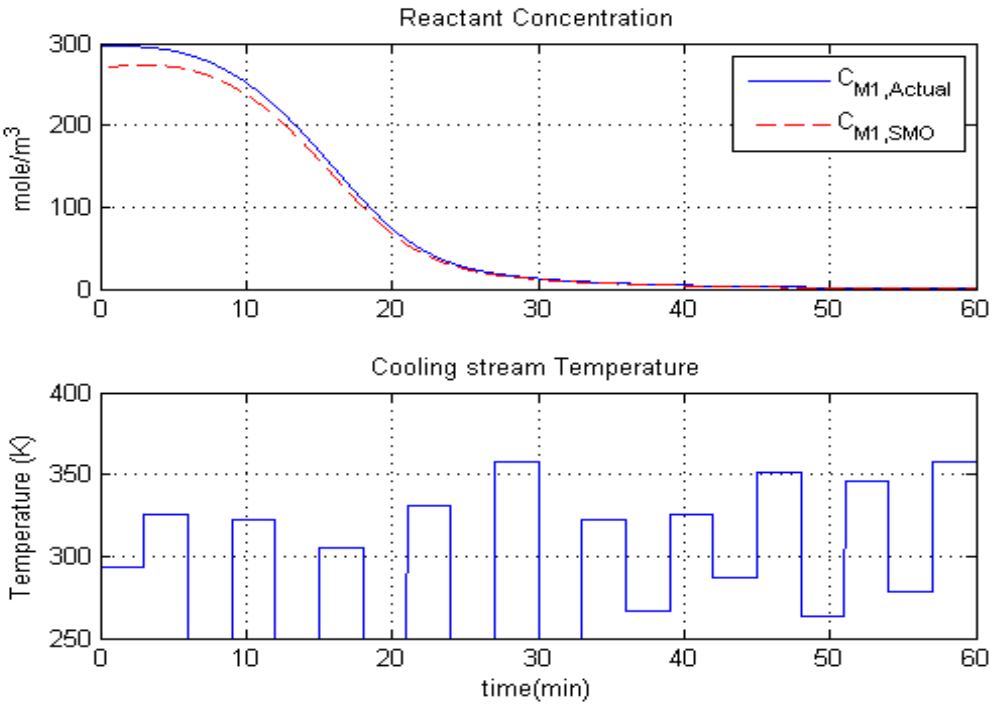


Figure 4. 9 Second training data set for SMO-NN

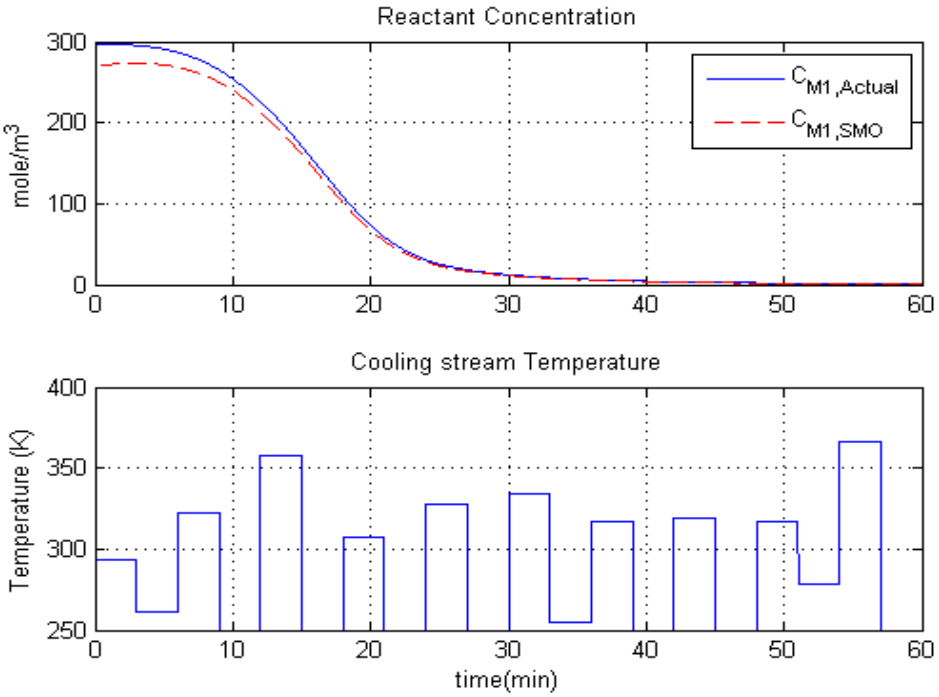


Figure 4. 10 Cross validation data set for SMO-NN

The performance of the SMO-NN hybrid estimator is compared with the SMO and the NN estimator under normal, noise and disturbance conditions which is discussed in the next chapter.

Table 4. 4 The components of hybrid neural network models

Parameters	Description
Network	Feed forward neural network
Performance function	MSE
Training algorithm	Levenberg-Marquardt
Epochs	300
Node in hidden layer	4
Activation function	Sigmoid function
Node in hidden layer	1
Activation function	Linear function

Chapter 5

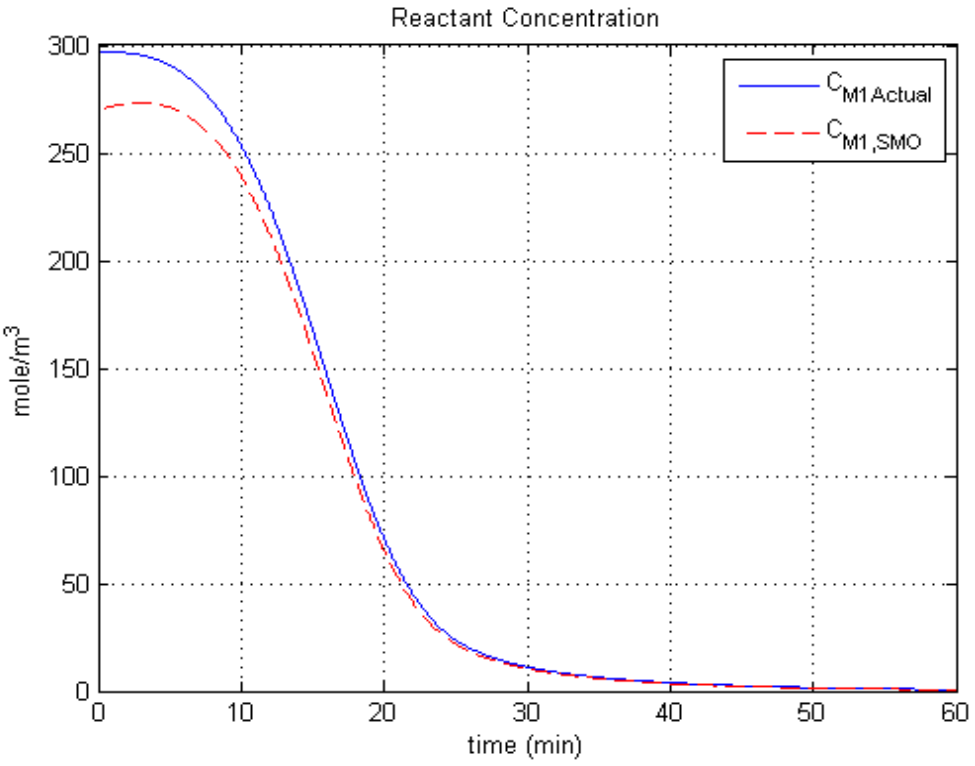
Simulation results

In this chapter, the SMO, the NN estimator and the SMO-NN hybrid estimator are applied to estimate the ethylene concentration in ethylene polymerization process. The performances and robustness of the all estimators are test with three conditions including the normal condition, noise condition and disturbance condition. In addition, the simulation results of SMO-NN hybrid estimator is compared with the SMO and the NN.

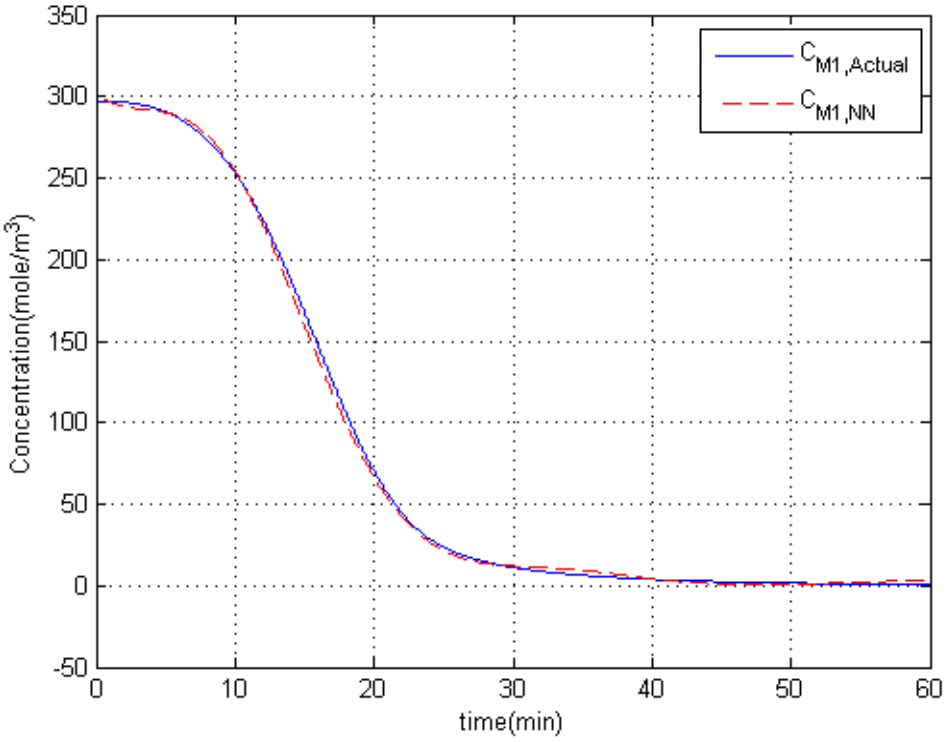
5.1 Normal condition

In this condition, the estimators provide the estimated ethylene concentration using the measured reactor temperatures which are calculated from the ethylene polymerization process models under the normal condition. The ethylene concentration estimation simulation results are demonstrated in Figure 5.1.

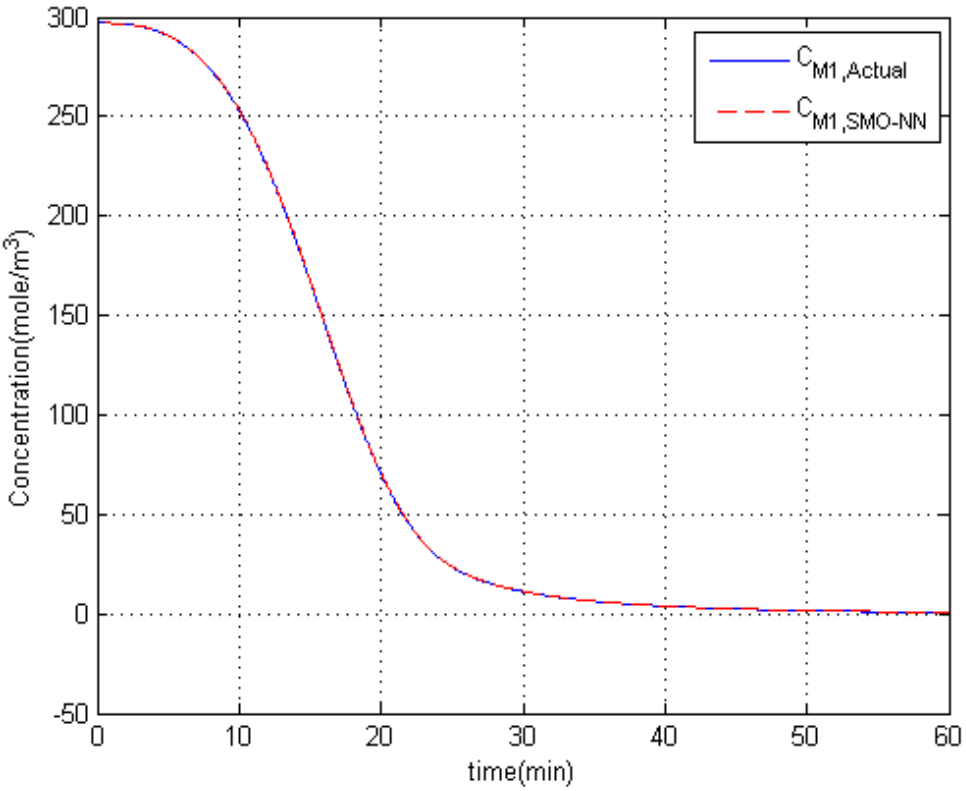
From Figure 5.1(a), sliding mode observer (SMO) is used to estimate the ethylene concentration. The simulation result shown that the SMO can estimate smooth estimation. The SMO used the dynamics of the estimation error to drive estimated value converge to actual data. However, the result indicated that the SMO has large error between the actual plant value and the estimated concentration. Due to, the primary of estimation, we assumed initially any values of estimated value. After that, the estimated value is recalculated by the SMO until the estimated value close to the actual value.


Reactant Concentration
$C_{M1,Actual}$
$C_{M1,SMO}$
mole/m3
time (min)
0
50
100
150
200
250
300
0
10
20
30
40
50
60

(a)


$C_{M1,Actual}$
$C_{M1,NN}$
Concentration(mole/m3)
time(min)
-50
0
50
100
150
200
250
300
350
0
10
20
30
40
50
60

(b)



(c)

Figure 5. 1 The estimation of the ethylene concentration under normal condition: a) SMO, b) NN estimator and c) SMO-NN hybrid estimator

Based on Figure 5.1(b), the ethylene concentration is estimated by neural network (NN) estimator. The optimal NN estimator consists of 4 nodes of input layer, 5 nodes of one hidden layer and one node of output layer (4-5-1 configuration). The training target data are the ethylene concentration (C_{M1}), produced from the simulation. The activation functions which are used in hidden layer as sigmoid function and output layer as linear function. The simulation result has shown that the NN estimator can be estimated the ethylene concentration and the estimated value approximate the actual data. However, the result of estimation has small error between the estimated value and the actual value and unsmooth. In order that, the

inputs of the NN estimator which are temperature of reactor and temperature of recycle stream are not sufficient sensitivity, so it has an affect on the accuracy estimation.

Table 5. 1 The summary of performance comparison between the designed estimators under the normal condition, noise condition and disturbance condition

Condition	IAE		
	SMO	NN	SMO-NN
Normal condition	20,021.69	2,391.42	835.25
Noise condition (1K)	12,995.84	23,623.08	2,509.60
Disturbance condition#1 (F_{M1}+5%)	20,164.77	7639.92	761.55
Disturbance condition#2 (F_{M1}+10%)	20,305.20	13,643.51	573.89

From Figure 5.1(c), the SMO-NN hybrid estimator is designed for estimating the ethylene concentration to improve performance of the SMO and the NN estimator. The SMO found problem about initially error, so the NN estimator combined into the SMO for increasing accuracy. The simulation result show that the SMO-NN hybrid estimator is capable of estimating the ethylene concentration excellent. The result of the estimation of the SMO-NN hybrid estimator showed fast to drive estimated value close to actual value and can be estimated smoothly. The SMO-NN estimator, the SMO and the NN estimator are compared performance of estimation by calculation Integral Squared Error (IAE) value. The IAE value of the SMO-NN estimator, the SMO and the NN estimator are 20,021.69, 2391.42 and 835.25, respectively. From the IAE value show that the SMO-NN hybrid estimator has the least value as shown

in Table 5.1. As the result, in normal condition, the SMO-NN hybrid estimator is the best of estimator.

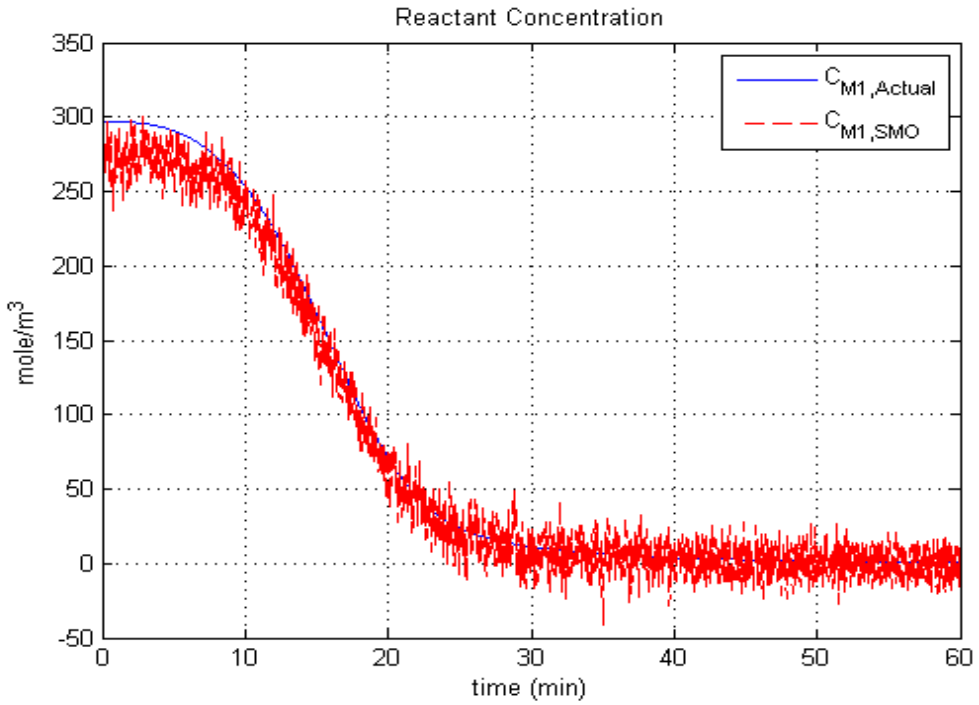
5.2 Noise condition

For this condition, noise is presented in the system. Random noises accounting to 1 K from the temperature of reactor are introduced into the measured temperature of reactor to evaluate robustness and performance of the estimators under real situations.

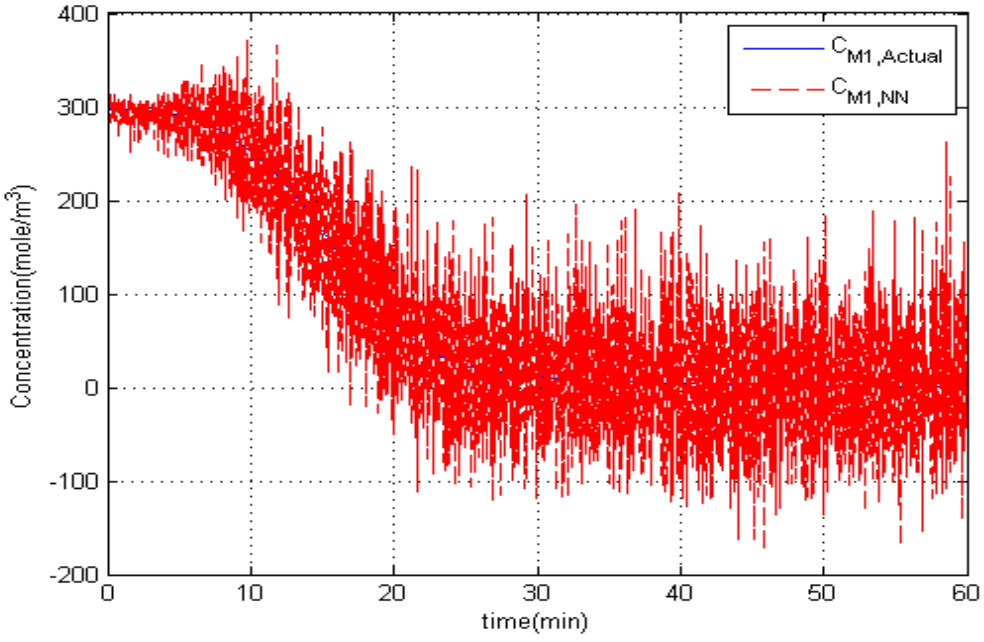
As shown in Figure 5.2(a), the result of estimation shows that the SMO can provide to acceptable estimate the ethylene concentration. The SMO used the sign of the error to drive the observer, thus it becomes insensitive to many forms of noise. However, the initial of estimation is far away from actual data. From Figure 5.2(b), the NN estimator cannot provide for estimating the ethylene concentration because noise signal strongly affects to the inputs of NN which is sensitively. Hence, the NN estimator do not appreciate to apply to estimate the ethylene concentration in this noise condition.

The simulation result of the SMO-NN hybrid estimator is shown in Figure 2.2(c). The SMO-NN hybrid estimator still estimates the ethylene concentration even noise signal is added to system. Because of advantage of the SMO and NN estimator, the SMO-NN is able to estimate concentration against noise. Advantages of SMO are provide fast convergence and robustness. On the other hand, benefits of NN are accuracy estimated and suitable for nonlinear system. Because of NN sensitivity, the SMO is design first for support noise condition. After that, NN is design later for approve accuracy estimated value from SMO. For this reason, the SMO-NN hybrid estimator

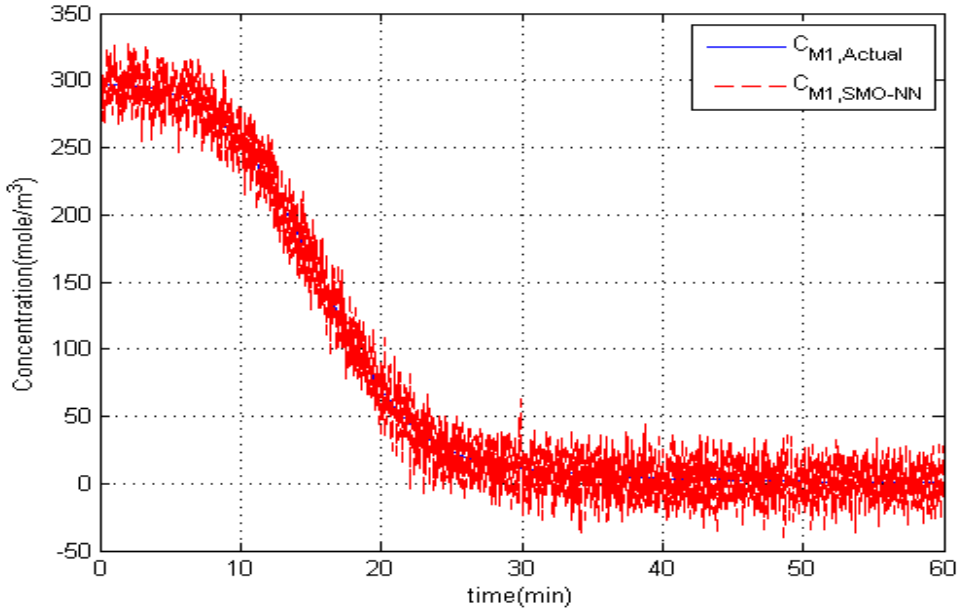
can estimate the ethylene concentration in this condition. In addition, the IAE value represents that the SMO-NN hybrid estimator has the least IAE value when compare with the SMO and the NN estimator in noise condition as shown in Table 5.1.



(a)



(b)



(c)

Figure 5. 2 The estimation of the ethylene concentration under noisy condition: a) SMO, b) NN estimator and c) SMO-NN hybrid estimator

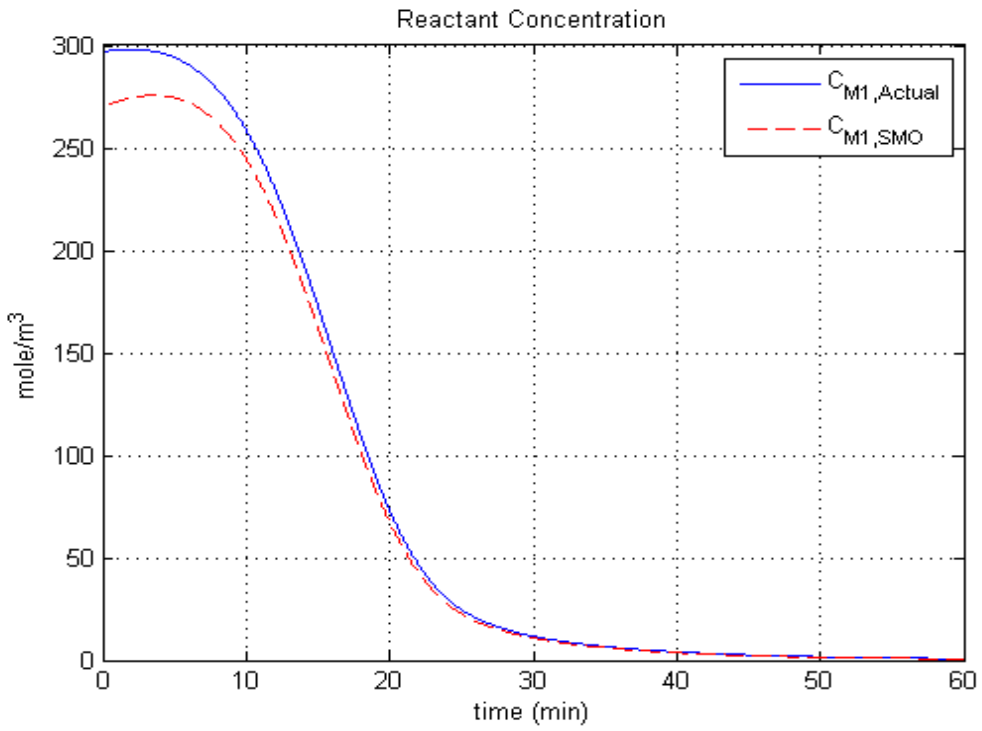
5.3 Disturbance conditions

The designed estimators are also evaluated involving several disturbances. For the disturbance condition, the molar flow rates of ethylene (F_{M1}) are increased by 5% and 10% from the normal value. The two case simulation results are discussed in below section.

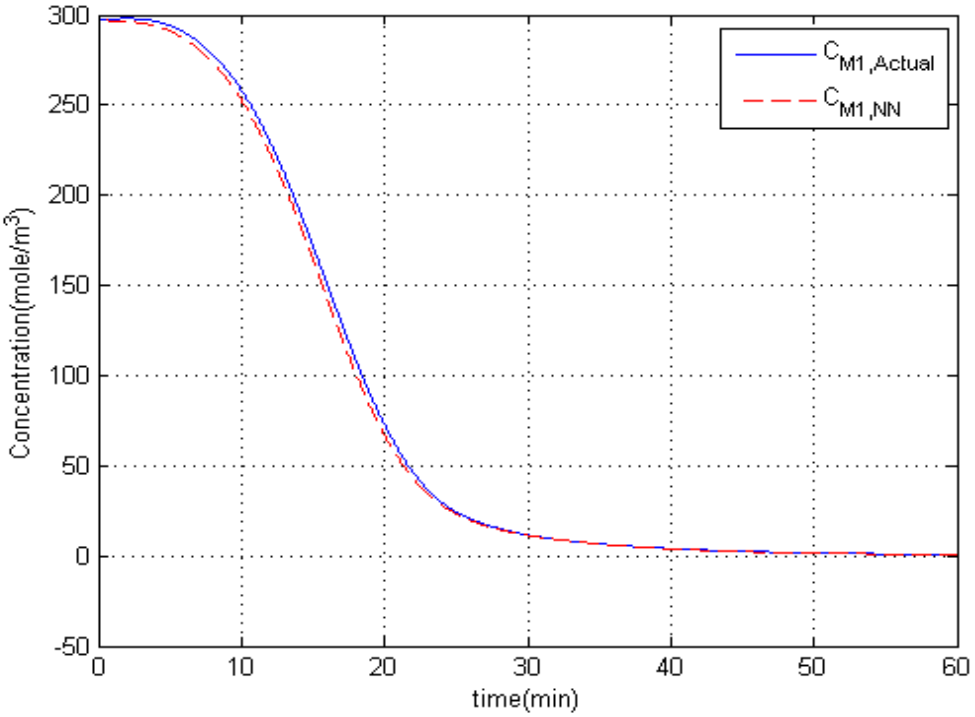
5.2.1 5% increasing of the molar flow rates of ethylene

First, the process is simulated by using the ODEs equation and parameters as shown in Table 4.1 and Table 4.2 but the molar flow rates of ethylene parameter is increased by 5% from 131.13 mol/s to 137.69 mol/s. This simulation information is used to the actual data for comparing with the designed estimator in this case.

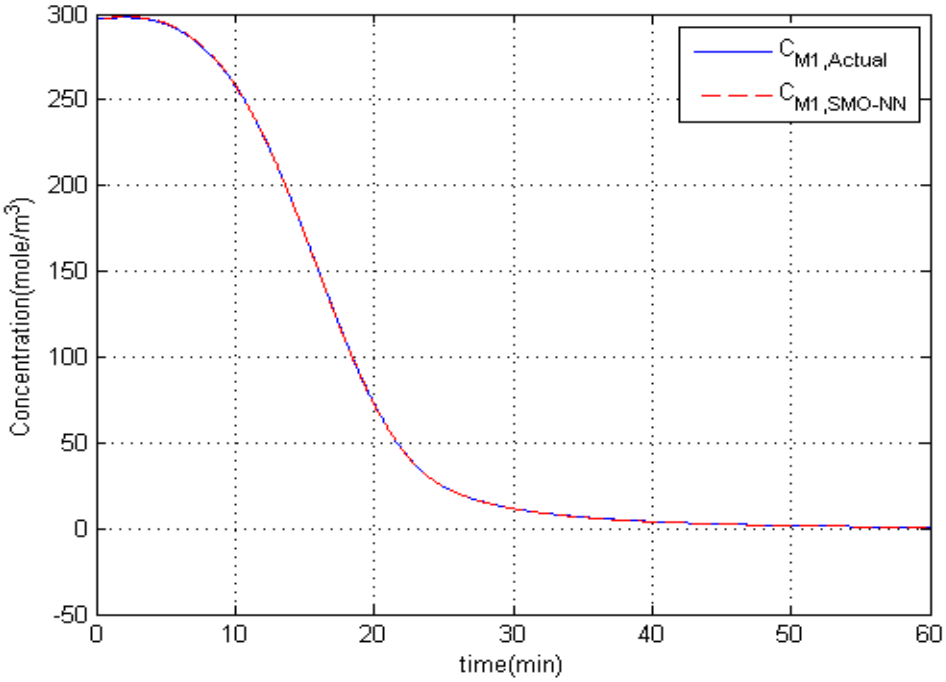
Based on Figure 5.3, the simulation shows the results of the SMO, the NN estimator and the SMO-NN hybrid estimators for estimating the ethylene concentration with introduced F_{M1} disturbance. From Figure 5.3(a), the simulation result of the SMO shows that the SMO can estimate the ethylene concentration like the normal condition. Due to dynamics of the estimation error term, the SMO has more robustness. However, it still has large error initially because the initial estimated value is assumed. On the other hand, the results of the NN estimator and the SMO-NN hybrid estimator show that they can give the estimate of the ethylene concentration accurately while the NN estimator shows the small discrepancy between the estimated value and the actual value. The comparative performance of the SMO-NN hybrid estimator, the SMO and the NN estimator are compared by IAE value as shown in Table 5.1.



(a)



(b)

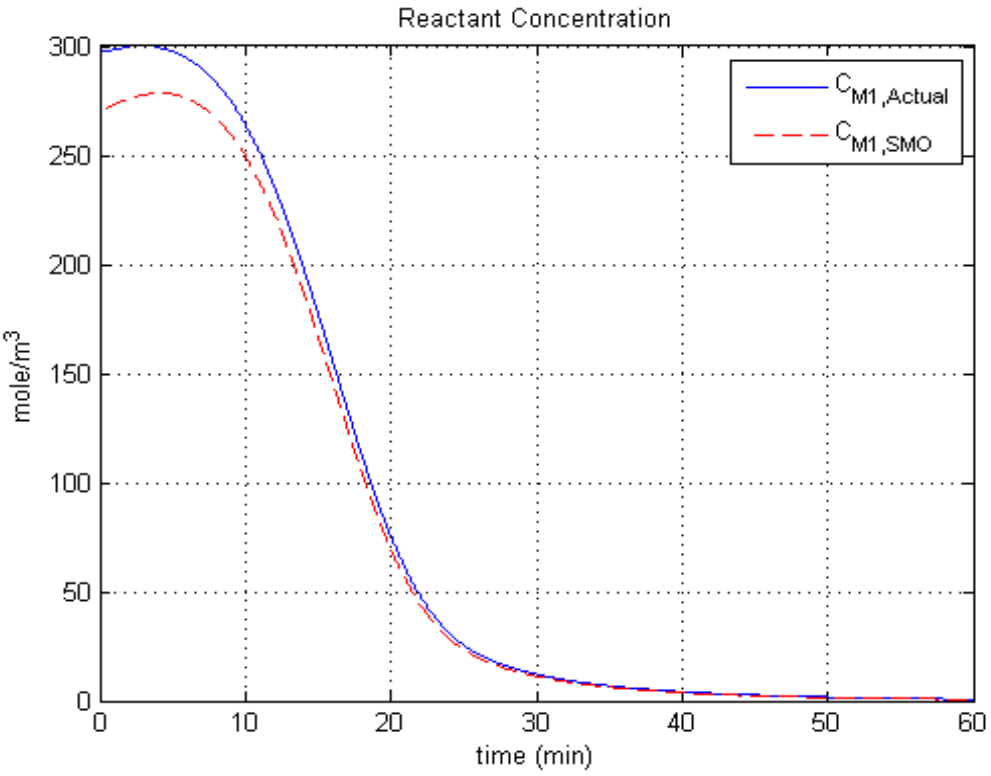


(c)

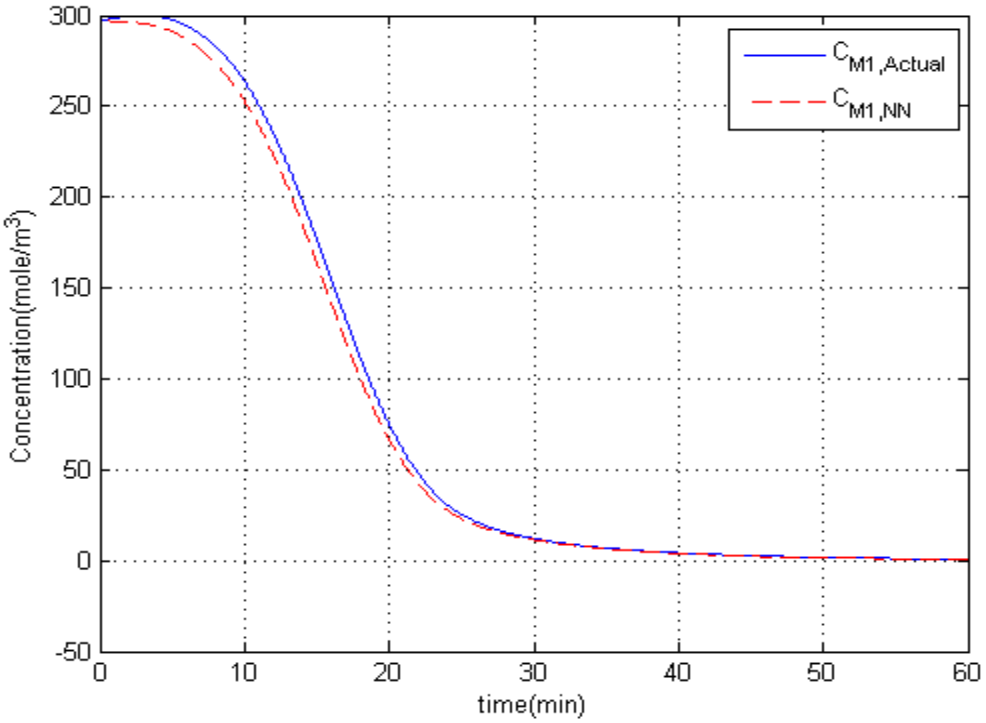
Figure 5. 3 The estimation of the ethylene concentration under disturbance condition (5% increasing of F_{M1}): a) SMO, b) NN estimator and c) SMO-NN hybrid estimator

5.2.2 10% increasing of the molar flow rates of ethylene

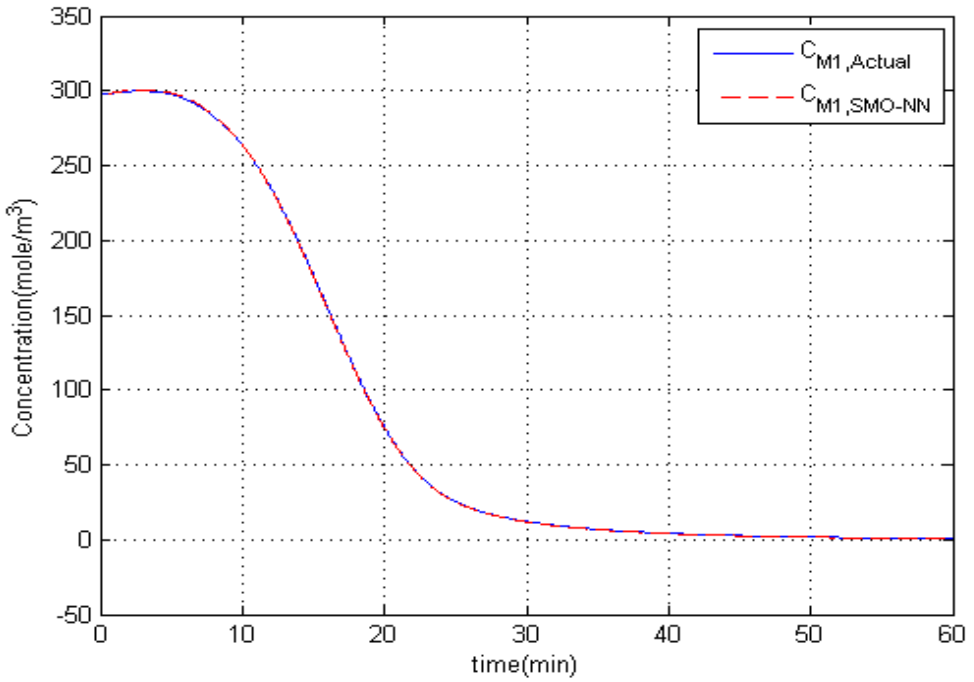
Like the 5% increasing of the molar flow rates of ethylene case, we run the process simulation using the condition as given in Table 4.1 and Table 4.2 but the molar flow rates of ethylene parameter are increased by 10% from 131.13 mol/s to 144.24 mol/s. The process model is run in order to find the new actual value that this value is used to compare with the ethylene concentration estimated by all estimators.



(a)



(b)



(c)

Figure 5. 4 The estimation of the ethylene concentration under disturbance condition (10% increasing of F_{M1}): a) SMO, b) NN estimator and c) SMO-NN hybrid estimator

In this case, the molar flow rates of ethylene (F_{M1}) are increased by 10%. The simulation results of this case are shown in Figure 5.4. From Figure 5.4, the simulations show result of the ethylene concentration estimation of the SMO, the NN estimator and the SMO-NN hybrid estimator. Their results have shown that all the proposed estimator can estimated the ethylene concentration smoothly like the 5% increasing of the molar flow rates of ethylene case. However, in all the proposed estimator, the SMO-NN hybrid estimator give the best of the estimation. In addition, the IAE value of the SMO-NN estimator indicates that it has the least of value when comparing with the SMO and the NN estimator in this case.

Chapter 6

Conclusion and Recommendations

6.1 Conclusion

In this work, the proposed hybrid estimator which combined between sliding mode observer (SMO) and neural network (NN) is designed for estimating the ethylene concentration of the ethylene polymerization process. The structure of hybrid estimator, which is SMO-NN hybrid estimator is studied. The first part of the SMO-NN hybrid estimator, SMO that provided fast and accurate estimation used applied to estimate all state variables and its output are sent to be NN input. The second part, the NN estimator estimates the ethylene concentration again from SMO output. The performance of the SMO-NN is compared with the performance of the single SMO and the NN. The performance is compared with three conditions, which are normal, noisy and disturbance condition, respectively.

Simulation results have shown that proposed SMO-NN hybrid estimator has provided stable, fast and accurate estimation in spite of noise case when compared with the SMO and the NN estimator. The single SMO can smooth estimated the ethylene concentration. However, it has error because it is assumed with any values initially. In contrast, the NN estimator can provide estimation accurately in normal condition. Nonetheless, it has the differences between the estimated value and the actual value because of selecting and number of NN input node. As a result, in the ethylene polymerization process, the SMO-NN hybrid estimator is the best

approached in estimating the ethylene concentration and provide fast convergence and can handle noise when compared with the SMO and the NN estimator.

6.2 Recommendation

In this work, the SMO-NN hybrid estimator is only used to estimate the ethylene concentration. As for the future work, the SMO-NN will estimate other polymerization parameters such as molecular weight distribution (MWD) and heat transfer coefficient.

In model predictive control, the parameters which is estimated will apply for approve control performance.

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APPENDIX

VITA

Mr.Thanawat Kaewsanmuang was born in Khonkaen, Thailand on October 2, 1992. After graduating high school from Darasamutr school, he entered Burapha University in June 2010 and received his Bachelor of Engineering degree in Chemical Engineering in July 2014. After that he continued to study in the Graduate school of Chulalongkorn University and joined Control and Systems Engineering Research Laboratory in the Department of Chemical Engineering.