HYBRID FUZZY-SLIDING MODE OBSERVER DESIGN FOR ESTIMATION AND ADVANCED CONTROL OF AN ETHYLENE POLYMERIZATION PROCESS

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**FACULTY OF ENGINEERING
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ABSTRACT

Observers are computational algorithms designed to estimate unmeasured state variables due to the lack of appropriate estimating devices or to replace the high-priced sensors in a plant. It is always important to determine those unknown variables before developing state feedback laws for control, preventing process disruptions and plant shutdowns. Due to high-nonlinearities of the chemical process systems, a single observer may not be sufficient to estimate the variables resulting in offsets and slow estimation rates. Therefore, a hybrid approach will be the best solution. In this research, a hybrid observer is designed using the combination of artificial intelligence (AI) algorithm and conventional observer. The conventional observer chosen is the sliding mode observer (SMO) and it is merged with fuzzy logic to become the hybrid fuzzy-sliding mode observer or fuzzy-SMO. The fuzzy-SMO is designed in such a way that it can be adjusted to estimate several parameters without re-designing the overall structure of the observer. This feature is unique and different from the observers available in the literature. The estimated parameters are then used as the measured parameters to develop a model predictive control (MPC) for overall control of the process system. The MPC is embedded with an integrator to avoid offsets and is designed in three cases to imitate ideal and practical conditions. The first case is the known initial state without constraint, which is the ideal case for study or more likely for programming validation purposes. The second case is the unknown initial state without constraint, which also include the proposed hybrid fuzzy-SMO. The third case is the unknown initial state with input and output constraints incorporated in the system. Both the second and third cases are behaving like practical cases. Polymerization reactor for producing polyethylene plant is chosen as the case study to observe the performances of both the fuzzy-SMO and the embedded integrator MPC. In addition, the estimator is also validated using the experimental data

from the polymerization pilot plant to observe the precision of the simulated data towards the real plant.

ABSTRAK

Pemerhati merupakan satu algoritma pengiraan yang dibentuk bagi menganggarkan pemboleh ubah yang tidak dapat diukur kerana terdapat kekurangan alat-alat penganggar yang sesuai ataupun untuk menggantikan sensor yang mahal di dalam sesebuah loji kimia. Pemboleh ubah tersebut amat penting untuk dianggarkan sebelum mendapatkan maklum balas bagi sistem kawalan, mencegah gangguan proses dan penutupan loji. Proses kimia merupakan proses yang tidak linear, oleh itu pemerhati tunggal sahaja tidak mencukupi bagi menganggarkan pemboleh ubah dan boleh menyebabkan ofset serta memperlahankan kadar penganggaran, maka pendekatan hibrid merupakan penyelesaian yang terbaik. Dalam kajian ini, pemerhati hibrid yang direka menggabungkan ‘artificial intelligence’ (AI) dan pemerhati konvensional untuk menganggarkan pemboleh ubah tersebut. Pemerhati konvensional yang dipilih adalah ‘sliding mode observer’ (SMO) dan digabungkan dengan ‘fuzzy logic’ untuk menjadi hibrid ‘fuzzy-sliding mode observer’ atau ‘fuzzy – SMO’. Pemerhati fuzzy – SMO ini dibentuk sedemikian rupa agar dapat diselaraskan untuk menganggarkan beberapa parameter tanpa mengubah keseluruhan strukturnya. Ciri ini adalah unik dan berbeza daripada pemerhati lain yang terdapat dalam kesusasteraan. Parameter yang telah dianggarkan akan digunakan sebagai parameter terukur bagi membentuk ‘model predictive control’ (MPC) bertujuan mengawal keseluruhan proses. MPC ditambah dengan penyepadu bagi mengelakkan ofset dan dibentuk dalam tiga kes yang berbeza untuk menunjukkan keadaan yang ideal dan praktikal. Kes pertama merupakan keadaan awal yang dikenali tanpa had kekangan, yang merupakan kes ideal atau bertujuan untuk mengkaji keberkesanan program simulasi. Kes kedua adalah keadaan awal yang tidak diketahui tanpa had kekangan serta melibatkan penggunaan pemerhati hibrid ‘fuzzy – SMO’. Kes ketiga adalah keadaan awal yang tidak diketahui dengan had kekangan terhadap input dan keluaran yang dimasukkan ke dalam sistem. Kes kedua dan ketiga adalah bercirikan kes yang praktikal. Reaktor pempolimeran

bagi penghasilan polietilena dipilih sebagai kes kajian untuk menentukan prestasi kedua-dua fuzzy-SMO dan MPC dengan penyepadu. Keberkesanan pemerhati juga dikenalpasti dengan menggunakan data dari eksperimen yang dijalankan pada reactor pempolimeran berskala kecil. Ini dilaksanakan bagi menetukan kepadanan data dari program simulasi dengan data sebenar.

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LIST OF SYMBOLS AND ABBREVIATIONS

M_1	:	Ethylene
M_2	:	Butene
M_3	:	Hydrogen
M_4	:	Nitrogen
a_c	:	Active site concentration
B_t	:	Bleed flow rate
C_{M_1}	:	Ethylene concentration
C_{M_2}	:	Butene concentration
C_{M_3}	:	Hydrogen concentration
C_{M_4}	:	Nitrogen concentration
Cp_{M_1}	:	Ethylene heat capacity
Cp_{M_2}	:	Butene heat capacity
Cp_{M_3}	:	Hydrogen heat capacity
Cp_{M_4}	:	Nitrogen heat capacity
Cp_g	:	Recycle gas heat capacity
Cp_p	:	Polymer heat capacity
Cp_w	:	Water heat capacity
F_c	:	Catalyst flow rate
F_w	:	Cooling water flow rate
F_g	:	Recycle gas flow rate
F_{M_1}	:	Ethylene flow rate
F_{M_2}	:	Butene flow rate
F_{M_3}	:	Hydrogen flow rate

F_{M_4}	:	Nitrogen flow rate
O_p	:	Polymer outlet rate
M_{w_1}	:	Molecular weight of ethylene
M_{w_2}	:	Molecular weight of butene
x_{M_1}	:	Mole fraction of ethylene
x_{M_2}	:	Mole fraction of butene
x_{M_3}	:	Mole fraction of hydrogen
x_{M_4}	:	Mole fraction of nitrogen
er	:	Process error
Δer	:	Change of process error
e_f	:	Error output from fuzzy logic
k_d	:	Deactivation rate constant
k_{p1}	:	Ethylene propagation rate constant
k_{p2}	:	Butene propagation rate constant
M_g	:	Eater holdup in heat exchanger
$M_r Cp_r$	:	Thermal capacitance of reaction vessel
R_{M_1}	:	gas constant (depends on k_{p1})
R_{M_2}	:	gas constant (depends on k_{p2})
R	:	Ideal gas constant
T_r	:	Bed temperature
T_f	:	Feed temperature
T_{ref}	:	Reference temperature
T_{gin}	:	Recycle stream temperature before cooling
T_g	:	Recycle stream temperature after cooling

HF	:	Sensible heat of fresh feed
HG	:	Sensible heat of recycle gas
HT_r	:	Sensible heat of bed
HP	:	Sensible heat of product
HR	:	Enthalpy generated from the polymerization
$\mathcal{M}$	:	Characteristics equation for the closed loop poles of the system
MI	:	Melt index
P_t	:	Total pressure
T_{win}	:	Cooling water temperature before cooling
T_{wout}	:	Cooling water temperature after cooling
Y_c	:	Number of moles of catalyst site
ΔH_r	:	Heat of reaction
E	:	Activation energy for propagation
V_g	:	Reactor volume
U	:	Overall heat transfer coefficient
A	:	Heat transfer area
$\mathscr{r}$	:	Tuneable parameter
$\mathscr{k}$	:	Constant parameter
x	:	State variable
u	:	Input variable
y	:	Measured variables
A	:	State space matrix
B	:	State space matrix
C	:	State space matrix
A_m	:	Augmented state space matrix

B_m	:	Augmented state space matrix
C_m	:	Augmented state space matrix
K_{ob}	:	Observer gain
x_m	:	Initial assumed value
$\hat{x}_m$	:	Estimated value
$\hat{x}_{m_f}$	:	Estimated value using fuzzy-SMO
x_p	:	Actual plant value
NV	:	Negative
ZV	:	Zero
PV	:	Positive
n	:	State space order number
U_1, U_2	:	External transfer vector
O	:	Observability matrix
R_v	:	Covariance of measurement noise
P_{k-1}	:	Covariance at time $k-1$
F_{k-1}	:	Nonlinear state transition function
Z	:	Process vector
ξ	:	Auxiliary variable
$\widehat{D}(s)$	:	Estimated disturbance
d	:	Discrete
F	:	Constant matrix for control signal
i	:	Number of row in a matrix
f	:	Matrix coefficient
I	:	Identity matrix
H	:	Constant matrix

J	:	Cost function
j	:	Number of column in a matrix
N_c	:	Control Horizon
k	:	Discrete-time
N_p	:	Prediction Horizon
r_w	:	Tuning parameters for the desired closed loop
R_s	:	Vector with set points information
$\emptyset$	:	Constant matrix for control signal
$w\ (t+k)$	:	Reference Trajectory
Δu	:	Incremental variation of input
Δu^{min}	:	Lower limit of input incremental variation
Δu^{max}	:	Higher limit of input incremental variation
SMO	:	Sliding mode observer
ELO	:	Extended Luenberger observer
EKF	:	Extended Kalman filter
KF	:	Kalman filter
DOB	:	Disturbance observer
MDOB	:	Modified disturbance observer
ASO	:	Adaptive state observer
UKF	:	Unscented Kalman filter
EnKF	:	Ensemble Kalman filter
SSKF	:	Steady state Kalman filter
AFKF	:	Adaptive fading Kalman filtering
UIO	:	Unknown input observer
MHE	:	Moving horizon estimator
NUIO	:	Nonlinear unknown input observer

EUIO	:	Extended unknown input observer
AO	:	Asymptotic observer
CSTR	:	Continuous stirred-tank reactor
QUIO	:	Quasi-unknown input observer
UIFDO	:	Unknown input fault detection observer
MPC	:	Model predictive control
AI	:	Artificial intelligence
ANN	:	Artificial neural network
FFN	:	Feed forward neural network
IRN	:	Internally recurrent net
RBFNN	:	Radial basis function neural networks
ERN	:	Externally recurrent net
RTNN	:	Recurrent trainable neural network
HNN	:	Hybrid neural network
ANFIS	:	Adaptive neuro-fuzzy inference systems
ES	:	Expert system
GA	:	Genetic algorithm
SAHNN	:	Structure approaching hybrid neural network
MNN	:	Shape-tunable neural network
RNNM	:	Recurrent neural network model
RANN	:	Recurrent artificial neural network
DNNO	:	Differential neural network observer
MLPFF	:	Multilayer perceptron feedforward

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CHAPTER 1: INTRODUCTION

1.1 Chapter overview

In this first chapter of the thesis, the background on the necessity of the observer, controller and its validation have been introduced. The problem statements that lead to the motivations are also emphasized, which has initiated the five important objectives of the work. Besides that, the overview of each chapter is also given as an early indication of the research.

1.2 Background

All state variables being accessible through online measurement is a common assumption before implementing a feedback control law in a plant. However, in practice, some of them are unmeasured due to the lack of appropriate sensors. Nevertheless, it is important to identify these variables to prevent process disruption and fault, which in the worst scenario may lead to plant shutdown. Therefore, devices known as observers or estimator are developed to estimate those difficult-to-measure variables. They are software-based computational algorithms designed to cater for the lack of appropriate estimating devices as well as replacement of the high-priced hardware sensors. It is also an effort to reduce the parametric error within the process since the states are continuously being predicted at the current time. Those observers are also applied to estimate the actual states and feedback to the system to provide an early warning before system failures or emergency shutdown occur in the plant.

Observers are initially developed using linear formulation or better known as linear observers. They have been applied to estimate states or unknown variables in linear processes with the presence of noise and disturbances (Bara et al., 2001; Bejarano et al., 2007; Bejarano & Fridman, 2010; Bodizs et al., 2011; Busawon & Kabore, 2001; Assoudi et al., 2002; Fissore, 2008; Jafarov, 2011; Lee, 2011; Oya & Hagino, 2002; Vries et al., 2010). Later, nonlinear observers have been introduced in order to adapt to the highly nonlinear behavior exhibits in most chemical processes (Bitzer & Zeitz, 2002; Boulkroune et al., 2009; Busawon & Leon-Morales, 2000; Assis & Filho, 2000; Ciccio et al., 2011; Dong & Yang, 2011; Farza et al, 1997, 2011; Floquet et al., 2004; Hashimoto et al., 2000; Kalsi et al., 2009; Kazantzis & Kravaris, 1998, 2001; Kazantzis et al., 2000; Ko & Wang, 2007; Kravaris et al., 2007; Maria et al., 2000; Schaum et al., 2008).

After that, researchers have utilized artificial intelligence (AI) algorithms as estimators (Mohd Ali, Hussain, Tade, & Zhang, 2015). By definition, AI is the capability of computers to perform tasks which require human intelligence and expertise. It has been widely used in many fields such as medicine, science, education, manufacturing, finance and engineering including process control. In process control specifically, AI has not only been applied to control and modeling but also as estimators. Those AI elements such as expert systems (ES), , fuzzy logic, artificial neural network (ANN) and genetic algorithm (GA) have been successfully applied as estimators in chemical process systems according to several works by various researchers (Ahmad et al., 2004; Araúzo-Bravo et al., 2004; Beigzadeh & Rahimi, 2012; Islamoglu, 2003; Molga & Cherbański, 2003; Patnaik, 1997; Rezende et al., 2008; Rivera et al., 2010; Shen & Chouchoulas, 2001; Singh et al., 2005, 2007; Sivan et al., 2007; Turkdogan-Aydınol & Yetilmezsoy, 2010). (Chuk et al., 2005; Kumar & Venkateswarlu, 2012).

Such use of single observers, however, may produce unsatisfactory results such as offsets and slow estimation rate especially due to the highly nonlinear behavior in many systems. Therefore, the hybrid approach has emerged as one of the solutions in order to overcome those limitations. Hybrid observers have been developed based on three combinations. The first combination is the merging between two or more conventional observers to improve the estimation performances. For example, extended Luenberger observer (ELO) is coupled with the asymptotic observer whereas sliding mode observer (SMO) is combined with the proportional observer (Aguilar-López & Maya-Yescas, 2005; Goffaux, Wouwer, & Bernard, 2009; Hulhoven & Bogaerts, 2002; Hulhoven, Wouwer, & Bogaerts, 2006). The second combination is the merging between conventional observers and AI algorithms. In this combination, for instance, fuzzy logic is combined with the extended Kalman filter (EKF) to produce the hybrid fuzzy Kalman filter (FKF) (Chairez, Poznyak, & Poznyak, 2007; Porru, Aragonese, Baratti, & Alberto, 2000; Poznyak, García, Chairez, Gómez, & Poznyak, 2007; Senthil, Janarthanan, & Prakash, 2006). The last combination is the merging between two or more AI algorithms such as when fuzzy logic is merged with ANN to establish fuzzy-neural network (fuzzy-NN) for improving the estimation (Chitanov, Kiparissides, & Petrov, 2004; Khazraee & Jahanmiri, 2010; Ng & Hussain, 2004; Wilson & Zorzetto, 1997; Yarlagadda & Teck Khong, 2001).

In this work, I apply the second combination type, which is combining the conventional observer with an AI algorithm. The conventional observer used is the sliding mode observer (SMO) while the AI algorithm utilized is the fuzzy logic. SMO is selected since it is a type of observer that provides a stable, fast and accurate estimation. Besides that, it does not require precise input assumptions during the design procedure and is suitable for complex nonlinear systems (Spurgeon, 2008). On the other hand, fuzzy logic is chosen since it is a simple algorithm compared to other AI elements such as genetic algorithm (GA) and neural network (NN) when applied in the hybrid observer design framework. Fuzzy logic has rules that can be easily manipulated in search of the best results without changing other parameters such as the membership function and defuzzification type in the fuzzy framework. However, when NN is applied all the training steps must be repeated to find the best solutions and the whole network may also need to be changed. In addition, if GA is combined with SMO, the reproduction, crossover and mutations steps must be redefined to achieve the best generation (output) since the first generation is always based on random numbers or values (Hussain & Ramachandran, 2003).

The motivation behind choosing this second combination is to improve the estimation performances shown by the single SMO in such a way that simpler formulation and computation methods are utilized. Furthermore, the hybrid framework must be flexible to allow expansion for estimating more variables, thus it can be applied in chemical process systems that deal with many unknown parameters such as the polymerization process utilized as the case study for this research. The ethylene polymerization process is used as a medium to observe the performances of the hybrid observer. The difficult-to-measure parameters including the ethylene concentration, butene concentration and melt flow index (MFI) in the process are estimated for this purpose. Once the observer has been successfully designed and applied, a controller is added for overall control of the system.

A controller may be required to enhance the overall control of the process system and an appropriate controller design shall be based on the measured states. Unfortunately, not all states are measurable therefore observer will estimate them prior to design the controller. The observer will help in improving the performance of the controller by first estimating the unknown parameters and then convey the information to the controller during its application. In this research, to enhance the overall control of the ethylene polymerization process, the embedded integrator model predictive control (MPC) strategy is applied to control the temperature of the reactor. The reactor temperature is controlled to achieve the desired product and to maintain the quality of the polyethylene product.

MPC is a model-based control strategy, which uses a model to predict the future output of a process and calculates the future control signals by minimizing an objective function as the system output approaches a reference trajectory (Camacho & Bordons, 2004). The optimization penalizes deviation of the future output from the intended future trajectory and the control effort within a specified number of output predictions (prediction horizon) and control moves (control horizon). However, out of all the calculated future control signals, only the first set of signals are applied in the multiple-input multiple-output (MIMO) system. In the next instant, the control moves for the whole control horizon are recalculated and the first of these optimum control moves are then applied to the system. This is the concept of receding horizon, which continuously repeats the calculation at each instant and implements only the first set of control signals on the system (Green & Perry, 2008). In addition, MPC is also suitable for MIMO control problems as it interacts between manipulated and controlled variables for finding the optimum control moves. It will accommodate inequality constraints on both input and output variables efficiently (Green & Perry, 2008). These inequality constraints include the upper and lower limits to restrict the parameter to a certain range of value, which is a common practice in the real plant (Camacho & Bordons, 2004).

This advanced control strategy is also capable of withstanding several industrial challenges especially tighter specification of the products' quality, rising and rapid changes in the demand for productivity and new environmental regulations set by the authority. In addition, MPC is also favorable in the industry mainly to be operated by employees with low expertise on control. This is because of its intuitive concepts and easy tuning methods. MPC can also be applied for controlling varieties of processes ranging from that with simple dynamics to high complex systems, which include unstable, non-minimum phase and long-time delay elements. MPC in this work is included with an integrator by modifying the state space model formulation as an alternative to guaranteeing offset free results from the controller during application. State space model is chosen as the prediction model in developing the MPC controller.

Both the hybrid observer and controller will be first designed in the simulation environment. This is important to test the formulation and readiness of the designs before they can be verified or implemented on-line. The real data from the polymerization pilot plant will be used to validate the hybrid observer. Validation is a method to decide whether the model represents the correct conceptual description of the process system (Trucano, Swiler, Igusa, Oberkampf, & Pilch, 2006). Validation is often carried out as a preliminary step before implementing the design in the real plant. In this work, the experimental data obtained from a polymerization pilot plant is considered as the validation benchmark to validate the effectiveness of the proposed observer.

1.3 Problem statement

The highly nonlinear behavior of an ethylene polymerization reactor is a factor that triggering the existence of many unknown parameters, which can disrupt the process and may lead to failures if they are not measured. Although the plant has always been equipped with sensors, they are expensive and are unreliable to estimate unknowns that appear unexpectedly due to disturbances and mismatches. Therefore, observers or estimators have been designed to reconstruct the state vector for estimating those parameters and help in reducing the usage of the high-priced hardware sensors. Those software-based sensors are cheaper, accurate, easy to design and retune.

Nevertheless, unsatisfactory results can also be observed from some conventional observers. Therefore, an alternative way has been introduced, which is to hybrid the observer for enhancing the performances. Although several hybrid observers have been successfully applied, the formulation of the observers is complicated and frequently limiting to a particular parameter estimation. If more parameters are required to be estimated, the whole structure of the observer must be modified. Furthermore, selecting the type of observers to be merged can be very challenging and time-consuming. In order to cater for these issues, it is essential to design a hybrid observer with a simple formulation and is able to estimate several parameters without redesigning the structure of the observer.

Furthermore, it is significant to control and maintain the product quality in a process by using a controller and is coupled with an observer for better control. The observer will estimate the parameters and deliver the information to the controller allowing it to receive only states at the current time for optimum performances. Choosing a controller to be used is often a tedious task and dependent on the type of process and controlled variables. Besides that, a controller tends to deviate from the setpoint producing poor results and offsets. Therefore, it is important to develop a suitable controller to be combined with the observer and at the same time eliminating the limitation for maintaining good results by adding an integral factor or integrator in the formulation.

In addition, simulation environment may not be sufficient enough to prove the effectiveness of the observer especially when there is a plan for on-line implementation in the future. Therefore, validation is necessary and will help in verification of the simulation programming or coding for this case.

1.4 Objective

This research has five objectives as follows:

i. To design a hybrid observer, which combines the conventional observer and AI element for several parameters estimation without redesigning the whole structure of the observer in an ethylene polymerization process.
ii. To compare the hybrid observer with other single-based observers, the AI element used in the proposed observer and another hybrid observer to highlight its effectiveness.
iii. To develop an embedded integrator MPC controller using state space model as the prediction model to control the reactor temperature for maintaining the product quality based on the measured states estimated from the hybrid observer as well as an additional advantage of the controller to guarantee free of offsets during application.
iv. To compare the MPC with conventional control method, MPC without integrator and MPC without both observer and integrator to highlight its advantages.
v. To validate the hybrid observer using the experimental data from a polymerization pilot plant.

1.5 Thesis overview

This thesis is organized as follows:

Chapter 1 is the introduction section that explains the background, motivation, problem statements, objectives, the scope of the research and the overview of the thesis.

Chapter 2 is the literature review section, which emphasizes on the previous works related to the various types and application of observers in chemical process systems that initiates and motivates this research.

Chapter 3 is the methodology section that provides the overview of the methods applied in designing the hybrid observer, the MPC controller and the validation testing.

Chapter 4 is the hybrid fuzzy-sliding mode observer (fuzzy-SMO) design section, which shows the step by step formulation of the hybrid observer and its performances in estimating parameters in the ethylene polymerization reactor.

Chapter 5 describes the design of the embedded integrator model predictive control (MPC) section that provides the formulation of the MPC design and its performances in controlling the reactor temperature in the reactor.

Chapter 6 describes the estimator validation using experimental data section, which provides the validation of the hybrid observer based on the experimental data from the polymerization pilot plant.

Chapter 7 includes the conclusions and future work sections that summarize the work and provide suggestions for the future of the research.

CHAPTER 2: LITERATURE REVIEW

2.1 Chapter overview

In this second chapter, observers applied in chemical process systems are reviewed. These observers are classified into six classes based on their structure and formulations. Next, the study of the artificial intelligence (AI) algorithm applied as observers in the chemical process systems is carried out. This is followed by the survey of the model predictive control (MPC). Summary and analysis are provided after the review to highlight and decide the best method to be used.

2.2 Applications of observers in chemical process systems

David G. Luenberger was the person responsible for introducing the observers since 1960's through his famous theories, the Luenberger observer while Rudolf E. Kalman had developed Kalman filter (KF) also in 1960 (Luenberger, 1964, 1966, 1967, 1971; Welch & Bishop, 1995). Many observers today, are the modification and extended version of the Luenberger observer or KF (Mohd Ali, Hoang, Hussain, & Dochain, 2015). Over the years, observer research areas have becoming popular and challenging because of their accuracy, good performances, cheap, easy to retune and to maintain (Gonzalez, Aguilar, Alvarez-Ramirez, & Barren, 1998; Lombardi, Fiaty, & Laurent, 1999). Various types of observers designed have been proven to accurately estimate variables in linear and nonlinear processes including the fixed gain observers, periodic resetting based and for on-line estimation usage (Aguirre & Pereira, 1998; del-Muro-Cuellar, Velasco-Villa, Jiménez-Ramírez, Fernández-Anaya, & Álvarez-Ramírez, 2007; Huang, Patwardhan, & Biegler, 2010; Pedret, Alcántara, Vilanova, & Ibeas, 2009). They have also been utilized either theoretically or practically through simulation and real plant testing respectively.

Researchers have also designed observers due to the requirement of a system to handle uncertainties including disturbances and mismatches. Nowadays, many different types of observers but with closely similar design formulations, aiming at overcoming the limitations of one another have been developed (Mohd Ali, Hoang, Hussain, & Dochain, 2015). For instance, to estimate disturbances, the disturbance observer (DOB) has initially been introduced followed by the perturbation observer (POB) (Radke & Zhiqiang, 2006), extended state observer (ESO), modified disturbance observer (MDOB) (Yang, Li, Chen, & Li, 2011), fractional-order disturbance observer (FO-DOB) and Bode-ideal-cut-off observer (BICO-DOB) (Olivier, Craig, & Chen, 2012). Another example is the fault detection based observer where the unknown input observer (UIO) (Sotomayor & Odloak, 2005) has first been designed followed by the nonlinear unknown input observer (NUIO) (Zarei & Poshtan, 2010), quasi-unknown input observer (QUIO) (Rocha-Cózatl & Wouwer, 2011) and unknown input fault detection observer (UIFDO) (Zarei & Poshtan, 2010). Besides UIO, the proportional observer has also applied for estimating error and faults with its extended version such as the proportional-integral observer (Nagy Kiss, Marx, Mourot, Schutz, & Ragot, 2011).

In chemical process systems, Alvarez-Ramirez has constructed a Luenberger observer for estimating concentration in CSTR and applied numerical simulation for monitoring the performance. It was found to be robust against modeling deviation and bounded to additive noise (Alvarez-Ramírez, 1995). Luenberger observer has been utilized for reconstructing concentration and temperature in an unstable tubular reactor resulting in a stable convergence factor (Alonso, Kevrekidis, Banga, & Frouzakis, 2004). Besides that, extended Luenberger observer (ELO) has been applied in estimating crystal mass in a sugar crystallization unit and has shown good estimation even without perfect initial condition (Damour, Benne, Boillereaux, Grondin-Perez, & Chabriat, 2010). Whereas in a fed-batch crystallizer, ELO has been used to estimate solutes concentration with high accuracy that is robust against modeling error (Mesbah, Huesman, Kramer, & Van den Hof, 2011). Another approach involving ELO was studied by Quintero-Marmol et al. for controlling multi-component batch distillation column and predicting compositions in reboiler, trays and reflux drum using measured feed, tray pressure and temperature based on only one gain value (Quintero-Marmol, Luyben, & Georgakis, 1991). In addition, ELO has been applied to estimate polymer concentration, mass transfer coefficient and specific surface in a polymerization reactor with satisfactory convergence rate (Appelhaus & Engell, 1996). Furthermore, Appelhaus and Ensell have also developed EKF in similar work to improve the rate of convergence in the process (Appelhaus & Engell, 1996).

Scali et al. has utilized the extended Kalman filter (EKF) for measured and unmeasured disturbances estimation in a polymerization reactor (Scali, Morretta, & Semino, 1997) while in a freeze-drying (lyophilisation) process, EKF has been applied in predicting the dynamic temperature interface within the primary drying stage (Velardi, Hammouri, & Barresi, 2009). Apart from that, EKF has been used in an isothermal batch reactor (Terwiesch & Agarwal, 1995), a reactive distillation column (Olanrewaju & Al-Arfaj, 2006) and a fed-batch crystallizer (Mesbah et al., 2011) to estimate reactant concentration, liquid compositions and solutes concentration respectively. Furthermore, the unscented Kalman filter (UKF) has been applied in a fed-batch crystallizer to accurately estimate the solutes concentration (Mesbah, Huesman, Kramer & Van den Hof, 2011) and in a semi-batch reactor for particle size distribution estimation (Mangold et al., 2009). The ensemble Kalman filter (EnKF) has also been employed to estimate similar solutes concentration in the fed-batch crystallizer as a comparison to the UKF (Mesbah, Huesman, Kramer & Van den Hof, 2011).

On the other hand, the sliding mode observers have been applied in both papers by Pico et al. and De Battista et al. in a fed-batch bioreactor and a fermentation process respectively (De Battista, Picó, Garelli, & Vignoni, 2011; Picó, De Battista, & Garelli, 2009). Relay-based sliding mode observer (Hajatipour & Farrokhi, 2010) has been applied in a bioreactor to estimate uncertainties of the process where the estimator has guaranteed stability and good convergence performances. Besides that, Sheibat-Othman et al. have used the adaptive state observer (ASO) for estimating radical concentration in a polymerization process (Sheibat-Othman, Peycelon, Othman, Suau, & Févotte, 2008). Another application is in the debutanizer studied by Amiya et al. for estimating vapor flow rate, liquid flow rate and distribution coefficient in reboiler (Jana, Samanta, & Ganguly, 2009). Jana et al. have designed an ASO, which precisely estimated the plant parameters under mismatch condition and is suitable for on-line implementation (Jana et al., 2009). Apart from that, the adaptive high-gain observer was used in an aeration tank in a waste treatment plant for approximating uncertainties (Lafont, Busvelle, & Gauthier, 2011).

In addition, Aamo et al. have developed a reduced order observer for state estimation in a gas-lift well to estimate the downhole pressure where the estimated pressure is able to be stabilized (Aamo, Eikrem, Siahaan, & Foss, 2005). The approach has been continued later by Salehi and Shahrokhi, which developed a reduced-order observer to control the temperature in a CSTR by first estimated the reactor concentration (Salehi & Shahrokhi, 2008). Further used of the reduced-order observer is to estimate the substrate concentration in a bioreactor designed by Kazantzis et al. (Kazantzis, Huynh, & Wright, 2005). After that, Jana has used this similar observer for top tray compositions estimation (Jana, 2010). Whereas an interval observer has been used to estimate reactant concentration in both the plug flow reactor and the mineral separator unit (Aguilar-Garnica, García-Sandoval, & González-Figueredo, 2011; Meseguer, Puig, Escobet, & Saludes, 2010).

Unknown disturbances can disrupt the process systems and lead to failure, therefore disturbance observers such as MDOB, FO-DOB and BICO-DOB have been developed specifically to estimate those disturbances (Olivier et al., 2012; J. Yang et al., 2011). DOB has been used to estimate disturbance in a solid feeding conveyor in a grinding mill resulting in a smooth estimation (Chen, Yang, Li, & Li, 2009) while Yang et al. have applied MDOB for disturbance estimation in a jacketed stirred tank heater (Yang et al., 2011). Besides that, in a cyclone also in a grinding mill, the observer is used together with the Q-filter that offers an additional tuning freedom in optimizing the performance even in the presence of disturbances (Olivier et al., 2012). Olivier et al. have also developed the FO-DOB and BICO-DOB to approximate those disturbances (Olivier et al., 2012).

Researchers have then developed the fault detection observers to estimate fault and unknown parameters for diagnosing the fault in the process units. In a CSTR, the modified proportional observer has been introduced to verify the state variables and satisfactory performance has been observed in both the simple and complex systems during application (Aguilar-López & Martinez-Guerra, 2005). On the other hand, for fault diagnosis in the polymerization reactor, an unknown input observer (UIO) has been used to estimate states (Sotomayor & Odloak, 2005) while Zarei and Poshtan have developed the UIO to detect sensor's fault in a CSTR (Zarei & Poshtan, 2010). Besides that, Zarei and Poshtan have also highlighted few types of fault detection observers including robust observer, extended unknown input observer (EUIO) and nonlinear unknown input observer (NUIO). Another extended version of UIO has also been introduced namely the quasi-unknown input observer (QUIO) for estimating concentration, flow rates and light intensity in phytoplantonic cultures with satisfactory results achieved in both simulation and experimental testing (Rocha-Cózatl & Wouwer, 2011). The robust observer has been applied to estimate the average molecular weight and mass fraction in a CSTR and distillation column respectively for fault analyzing in the process systems (Zambare, Soroush, & Ogunnaike, 2003).

Furthermore, researchers have introduced the hybrid observer to overcome the limitations of the single-based observers. Hybrid observer, looking at its name, is a combination of more than one observer to obtain better estimating performances, for instance, ELO is merged with an asymptotic observer (AO) (Hulhoven, Wouwer, & Bogaerts, 2006). The type of observers to be combined is based on their advantages as given in Table 2.1. The hybrid observer has been applied in approximating biomass concentration in a bioreactor according to the work carried out by Hullhoven et al. (Hulhoven et al., 2006) while Aguilar-Lopez et al. have applied a continuous-discrete observer also for biomass concentration estimation in a batch reactor. (Aguilar-López & Martínez-Guerra, 2007). A continuous-discrete observer has also been applied by Elicabe et al. for reaction rate estimation in a semi-continuous reactor (Elicabe, Ozdeger, Georgakis, & Cordeiro, 1995).

Moreover, Ricardo et al. have estimated the monomer concentration, molecular weight of the polymer and the temperature in a polymerization reactor using a proportional-type sliding mode observer (Aguilar-López & Maya-Yescas, 2005). Whereas, a continuous-discrete interval observer has been found to be good at managing uncertainties in green algae cultures according to the work done by Goffaux et al. (Goffaux, Wouwer, & Bernard, 2009). A continuous-discrete observer has also been combined with EKF for biomass and substrate concentration in a bioreactor while a proportional integral observer was applied to estimate uncertainties in waste water treatment plant (Bogaerts & Wouwer, 2004; Kiss et al., 2011).

Another type of hybrid observer is the combination of the conventional observers with the AI elements. In their work, Prakash and Senthil have designed the fuzzy Kalman filter

(FKF) and state fuzzy Kalman filter (ASFKF) for estimating the temperature and concentration in a CSTR (Prakash & Senthil, 2008). It is a combination of KF with the 'IF-THEN' rules of the fuzzy logic. First, the FKF was designed, but since it had shown unfair results during the presence of disturbances in the input and output, ASFKF mechanism has been established to handle mismatches. Two more examples are the differential neural network observer (DNNO), which has been applied in a contaminated model soil for estimating contaminant and ozone concentration (Poznyak, García, Chairez, Gómez, & Poznyak, 2007) and the combination between EKF and neural model to approximate the outlet reactor concentration in a heterogeneous gas-solid reactor (Porru, Aragonese, Baratti, & Alberto, 2000).

Table 2.1: Advantages of observer for hybrid purposes

Observer	Advantages of observers for hybrid purposes
EKF	Fast convergence time
ELO	Good convergence time but need accurate model kinetics
Asymptotic observer	Do not need kinetic data but dynamics depends on operating condition
SMO	Fast convergence and stable, do not need unknown input assumptions
Interval observer	Robust against disturbances
Exponential observer	Do not need kinetic data but dynamics do not depend on operating conditions
Proportional observer	Good for fault detection
Backstepping observer	Guaranteed convergence
Geometry observer	Can overcome ill-condition
Disturbance observer	Good for predicting disturbances
Moving horizon	Robust against model deviation
Specific observer	Robust against modelling error
Generic observer	Robust against modelling error
High-gain observer	Less oscillations
Adaptive state observer	Good convergence factor
Low-order observer	For high dimensional systems
Reduced-order observer	For certain parameters estimation only
Integral observer	Easy implementation and robust against uncertainties
Continuous observer	Mainly for continuous process
Discrete observer	Mainly for discrete-time process

All the observers that have been applied in chemical process systems above can be classified into six classes according to their structure and formulations as tabulated in Table 2.2. These classes consist of the Luenberger-based observers, the finite-dimensional system observers, the Bayesian estimators, the disturbances and fault detection observers, the artificial intelligence-based observers and the hybrid observers (Mohd Ali, Hoang, Hussain, & Dochain, 2015).

The Luenberger-based observers class is the first category. It combines all observers which designed are based on the Luenberger observer methodology (Alonso et al., 2004; Dochain, 2003; Fissore et al., 2007; Tronci et al., 2005; Vries et al., 2010). The extended Luenberger observer (ELO), adaptive state observer (ASO), sliding mode observer (SMO) and geometric observers are examples of observers in this class. This type of observer is relatively suitable for linear systems with less complex and simpler computation (Bejarano et al., 2007).

The finite-dimensional system observers class is the second category that has been designed for chemical process systems whose dynamics are described by the ordinary differential equations (ODEs) such as the reduced-order, low-order, high-gain and exponential observers (Bitzer and Zeitz, 2002). Their implementations are easy and straightforward, thus suit systems that are less kinetic information. Nevertheless, the accuracy of the convergence rate is often uncertain, for example, the convergence rate of the asymptotic and exponential observers can only be obtained if the operating conditions are bounded by the dilution rate (Dochain et al., 1992; Dochain, 2000; Sadok and Gouze, 2001; Hoang et al., 2013).

On the other hand, the third class is the Bayesian estimators, which is based on the probability distribution estimation of the state variables using available data from the system (Chen et al., 2004). Here, all variables are assumed as stochastic in nature, thus the distribution of the state variables is achievable through the measured variables (Mohd Ali, Hoang, Hussain, & Dochain, 2015). The examples of the Bayesian estimators are the particle filter (PF), extended Kalman filter (EKF) and moving horizon estimator (MHE). Since they are based on the probability distribution, they are consistent and versatile estimators that are highly recommended for fast estimation (Abdel-Jabbar et al., 2005; Fan and Alpay, 2004; Patwardhan and Shah, 2005).

The fourth class is the disturbance and fault detection observers. Both observers are combined in the same class since they are frequently applied to estimate irregularities in the system, either through disturbances or faults (Olivier et al., 2012). Fault detection observers have also been used for estimating parameters prior to diagnosing fault in chemical process systems. The examples of the disturbance and fault detection observers are the disturbance observer (DOB), the modified disturbance observer (MDOB) and the nonlinear unknown input observer (NUIO) (Mohd Ali, Hoang, Hussain, & Dochain, 2015). These observers focus only on estimating variables related to disturbances and fault detection (Chen et al., 2009; Rocha-Cozatl and Wouwer, 2011; Sotomayor and Odloak, 2005; Yang et al., 2011). They are mostly suitable to estimate disturbances and faults to provide an early warning before disruptions occur to the systems (Sotomayor and Odloak, 2005; Zarei and Poshtan, 2010).

Next class is the artificial intelligence (AI)-based observers, which consists of AI algorithms such as expert systems (ES), fuzzy logic, genetic algorithm (GA) and artificial neural network (ANN). However, here it focuses only on the AI-based observers that coupled with the conventional observers such as fuzzy Kalman filter (FKF) and the EKF-neural network observers (Porru et al., 2000; Prakash and Senthil, 2008). These AI-based observers will help to overcome the limitations of the single-based observers and are appropriate for systems with incomplete model structure and lack of information.

However, the development of the formulation of these AI-based observers may be difficult and time-consuming compared to the other type of hybrid observers depending on the type of the systems (Senthil et al., 2006). Furthermore, the AI elements must be adapted before being implemented on-line (Himmelblau, 2008; Lashkarbolooki et al., 2012; Rivera et al., 2010).

The final or the sixth class is the hybrid observers, which are combinations of two or more observers for improving the estimation performances. For example, the combination of the asymptotic observer (AO) and the extended Luenberger observer (ELO) (Hulhoven et al., 2006). AO can estimate parameters without needing the kinetics data while ELO provides good convergence factors. Therefore, their combination will result in an improved observer which replicates both features. Hybrid observers are capable of overcoming the limitations of the single observer, even though finding the appropriate combination can be tedious and time-consuming (Lopez and Yescas, 2005; Bogaerts and Wouwer, 2004; Goffaux et al., 2009). This class of observer is usually suitable when the single-based observer has provided less accuracy in the estimation, for instance, to compensate offsets resulting from the use of the single observer for parameter estimation (Hulhoven et al., 2006). The applications of these observers in chemical process systems under their classes are listed in Table 2.3 while their comparisons in terms of attributes, advantages and limitations are tabulated in Table 2.4.

Table 2.2: Observers categorized under different classes (Mohd Ali, Hoang et al., 2015)

Class	Luenberger-based observers	Finite-dimensional system observers	Bayesian Estimators	Disturbance and Fault Detection observers	Artificial Intelligence- based Observers	Hybrid Observers
Specific Observer	1. Extended Luenberger observer (ELO) 2. Sliding Mode observer (SMO) 3. Adaptive State observer (ASO) 4. Zeitz nonlinear observer 5. Discrete-time nonlinear recursive observer (DNRO) 6. Geometric observer 7. Backstepping observer	1. Reduced-Order observer 2. Low-Order observer 3. High gain observer 4. Asymptotic observer 5. Exponential observer 6. Integral observer 7. Interval observer	1. Particle Filter (PF) 2. Extended Kalman Filter (EKF) 3. Unscented Kalman Filter (UKF) 4. Ensemble Kalman Filter (EnKF) 5. Steady state Kalman Filter (SSKF) 6. Adaptive Fading Kalman Filtering (AFKF) 7. Moving horizon estimator (MHE) 8. Generic observer 9. Specific observer	1. Disturbance observer 2. Modified Disturbance observer (MDOB) 3. Fractional- Order Disturbance observer 4. Bode-Ideal Cut-off observer 5. Unknown input observer (UIO) 6. Nonlinear unknown input observer 7. Extended unknown input observer 8. Modified proportional observer	1. Fuzzy Kalman Filter 2. Augmented Fuzzy Kalman Filter 3. Differential Neural Network observer 4. EKF with Neural Network model	1. Extended Luenberger-Asymptotic observer 2. Proportional-Integral observer 3. Proportional-SMO 4. Continuous-Discrete observer 5. Continuous-Discrete- Interval observer 6. Continuous-Discrete-EKF 7. High-gain-continuous-discrete

Table 2.3: Application of observers in chemical process systems under different classes (Mohd Ali, Hoang et al., 2015)

Class 1: Luenberger-based Observers

Observer	Objective /Estimate(s)	System	Positive Highlight(s)	Ref
ELO	Crystal mass	Crystallization unit	Good estimation without perfect initial condition	Damour et al. (2010)
ELO	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
ELO	Process kinetics, influent concentrations	Fixed bed reactor	Easy to implement, simple structures	Mendez-Acosta et al. (2008)
SMO	Substrate concentration, specific growth rate	Fermentation process	Smooth estimates	Pico et al. (2009)
SMO	Specific growth rate	Fed-batch bioreactor	Accurate and error free estimation	Battista et al. (2011)
SMO	Substrate concentration	Bioreactor	Proven stability factor	Gonzalez et al. (2001)
SMO	Biomass and substrate concentration	Bioreactor	Proven stability factor	Hajatipour & Farrokhi (2010)
DNRO	Reactor parameters	CSTR	Stable estimator	Huang et al. (2010)
ASO	Growth rate, kinetic coefficient	Bioreactor	Guaranteed convergence factor	Zhang & Guay (2002)
ASO	Liquid, vapor flow rate, reboiler coefficient	Debutanizer	Precise estimates under mismatch condition	Jana et al. (2009)
ASO	Radical concentration	Polymerization process	Estimates without information of initiator	Othman et al. (2008)
ASO	Distribution coefficients	Distillation column	Guaranteed convergence factor	Jana et al. (2006)
ASO	Compositions, partially known parameters	Batch distillation column	Good convergence factor	Murlidhar & Jana (2007)
Backstepping	Concentrate and tailing grade	Solid-solid separation unit	Guaranteed convergence, zero estimation error	Benaskeur & Desbiens (2002)

Class 1: Luenberger-based Observers (continued)

Zeitz nonlinear observer	Nitrogen oxide (NO_x) inlet concentration, outlet reactant conversion	Loop reactor	Fast, reliable estimates	Fissore et al. (2007)
Geometric	Product compositions	Distillation column	Overcomes ill-conditioning of the observability matrix	Tronci et al. (2005)
Geometric	Compositions, solid mass fraction, production rate	Copolymerization reactor	Accurate estimation	Lopez & Alvarez (2004)

Class 2: Distributed Parameter System Observer

Observer	Objective /Estimate(s)	System	Positive Highlight(s)	Ref
Reduced-order	Down hole pressure	Gas-lift well	Stable estimates	Aamo et al. (2005)
Reduced-order	Reactor concentration	CSTR	Good concentration estimates	Salehi & Shahrokhi (2008)
Reduced-order	Substrate concentration	Bioreactor	Robust estimation	Kazantzis et al. (2005)
Low-order	Steady state profiles	30-tray distillation column	Robust against noise	Singh and Juergen Hahn (2005b)
High-gain	Reaction heat	CSTR	Robust against noise and disturbances	Aguilar et al. (2002)
High-gain	Reactor concentration and temperature	CSTR	Precise estimates	Biagiola & Figueroa (2004b)
Exponential	Reactor concentration	Tubular reactor*	Good estimation without process kinetics	Dochain (2000)
Exponential	Top tray compositions	Batch distillation column	Good convergence properties	Jana (2010)
Exponential	Microorganisms concentration	Bioreactor	Guaranteed convergence	Assoudi et al. (2002)
AO	Concentrations, enthalpy	CSTR	Good estimation, not sensitive to noise	Dochain et al. (2009)

Class 2: Distributed Parameter System Observer (continued)

AO	Reactor concentration	Tubular reactor[*]	Good estimation without process kinetics	Dochain (2000)
AO	Growth rate	Activated sludge process	Precise estimation without process kinetics	Sadok & Gouze (2001)
Interval	Organic concentration, growth rates	Activated sludge process	Converge towards bounded interval	Sadok & Gouze (2001)
Interval	Reactant concentration	Plug flow reactor[*]	Robust estimation	Garnica et al. (2011)
Interval	Residual parameters	Separator (grinding process)	Good convergence factor	Meseguer et al. (2010)
Integral	Heat of reaction	CSTR	Robust estimation	Lopez (2003)

Class 3: Bayesian Estimators

Observer	**Objective /Estimate(s)**	**System**	**Positive Highlight(s)**	**Ref**
SSKF	Time-delay	Stirred tank heater	Consistent estimates even with noise	(Patwardhan & Shah, 2005)
SSKF	Product compositions	Batch distillation column	Stable estimation	(Venkateswarlu & Avantika, 2001)
EKF	Interface temperature	Freeze-drying process	Good estimation without perfect initial condition	Velardi et al. (2009)
EKF	Component's concentration	Batch distillation column	Simple observer design yet accurate estimation	Yildiz et al. (2005)
EKF	Product compositions	Batch distillation column	Precise estimate even with noise	(Venkateswarlu and Avantika, 2001)
EKF	Outlet reactor concentration	CSTR	Accurate concentration estimation	(Himmelblau, 2008)

Class 3: Bayesian Estimators (continued)

EKF	Liquid compositions	Reactive distillation column	Robust against modeling error	(Olanrewaju & Al-Arfaj, 2006)
EKF	Top tray compositions and flow rates	Distillation column	Guaranteed convergence factor	Jana et al. (2006)
EKF	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
UKF	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
UKF	Particle size distribution	Semi-batch reactor	Good estimation without accurate model	Mangold et al. (2009)
UKF	Biomass concentration	Fermentor	Effective estimation despite using the simplified mechanistic model	Wang et al. (2010)
UKF	Uncertain parameters	Hybrid tank system	Effective control and good estimation	Prakash et al. (2010)
EnKF	Solute concentrations	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
EnKF	Unmeasured disturbances	Hybrid tank system	Effective control and good estimation	Prakash et al. (2010)
AFKF	Product compositions	Batch distillation column	Precise estimate despite noisy conditions	(Venkateswarlu & Avantika, 2001)
AFKF	Temperature	Heat exchanger	Good estimation without coefficient adjustment	Bagui et al. (2004)
PF	Yield parameter	Fermentor	Good estimation based on maximization algorithm theory	Chitralekha et al. (2010)
PF	Conditional density	CSTR	Few assumptions required for estimation	Negrete et al. (2011)
PF	Conditional density	Batch Reactor	Few assumptions required for estimation	Negrete et al. (2011)

Class 3: Bayesian Estimators (continued)

MHE	Solutes concentration	Fed-batch crystallizer	Robust against model deviation	Mesbah et al. (2011)
MHE	Molecular weight distribution	Polymerization reactor	Smooth estimates	(Negrete & Biegler, 2012)
MHE	Tray efficiencies	Binary distillation column	Able to handle constraint during estimation	(Negrete & Biegler, 2012)
MHE	Biomass concentration	Animal cell cultures	Accurate estimates	Raissi et al. (2005)
Generic observer	Carbon and nitrogen concentrations	Sequential batch reactor	Robust against modeling error	Boaventura et al. (2001)
Specific observer	Carbon and nitrogen concentrations	Sequential batch reactor	Robust against modeling error	Boaventura et al. (2001)

Class 4: Disturbances and Fault Detection Observers

Observer	Objective /Estimate(s)	System	Positive Highlight(s)	Ref
DOB	Disturbances related to time delay	Conveyor (grinding process)	Overcome the effect of internal disturbances	Chen et al. (2009)
FO-DOB	Disturbances due to mismatch	Cyclone (grinding process)	Optimize the estimation even with huge disturbances	Olivier et al. (2012)
BICO-DOB	Disturbances due to mismatch	Cyclone (grinding process)	Optimize the estimation even with huge disturbances	Olivier et al. (2012)
MDOB	Closed-loop system disturbances	Jacketed stirred tank heater	Smooth disturbances estimate	Yang et al. (2011)
Modified proportional	Uncertainties in reactive concentration, reactor and jacket temperature	CSTR	Robust against uncertainties	(Lopez & Guerra, 2005)
UIO	Fault in actuator and sensor	Polymerization reactor	Accurate estimation	(Sotomayor & Odloak, 2005)
UIO	Fault in input sensor	CSTR	Accurately estimating fault even in the presence of disturbances	(Zarei & Poshtan, 2010)

Class 4: Disturbances and Fault Detection Observers (continued)

QUIO	Faults in concentration, flow rates, light intensity	Bioreactor	Satisfactory estimates	(Cozatl & Wouwer, 2011)
NUIO	Fault in residuals	CSTR	Acting as alternative fault alarm	(Zarei & Poshtan, 2010)
EUIO	Fault in residuals	CSTR	Acting as alternative fault alarm	(Zarei & Poshtan, 2010)

Class 5: AI-based Observers

Observer	Objective /Estimate(s)	System	Positive Highlight(s)	Ref
FKF	Reactor temperature and concentration	CSTR	Unbiased estimation	(Prakash & Senthil, 2008)
ASFKF	Reactor temperature and concentration	CSTR	Satisfactory unbiased estimates	(Prakash & Senthil, 2008)
DNNO	Anthracene dynamics decomposition and contaminant concentration	Microreactor	Good agreement with the actual value	Poznyak et al. (2007)
DNNO	Formic acid, fumaric acid, maleic acid, oxalic acid	Wastewater treatment plant	Guaranteed small estimation error	Chairez et al. (2007)
EKF-NN	Outlet reactor concentration	Heterogeneous reactor	Further reduction in estimation error compared to EKF	Porru et al. (2000)

Class 6: Hybrid Observers

Observer	Objective /Estimate(s)	System	Positive Highlight(s)	Ref
ELO-AO	Biomass concentration	Bioreactor	Stable rate of convergence	Hulhoven et al. (2006)
Continuous-discrete	Biomass concentration	Batch reactor	Robust against modeling error	(Lopez & Guerra, 2007)
Continuous-discrete-interval	Process kinetics	Bioreactor	Avoids growth of interval sizes during estimation	Goffaux et al. (2009)
Continuous-discrete-EKF	Biomass, substrate concentration	Bioreactor	Accurate estimates, reduced error	(Bogaerts & Wouwer, 2004)
Proportional-SMO	Polymer molecular weight, monomer concentration, reactor temperature	Polymerization reactor	Robust against noise and uncertain parameters	(Lopez & Yescas, 2005)
Proportional-integral	Unknown inputs	Wastewater treatment plant	Stable estimation rate	Kiss et al. (2011)
High-gain-continuous-discrete	Rate coefficient	Polymerization process	Estimates without information of initiator	Othman et al. (2008)

Table 2.4: Observer's evaluation based on class (Mohd Ali, Hoang et al., 2015)

No.	Class of Observers	Example of Observer Equation	Attributes	Advantages	Limitations	Guidelines for practicing engineers
1	Luenberger-based observers	For sliding mode observer: $\dot{\hat{x}} = A\hat{x} + Bu + Lsign(y - C\hat{x})$	Extension of classical Luenberger observer	Simple computational methods	Design is always based on the perfect knowledge of system parameters	For less complex linear systems, this type of observer is sufficient for crucial parameter estimation
2	Finite-dimensional system observers	For exponential observer: $\frac{d\xi}{dt} = F\xi + Gx_1 - LU_1 + U_2$	Knowledge of process system kinetics is not necessary	Easy implementation and simple formulation	Convergence factor depends strongly on the operating condition	Suitable for systems with less kinetics information
3	Bayesian estimators	For Extended Kalman Filter: $P_{k\|k-1} = F_{k-1}P_{k-1\|k-1}F_{k-1}^{T} + R_v$	Based on probability distribution and mathematical inference of the system	Fast estimation based on prediction-correction method and versatile estimators	The complexity of their computational method is sometimes infeasible for high dimensional systems	For fast estimation results based on probability theory, Bayesian estimators may be applied

Table 2.4 (continued)

4	Disturbance and fault detection observers	For disturbance estimation: $\widehat{D}(s) = \widetilde{D}_1(s) + \widetilde{D}_2(s) + \cdots + \widetilde{D}_n(s)$	Focus on estimating disturbances and detecting faults within the system	Good at estimating disturbances and predicting faults before they can affect the unit operations of the plant	May ignore other uncertainties during the estimation process	If the objective is to estimate disturbances and parameters to predict faults, then these types of observers are the most appropriate
5	AI-based observers	According to AI-elements, example using fuzzy logic where the IF-THEN rule is: $IF\ e\ is\ negative\ small\ AND\ \Delta e\ is\ zer$ $THEN\ \hat{x}_{estimated} = x_{actual}$	Combination of observers with AI elements	Overcome limitations of single observer and suitable for systems with incomplete model structure	May be difficult and time consuming For online implementation, the AI elements must first be adapted to the system	For highly nonlinear systems with an incomplete or unknown model
6	Hybrid observers	For combination of extended Luenberger and asymptotic observer: $\frac{dZ(t)}{dt} = D(t)Z(t) + A_1u_1(t) + A_2u_2(t)$	Combination of two or more observers	Overcome the limitations of a single observer	Choosing appropriate combination may be tedious	This is suitable for systems where a single type of observer is not accurate enough

2.3 Artificial intelligence applied as estimator in chemical process systems

Artificial intelligence (AI), which has been established since 1934 have been utilized as estimators apart from other conventional observers explained in section 2.2. They are also addressed as virtual sensors, which involve several algorithms such as expert system (ES), fuzzy logic, genetic algorithm (GA) and artificial neural network (ANN). Those algorithms have been successfully used as estimators or observers in chemical process systems.

ANN has been applied as an estimator in a distillation column for predicting the distillate composition based on the research by Singh et al., where it is able to handle the multi-components in the system to provide accurate estimation (Singh, Gupta, & Gupta, 2005). Besides that, Gonzalez et al. have applied ANN for estimating the mole fractions of the distillate product while Canete et al. have estimated the product composition in binary distillation columns (de Canete, del Saz-Orozco, Gonzalez, & Garcia-Moral, 2012; González, Aguilar, Alvarez-Ramírez, Fernández, & Barrón, 1999). Furthermore, Bahar and Ozgen have predicted the product composition in a reactive distillation column using ANN with satisfactory results (Bahar & Özgen, 2010). Ana Frattini et al. have also applied it for estimating the reflux ratio, top and bottom compositions of a batch distillation column (Frattini, Fileti, Cruz, & Pereira, 2000). ANN has also been utilized for product composition estimation in batch and packed distillation columns (Sharma, Singh, Singhal, & Ghosh, 2004; Zamprogna, Barolo, & Seborg, 2001). Another study has been performed by Fortuna et al. that used ANN to estimate gasoline and butane concentrations in a debutanizer (Fortuna, Graziani, & Xibilia, 2005). Besides that, ANN has also been used for predicting density, viscosity and refractive index of a binary distillation system that results in less than 1% of errors (Mehlman, Wentzell, & McGuffin, 1998).

ANN has acted as estimators in several reactors such as bioreactor, batch reactor, continuous stirred tank reactor (CSTR) and polymerization reactor. Himmelblau has used ANN to predict the polymer product in a polymerization reactor and the outlet concentration of CSTR (Himmelblau, 2008) while Chen and Peng have utilized ANN for estimating the heat transfer coefficients and the heat of reaction in a CSTR (Chen & Peng, 1999). Furthermore, in bioreactors ANN has estimated several parameters including biomass concentration (Acuña, Latrille, Béal, & Corrieu, 1998), cellular concentration (Silva, Pinotti, Cruz, Giordano, & Giordano, 2008), kinetics parameters (de Assis & Filho, 2000), oxygen uptake rate and the evolution rate of carbon dioxide (Komives & Parker, 2003). Other applications of ANN as estimators can be found in stirred tank reactors (STR), fed-batch reactor and stirred cell reactor for estimating the mass transfer coefficient, the ethanol concentrations and the reaction rates accordingly (Gadkar, Mehra, & Gomes, 2005; García-Ochoa & Castro, 2001; Molga & Cherbański, 2003). On the other hand, in polymerization reactors ANN has been used to estimate several parameters including the chain length, reactive impurities, monomer concentration, fouling, heat of reactions, melt index and jacket temperature (Aziz, Hussain, & Mujtaba, 2000; Barton & Himmelblau, 1997; Horn, 2001; Kuroda & Kim, 2002; Yang, Chung, & Brooks, 1999; Zhang, 1999; Zhang, Morris, Martin, & Kiparissides, 1999; Zhang, Morris, Martin, & Kiparissides, 1998).

Besides reactors, ANN has also been applied to estimate ethanol concentration, chemical potency and sugar concentration. Rivera et al. have predicted the ethanol concentration while Dai et al. have estimated both the chemical potency and sugar concentration. (Dai, Wang, Ding, & Sun, 2006; Rivera, Atala, Filho, Carvalho da Costa, & Filho, 2010). Furthermore, Jin et al. have employed ANN for estimating glucose, galactose and carbon source concentrations while Yet-Pole et al. have used ANN to estimate optical density and sugar concentration, all of which in the fermentation processes (Jin, Ye, Shimizu, & Nikawa, 1996; Yet-Pole, Wen-Tengu, & Yung-Chuan, 1996). Further studies are performed to predict biomass concentration and to estimate process kinetics in fermenters (James, Legge, & Budman, 2002; Valdez-Castro, Baruch, & Barrera-Cortes, 2003).

Other parameters that has been estimated by ANN are the pressure drop in rotating fed bed, activated carbon cloth (ACC) in an absorber, the fluid particle temperature and Biot number (B_i) in fluid-particle systems, the conversion rate of iron oxide and the thermal conductivity in gas chromatography (Faur-Brasquet & Le Cloirec, 2003; Jalali-Heravi & Fatemi, 2000; Lashkarbolooki, Vaferi, & Mowla, 2012; Sablani, 2001; Wiltowski et al., 2005). On the other hand, heat transfer rate and heat flux are also predicted using ANN in heat exchangers (Islamoglu, 2003; Su et al., 2002). In addition, the particle size in a cyclone, coal combustion rate and hydrogen content have been estimated using ANN in combustion processes (Du, del Villar, & Thibault, 1997; Linko, Zhu, & Linko, 1999; Yao, Vuthaluru, Tadé, & Djukanovic, 2005; Zhu, Jones, Williams, & Thomas, 1999). ANN has also estimated the slurry velocity in a pipeline and dynamic process compositions in a chemical plant with satisfactory results (Lahiri & Ghanta, 2008; Yeh, Huang, & Huang, 2003). Whereas in an evaporator and membrane separator, ANN has been applied as estimator to estimate the conductivity in a sugar cane factory and to predict permeate and residue hydrogen concentrations respectively (Devogelaere, Rijckaert, Leon, & Lemus, 2002; Lei Wang, Shao, Wang, & Wu, 2006).

Several structures of ANN have been considered for estimating those parameters in chemical process systems such as the feed forward neural networks (FFN), internally recurrent net (IRN), externally recurrent net (ERN), radial basis function networks (RBFN), and the shape-tuneable neural network (MNN) (Chen & Chang, 1996). Each structure has their unique features and their comparisons are listed in Table 2.5 (Mohd Ali, Hussain, Tade, & Zhang, 2015).

Table 2.5: Comparisons of several ANN structures (Mohd Ali, Hussain et al., 2015)

No.	Types of ANN	Key Features	Advantages	Limitations
1	Feed forward neural networks (FFN)	▪ Fixed function and require large amount of training data	▪ Accurately approximate continuous functions ▪ Easy to implement	▪ Slow convergence ▪ Lack dynamics ▪ Mainly used for static function approximation
2	Internally recurrent net (IRN)	▪ Characterized by time-delayed feedback connections from output of hidden nodes back to inputs of hidden nodes	▪ Capable of estimating process with changing variable dynamics ▪ No limit for the number of states	▪ Difficult to initialize ▪ Training can be time consuming
3	Externally recurrent net (ERN)	▪ Contain time-delayed feedback connections from output layer to a hidden layer	▪ Easy to initialize ▪ Simple design and can use current values to initialize states	▪ Number of states must be the same as model outputs ▪ Training can be time consuming
4	Radial basis function neural networks (RBFNN)	▪ Basis function used can be Gaussian or wavelets ▪ Do not apply back-propagation for training	▪ Less sensitive to sensor noise ▪ Faster training	▪ Most suitable for classification problem ▪ Large number of hidden nodes needed
5	Recurrent trainable neural network (RTNN)	▪ Hidden layer is the recurrent layer and the other two layer is based on back propagation	▪ Faster convergence ▪ Less complexity in the design	▪ Not versatile ▪ Slow training due to sequential structure
6	Shape-tuneable neural network (MNN)	▪ Allow tuning of weight between neurons and its saturation function of each neurons simultaneously	▪ Sensitive to plant changes but still provide good estimation even with varied parameters	▪ Greatly depends on sampling time and initial parameters

Fuzzy logic is another AI algorithm that has been used as estimators. It is applied for estimating the specific O_2 uptake rate and the specific CO_2 evolution rate to obtain high yield and productivity in a fermentor (Hisbullah, Hussain, & Ramachandran, 2003). It is also used to estimate the energy efficiencies in a furnace (Geng, Han, Gu, & Zhu, 2012). Furthermore, fuzzy logic has approximated the population size of algae and fault in a wastewater treatment plant and digestion reactor accordingly (Cong, Yu, & Chai, 2010; Shen & Chouchoulas, 2001). In a pipeline, fuzzy has been applied as the estimator to predict heat flux while in a fed-batch reactor for estimating the product concentration (Chen & Lee, 2008; Patnaik, 1997). Besides that, fuzzy logic has also been utilized in a digester for biogas and methane production rate estimations and to predict faults in both residual evaluation and gasoline sample (Brudzewski, Kesik, Kołodziejczyk, Zborowska, & Ulaczyk, 2006; Frank & Köppen-Seliger, 1997; Turkdogan-Aydınol & Yetilmezsoy, 2010). Liu has also utilized fuzzy logic for estimating melt index in a fluidized bed reactor of LDPE plant while Genovesi et al. have applied fuzzy logic for estimating sensor and process faults in a digestion reactor (Genovesi, Harmand, & Steyer, 1999; J. Liu, 2007).

Apart from that, GA and ES have also been used as estimators. GA has been applied in several unit operations including distillation column and wastewater treatment plant. It has estimated the process input parameter with higher conversion and is able to increase the productivity (Rezende, Costa, Costa, Maciel, & Filho, 2008). In a CSTR, GA has been used to predict the reactor temperature, which provided superior ability as well as to predict the learning parameters in a fruit dehydration process (Abdul Wahab, Hussain, & Omar, 2007; Mohebbi, Shahidi, Fathi, Ehtiati, & Noshad, 2011). ES, on the other hand, has been applied for estimating the effluent colour of the waste produced for further treatment in a wastewater treatment process (Paraskevas, Pantelakis, & Lekkas, 1999). ES has also been utilized to predict product flow and temperature in a crude oil distillation column and to approximate probability of odour in a waste treatment plant (Kordon, Dhurjati, & Bockrath, 1996; Motlaghi, Jalali, & Ahmadabadi, 2008).

In addition, AI elements have been merged with one another to form hybrid estimators for increasing the estimation performances such as fuzzy neural network (FNN), hybrid neural network (HNN), expert system neural network (ES-NN) and adaptive neuro-fuzzy inference systems (ANFIS) (Sivan, Filo, & Siegelmann, 2007). ANFIS has been applied as estimator to predict compositions in a reactive distillation column and to estimate emulsion stability in the water-in-oil mixtures as well as to predict the friction factor in a coiled tubes (Beigzadeh & Rahimi, 2012; Khazraee & Jahanmiri, 2010; Yetilmezsoy, Fingas, & Fieldhouse, 2011).Whereas FNN has been used to estimate the fault in a valve, melt index and molecular weight average (M_w) in a polymerization reactor (Chitanov, Kiparissides, & Petrov, 2004; Korbicz & Kowal, 2007; X. Liu & Zhao, 2012). Besides that, FNN has also been applied to predict viscosity and biomass concentration in a bioreactor (Araúzo-Bravo et al., 2004). Moreover, fuzzy-rough set or FuREAP has also estimated the population size of algae in a wastewater treatment plant (Shen & Chouchoulas, 2001).

Furthermore, HNN has been utilized in several process systems such as to predict the production yield and gas compositions in fluidized bed gasifier, to estimate temperature and monomer concentration in a polymerization reactor, for pressure and injection time estimations in a plastic injection moulding process, to estimate the porosity in food drying process and to approximate the liquid heads in tanks (Guo, Li, Cheng, Lü, & Shen, 2001; Hussain, Rahman, & Ng, 2002; Ng & Hussain, 2004; Wilson & Zorzetto, 1997; Yarlagadda & Teck Khong, 2001). Besides that, a structure approaching hybrid neural network (SAHNN) has been applied in a batch reactor to predict the reactant concentrations with rapid convergence shown while hybrid mechanistic-neural network rate function model (HMNNRFM) has been utilized in a fixed bed reactor for estimating the reaction (Kumar & Venkateswarlu, 2012; Wang, Cao, Wu, Li, & Jin, 2011).

ANN has once been combined with GA known as GNN for critical heat flux estimation in the heated tubes (Wei, Su, Qiu, Ni, & Yang, 2010). Other combinations are the expert system with fuzzy (Fuzzy-ES) and neural network (ANN-ES). Fuzzy-ES has been applied to predict the froth density in a flotation column (Chuk, Ciribeni, & Gutierrez, 2005) while ANN-ES is used to estimate sulphur and silicon concentrations in a furnace (Radhakrishnan & Mohamed, 2000). Moreover, fuzzy logic has been merged with GA to estimate the kinetic parameters in a sulphuric acid catalyst preparation process (Yang & Yan, 2011). Both fuzzy logic and neural network have also been combined with GA in a plastic injection moulding process to estimate the weight distribution (Li, Jia, & Yu, 2002). The applications of all the AI elements applied as observers in chemical process systems above are tabulated in Table 2.6.

Table 2.6: Various application of AI as observers in chemical process systems (Mohd Ali, Hussain et al., 2015)

a) ANN as estimators in chemical process systems

Types	Objective /Estimate(s)	Systems Applied	Positive Highlights	Ref
FFN	Conductivity	Evaporator	Small validation error (7%)	(Devogelaere, et al., 2002)
ANN	Gasoline and butane concentration	Debutanizer	Able to overcome delay	(Fortuna, et al., 2005)
ANN	Distillate composition	Distillation column	Good for binary distillation without multi-component	(Singh, Gupta, & Gupta, 2005)
ANN	Distillate composition	Distillation column	Handle many inputs with accurate results	(Singh, Gupta, & Gupta, 2007)
Adaptive Neural Network	Product composition	Binary distillation column	High accuracy with faster response	(de Canete, et al., 2012)
ANN	Mole fraction of distillate product	Binary distillation column	Satisfactory estimation performance, help to enhance overall control	(González, Aguilar, Alvarez-Ramírez, Fernández, & Barrón, 1999)
ANN	Product composition	Reactive distillation column	Allow error refinement	(Bahar & Özgen, 2010)
ANN	Top, bottom composition, reflux ratio	Batch distillation	Able to speed up training for better prediction	(Frattini Fileti, Cruz, & Pereira, 2000)
RANN	Product compositions	Batch Distillation	Good agreement with actual value	(Zamprogna, Barolo, & Seborg, 2001)
ANN	Faults	Packed distillation column	Consistent results even with disturbances	(Sharma, et al., 2004)
IRN	Polymer product quality	Polymerization reactor	Excellent prediction especially in grade transition region	(Himmelblau, 2008)
IRN	Outlet reactor concentration	CSTR	Good prediction compare with Extended Kalman filter (EKF)	(Himmelblau, 2008)
MNN	Heat of reaction, heat coefficient	CSTR	Handle system with noise	(Chen & Peng, 1999)
ANN	Kinetic parameters	Bioreactor	Good estimation for on-line application	(de Assis & Filho, 2000)
RANN	Biomass concentration	Bioreactor	Stable estimation based on corrective action during training	(Acuña, Latrille, Béal, & Corrieu, 1998)

a) ANN as estimators in chemical process systems (continued)

MLPFF	Cellular concentration	Bioreactor	Accurate estimation at all three phases (lag, exponential, stationary)	(Silva, et al., 2008)
FFN	Oxygen uptake rate, carbon dioxide evolution rate	Bioreactor	High accuracy even the training data is reduced and save cost due to the reduction	(Komives & Parker, 2003)
ANN	Oxygen mass transfer coefficient	STR	Good prediction even with noise	(García-Ochoa & Castro, 2001)
ANN	Overall reaction rates of anhydrite	Stirred cell reactor	Good estimation even without initial assumption	(Molga & Cherbański, 2003)
ANN	Substrate, ethanol concentration	Fed-batch reactor (Experimental)	Estimation can be done outside domain	(Gadkar, Mehra, & Gomes, 2005)
ANN	Heat-released	Batch reactor	Accurate and fast estimation	(Aziz, Hussain, & Mujtaba, 2000)
FFN	Reactive impurities, polymer product quality	Polymerization reactor	Effective estimation if based only on the initial batch condition of reactive impurities	(Zhang, Morris, Martin, & Kiparissides, 1998)
Stacked NN	Reactive impurities, fouling	Polymerization reactor	Good prediction with impurities	(Zhang, Morris, Martin, & Kiparissides, 1999)
ANN	Initiator concentration, heat of reaction	Polymerization reactor	Only need measurement of one variable for training	(Horn, 2001)
ANN	Monomer, Initiator concentration	Polymerization reactor	Satisfactory estimation performance	(Yang, Chung, & Brooks, 1999)
MLRN	Chain length	Polymerization reactor	Good estimation that allow variety of measured variables during training	(Meert & Rijckaert, 1998)
ANN	Reactor temperature	Polymerization reactor	Small estimation error	(Kuroda & Kim, 2002)
Bootstrap NN	Weight and number of average MW	Polymerization reactor	Reduce estimation error	(Zhang, 1999)

a) ANN as estimators in chemical process systems (continued)

IRN	Polymer product quality	Polymerization reactor (Experimental)	Accurate prediction over wide range of transition period	(Barton & Himmelblau, 1997)
ANN	Ethanol concentration	Flash fermentor	Optimum performances	(Rivera, Atala, Filho, Carvalho da Costa, & Filho, 2010)
ANN	Sugar concentration, chemical potency	Fermentation process	Good agreement with the value from production process	(Dai, Wang, Ding, & Sun, 2006)
ANN	Glucose and Galactose concentration, residual carbon concentration	Fermentor (Experimental)	Error of estimation is almost zero (0.06%)	(Jin, Ye, Shimizu, & Nikawa, 1996)
ANN	Consumed sugar concentration, optical cell density	Fermentor (Experimental)	Satisfactory despite variation in substrate	(Yet-Pole, Wen-Tengu, & Yung-Chuan, 1996)
FFN, RBFNN	Biomass concentration	Fermentor	Good estimation even with variation in yield coefficient	(James, Legge, & Budman, 2002)
ANN	Fluid and particle temperature, Biot number (B_i)	Fluid-particle system	Able to reduce the error of estimation	(Sablani, 2001)
RNNM	Process kinetics	Fermentor (Experimental)	Reliable estimates and able to avoid over-fitting of NN during learning	(Valdez-Castro, Baruch, & Barrera-Cortes, 2003)
ANN	Density, viscosity, refractive index	Binary system (water-methanol-acetonitrile-tetrahydrofuran mixtures)	Small estimation error	(Mehlman, Wentzell, & McGuffin, 1998)
ANN	Heat transfer rate	Heat exchanger	Consistent prediction value compared with actual value	(Islamoglu, 2003)
ANN	Heat flux	Heat exchanger	Prediction is based on known experimental data	(Su, et al., 2002)
ANN	Pressure drop	Rotating fed bed	Accurate estimation compare with actual values in wet bed	(Lashkarbolooki, et al., 2012)
ANN	Activated carbon	Absorber	Satisfactory prediction performance	(Faur-Brasquet & Le Cloirec, 2003)

a) ANN as estimators in chemical process systems (continued)

ANN	Iron oxide conversion rate	Iron oxide reduction process	High convergence	(Wiltowski, et al., 2005)
ANN	Thermal conductivity response factor	Gas chromatography	Good agreement with actual value	(Jalali-Heravi & Fatemi, 2000)
ANN	Particle size	Cyclone (grinding process)	Simple formulation	(Du, et al., 1997)
FFN	Coal combustion rate	Coal combustion process	High accuracy and robust compared with actual value	(Zhu, Jones, Williams, & Thomas, 1999)
BPNN	Hydrogen content of coal	Coal combustion process	Prediction is based on proximate analysis	(Yao, Vuthaluru, Tadé, & Djukanovic, 2005)
ANN	Slurry velocity, solid concentration	Pipeline for conveying bulk material	Suitable for difficult model development process	(Lahiri & Ghanta, 2008)
FFN	Dynamic compositions	Tennessee Eastman plant	Reliable estimates upon calibration of the estimator	(Yeh, et al., 2003)
ANN	Lipase, biomass concentration	Enzyme process (Experimental)	Good estimation based only one online measured parameters	(Linko, Zhu, & Linko, 1999)
RBFNN	Permeate and residue hydrogen concentration, permeate gas flux	Gas membrane separator	Predict by omitting many boundary values	(Wang, et al., 2006)
FFN	Moisture content of bananas	Fruit dehydration process	Superior ability in predicting moisture content	(Mohebbi, et al., 2011)
ANN	Critical odour release	Waste water treatment plant (refinery)	Good prediction even when number of nodes are reduced	(Kordon, et al., 1996)

b) Fuzzy Logic as estimators in chemical process systems

Types	Objective /Estimate(s)	Systems Applied	Positive Highlights	Ref
Fuzzy Takagi-Sugeno (FTS)	Fouling parameters	Heat exchanger	Accurate estimate without any additional sensors	(Delrot, et al., 2012)
Fuzzy Takagi-Sugeno (FTS)	Specific CO_2 evolution rate, specific O_2 uptake rate	Fermentor	Eliminate defuzzification part since output can be directly obtained from rule part	(Hisbullah, Hussain, & Ramachandran, 2003)
Fuzzy	Energy efficiencies of ethylene	Furnace	High efficiencies, able to reduce more than 50% of the cost	(Geng, Han, Gu, & Zhu, 2012)
Fuzzy	Size of Algae population	Wastewater treatment plant	High accuracy that able to improve the runtime	(Shen & Chouchoulas, 2001)
Intelligent Fuzzy Weighted	Heat flux	Thermal fluid hollow cylinder pipeline	Fast convergence	(Chen & Lee, 2008)
Fuzzy	Product concentration	Fed-batch reactor	Easy design	(Patnaik, 1997)
Fuzzy matching	Cost	Chemical plant (Chem. Systems Ltd.)	Accurate with minimal estimation effort	(Petley & Edwards, 1995)
Fuzzy (Mamdani inferences)	Biogas, methane production rate	Digester	Satisfactory performance with small deviation	(Turkdogan-Aydınol & Yetilmezsoy, 2010)
Fuzzy c-means (FCM)	Melt index	Fluidized bed reactor	Reduce input variables dimension	(Liu, 2007)
Fuzzy (Mamdani inferences)	Fault on pH sensor and sodium hydroxide frequency	Digestion reactor (Experimental)	Satisfactory even with varied operating condition	(Genovesi, Harmand, & Steyer, 1999)

c) ES as estimators in chemical process systems

Types	Objective /Estimate(s)	Systems Applied	Positive Highlights	Ref
ES	Probability of odour	Waste water treatment plant	Good prediction even when number of nodes are reduced	(Kordon, et al., 1996)
ES	Effluent waste colour	Wastewater treatment plant	Provide early warning for further treatment process	(Paraskevas, Pantelakis, & Lekkas, 1999)
ES	Product flow, temperature	Crude oil distillation column	Able to minimise the error	(Motlaghi, Jalali, & Ahmadabadi, 2008)

d) GA as estimators in chemical process systems

Types	Objective /Estimate(s)	Systems Applied	Positive Highlights	Ref
GA	Size of Algae population	Wastewater treatment plant	High accuracy that able to reduce the cost	(Shen & Chouchoulas, 2001)
GA	Friction factor	Helically coiled tubes (Experimental)	High accuracy by improving the mean relative error	(Beigzadeh & Rahimi, 2012)
GA	Hydrogen concentration, temperature of coolant and reactant	Catalytic reactor	High conversion	(Rezende, Costa, Costa, Maciel, & Filho, 2008)
GA	Temperature	CSTR	Minimize error between the estimated and set point temperature	(Wahab, Hussain, & Omar, 2007)
GA	Moisture content of banana	Fruit dehydration process	Superior ability of on-line estimation	(Mohebbi, et al., 2011)
GA	Fuel input parameter	Palm oil mill	Consistent prediction	(Ahmad, Azid, Yusof, & Seetharamu, 2004)

e) Hybrid systems as estimators in chemical process systems

Types	Objective /Estimate(s)	Systems Applied	Positive Highlights	Ref
FuREAP	Size of Algae population	Wastewater treatment plant	High accuracy that able to improve the runtime	(Shen & Chouchoulas, 2001)
ANFIS	Compositions	Multi-component reactive distillation column	Reliable and accurate estimation	(Khazraee & Jahanmiri, 2010)
FNN	Fault signal in valve	Control valve	Good estimation despite model mismatch	(Korbicz & Kowal, 2007)
FNN	Melt index	Polymerization reactor (Experimental)	Able to settle the online training efficiency problem	(Liu & Zhao, 2012)
FNN	MW average	Polymerization reactor	Fast estimation	(Chitanov, Kiparissides, & Petrov, 2004)
FNN	Biomass concentration, viscosity	Bioreactor	Fast convergence	(Araúzo-Bravo, et al., 2004)
ANFIS	Emulsion stability	Water-in-oil mixtures	Satisfactory performance with small deviation	(Yetilmezsoy, et al., 2011)
ANFIS	Friction factor	Helically coiled tubes	High accuracy by improving the mean relative error	(Beigzadeh & Rahimi, 2012)
HNN	Injection time, injection pressure	Plastic injection moulding process	Small estimation error without the knowledge of injection moulding	(Yarlagadda & Khong, 2001)
HNN	Product yield, gas compositions	Fluidized bed gasifier	Powerful estimator especially for complex process	(Guo, Li, Cheng, Lü, & Shen, 2001)
HNN	Monomer concentration	Polymerization reactor	Accurate estimation without the knowledge of model structure	(Ng & Hussain, 2004)
HNN	Monomer concentration, temperature	Polymerization reactor	Good validation results, fast convergence	(Wei, Hussain, & Wahab, 2007)
HNN	Liquid heads	3-tanks in series	Able to handle noise and variation of the stochastic process	(Wilson & Zorzetto, 1997)
HNN	Food porosity	Food drying process (Experimental)	High accuracy based on increasing number of inputs	(Hussain, Rahman, & Ng, 2002)

e) Hybrid systems as estimators in chemical process systems (continued)

SAHNN	Reactants rates and concentration	Batch reactor	Fast convergence rate	(Wang, Cao, Wu, Li, & Jin, 2011)
HMNNRFM	Reaction rate	Fixed bed reactor	Good prediction without use of model equation	(Kumar & Venkateswarlu, 2012)
ANN-GA (GNN)	Critical heat flux	Heated tubes	Fast convergence, consistent prediction	(Wei, Su, Qiu, Ni, & Yang, 2010)
FFN-ES	Silicon, sulphur compositions	Furnace	Small estimation error	(Radhakrishnan & Mohamed, 2000)
Fuzzy-ES	Froth density	Flotation column (Experimental)	Satisfactory despite variation in feed rate	(Chuk, Ciribeni, & Gutierrez, 2005)
Fuzzy-GA	Kinetic parameters	Sulphuric acid catalyst preparation process	Effective convergence, able to avoid premature convergence	(Yang & Yan, 2011)
Fuzzy-Neural-GA	Injection velocity and cooling water temperature	Plastic injection moulding	Good generalization capabilities	(Li, Jia, & Yu, 2002)

2.4 Applications of model predictive control in chemical process systems

MPC has been applied in many industries such as in the distillation column, drying towers, cement industry and PVC plant. Various types of MPC algorithms have been developed such as Model Algorithmic Control (MAC), Generalized Predictive Control (GPC), Predictive Functional Control (PFC), Dynamic Matrix Control (DMC), Extended Prediction Self Adaptive Control (EPSAC), and Extended Horizon Adaptive Control (EHAC). Their characteristics and formulations in determining the control law that make them different from each other (Camacho & Bordons, 2004).

Cutler and Ramaker have developed the Dynamic Matrix Control (DMC), which has been widely used in various industries especially petrochemicals (Cutler & Ramaker, 1980). DMC uses the step response model for prediction. The process has to be assumed stable without integrators and DMC tends to show unusual dynamic behavior, which is incapable to be demonstrated by the transfer function model. However, the size of the model must be first identified, thus not suitable for the unstable process. Only the future error or both the future error and control effort will be included in the cost function of DMC as given in Eq. (2.1) (Camacho & Bordons, 2004).

$$\boldsymbol{J(N_1 N_2 N_u) = \sum_{j=N_1}^{N_2} \delta\,(j)[\hat{y}(t+j-t) - w(t+j)]^2 + \sum_{j=1}^{N_u} \lambda\,(j)[\Delta u(t+j-1)]^2} \quad (2.1)$$

On the other hand, the disturbances have remained the same along the control horizon and are equal to the measured value of output (y_m) minus the estimated model output ($\hat{y}(t|t)$). The predicted value is described in Eq. (2.2) (Camacho & Bordons, 2004).

$$\hat{y}(t+k|t) = \sum_{i=1}^{k} g_i \Delta u(t+k-1) + \sum_{i=k+1}^{N} g_i \Delta u(t+k-i) + \hat{n}(t+k|t) \quad (2.2)$$

Model Algorithmic Model (MAC) has been classified as the simplest and most intuitive MPC algorithm. It has been recognized as Model Predictive Heuristic Control (MPHC). MAC uses impulse response model, which is suitable for a stable process with equivalent disturbances along the horizon. MAC do not apply the control horizon concept since the number of control signals is similar to the number of future outputs. The output prediction is given in Eq. (2.3) (Camacho & Bordons, 2004).

$$\hat{y}(t) = \sum_{j=1}^{N} h_i u(t-j) = H(z^{-1})u(t) \tag{2.3}$$

Besides that, Predictive Functional Control (PFC) algorithm uses the state space model of the process that allows nonlinearity and instability. PFC has two characteristics namely the basis functions and the coincidence points. According to the basis function theory, the control signal is parameterized using a set of polynomial, which specifies the relative complex input profile over a huge range of horizon. A coincidence point, on the other hand, is a concept that simplifies the calculations by considering only a subset of points in the prediction horizon. In order to correspond to the point, the desired and predicted future outputs are required. The cost function needed for minimization has been given in Eq. (2.4). Here, $w(t+h_j)$ represents a first-order approach to a known reference (Camacho & Bordons, 2004).

$$J = \sum_{j=1}^{n_H} \left[\hat{y}(t+h_j) - w(t+h_j)\right]^2 \tag{2.4}$$

The remaining three algorithms of MPC use transfer function models and are applicable for unstable processes. The algorithms are the Extended Horizon Adaptive Control (EHAC), Extended Predictive Self Adaptive Control (EPSAC), and Generalized Predictive Control (GPC), which are differentiated by their disturbances. Disturbances of

EPSAC is measurable but not for GPC while EHAC is able to neglect the disturbances (Camacho & Bordons, 2004).

MPC has influenced process control during the past twenty years with its early technology evolved principally in industrial settings, followed by many types of research that analyze the theoretical basis (Froisy, 2006). Its methodology has been very appealing to the practitioner because input and state constraints are explicitly accounted in the controller. Many industrial applications have applied MPC using the integrated software including the QDMC, IDCOM-M, HIECON, SMCA and SMOC. All these have been commercialized as the new version of MPC (Qin & Badgwell, 2003).

AlGhazzawi and Lenox have emphasized that the sustaining performance of MPC in a system depended on various factors such as lack of experienced operators and support personnel, lack of condition monitoring, significant process modifications, poor controller tuning and inaccurate model as well as the unresolved basic PID control problem (AlGhazzawi & Lennox, 2009). Besides that, Wang and Young have proposed a new design of MPC, which is based on the non-minimal type of the state space model (Wang & Young, 2006). A state variable here has been chosen as a set of measured input and output variables alongside their past values. In addition, Palma and Magni have specified that MPC can be applied starting from the black box or other model structures (Di Palma & Magni, 2007).

In the polymerization process though, MPC has been developed with several approaches such as linear MPC (LMPC), nonlinear MPC (NMPC), neural network MPC (NNMPC) and INCA or the new technology of MPC to cater for the demand driven process (Brempt et al., 2001). All the approaches have been successfully applied to control the parameters including temperature, pressure, molecular weight distribution (MWD) and reaction rate of the process to obtain acceptable rate of the polymer produced

(Shamiri, Hussain, Mjalli, Mostoufi, & Hajimolana, 2013). Emad and Mohammad have applied NMPC to control the MWD of the polyethylene process in a gas-phase reactor by manipulating the hydrogen content and the catalyst (Ali & Ali, 2010). NMPC has also been applied by Seki at al. to control the temperature to maximize the monomer feed rate in a semi-batch polyethylene reactor (Seki et al., 2001). They applied the NMPC using successive linearization approach.

In the fluidized bed catalytic reactor (FCR), MPC has been applied to control the emulsion temperature and the propylene production rate (Ho, Shamiri, Mjalli, & Hussain, 2012) and to minimize the set point error (Ibrehem, Hussain, & Ghasem, 2008). In addition, Ali et al. have used the NMPC to control bed temperature and total pressure of an ethylene polymerization reactor by manipulating the bleed and inlet coolant flow (Ali, Al-Humaizi, & Ajbar, 2003). Temperature is one of the common industrial controls besides the total pressure because of the perseverance of the total mass and energy as well as steady state operation it has provided (Ali et al., 2003). In several MPC designs, researchers have also included the estimation techniques such as Extended Kalman Filter (EKF) to reduce the amount of parametric error that lead to model-plant mismatches (Ali et al., 2003) and causing offsets and persistence oscillation (Ahn, Park, & Rhee, 1999; Hedengren, Allsford, & Ramlal, 2007; Jacob & Dhib, 2012; Ramlal, Allsford, & Hedengren, 2007). The applications of different types of MPC in chemical process units are also summarized in Table 2.8.

Table 2.7: MPC applications in chemical process systems

Type of MPC	Objective /Estimate(s)	Systems Applied	Positive Highlights	Ref
NMPC	Stream temperature	Heat exchanger	Increase the flexibility and resiliency of the heat exchanger	(Akman & Uygun, 1999)
NMPC	Electrical circuits/ electrodes	Electric arc furnace	Efficient in environment protection, extract hazardous gas	(Bekker, Craig, & Pistorius, 2000)
On-Off MPC	pH control, minimise CO_2 lost	Micro-algal tubular photo-bioreactor	Avoid cycle time delay, reduce oscillation at appropriate sampling time	(Berenguel, Rodríguez, Acién, & García, 2004)
Constrained DMC	Feed flowrate, dilution water flowrate	Grinding process (Ball mill grinding	Overcome sluggish due to imperfect model	(Chen, Li, & Fei, 2008)
NMPC	Set point tracking of crystal mass	Crystallization process (CSTR)	Good set point tracking even in the presence of vacuum accident data	(Damour, Benne, Grondin-Perez, & Chabriat, 2010)
DMC	Permeate flux, flowrate, conductivity	Desalination unit	Good control even with large variation of process gain	(Abbas, 2006)
Linear MPC	Particle size distribution	Continuous granulation plant	Robustness and efficiency increased	(Glaser et al., 2009)
NMPC	Dissolved O_2 concentration	WWTP (aerobic reactor)	Good performance in controlling the concentration	(Holenda, Domokos, Rédey, & Fazakas, 2008)
Linear MPC	Product concentration	Bioreactor	Good control and achieve high concentration of product	(Ashoori, Moshiri, Khaki-Sedigh, & Bakhtiari, 2009)
NMPC	Control MWD of online polymer, manipulate H2 content	Gas-phase PE reactor	Achieve good control even when there is model errors	(Ali & Ali, 2010)
MPC (INCA)	Melt index, density, temperature and prod rate	Gas-phase fluidized bed PE reactor (HDPE)	Low implementation cost, present new method of off-line trajectory optimization with feedback control	(Brempt et al., 2001)

Table 2.7 (continued)

NMPC using successive linearization	Maximize monomer feed rate, Temperature	CSTR (Semi-batch polypropylene reactor)	Satisfactory result with heat removal constraints	(Seki et al., 2001)
NNMPC (neural network MPC)	Minimize setpoint error	Fluidized bed catalytic reactor	Small offsets, small oscillation compare to PID	(Ibrehem et al., 2008)
APMBC (Adaptive predictive model based control)	Control propylene production rate, emulsion phase temperature	Fluidized bed reactor (propylene)	Excellent regulatory control properties	(Ho et al., 2012)
NMPC	Bed temperature, total pressure	Gas-phase polyethylene reactor	Multivariable control of PE reactor using two approaches	(Ali et al., 2003)

2.5 Summaries and analysis of the literature review

Based on the review, observers have been widely applied in chemical process systems to estimate parameters or unknown states. Those observers include the six classes as discussed in section 2.2 and the AI elements applied as estimators explained in section 2.3. The trend of those observers has changed from single to hybrid as depicted in Figure 2.1. Although single-based observers will still be used, its pattern is inconsistent and is limited to particular estimation in certain systems.

On the other hand, the hybrid observers, which made its debut around 2000 have shown increasing in usage. The existence of many types of observers that can be merged and the availability of software are among the reasons for the increased. Besides that, those hybrid observers also tend to produce better results such as improving the rate of estimation. Therefore, it is clear that hybrid observers are significant contributions for adding knowledge to the whole observer related research area.

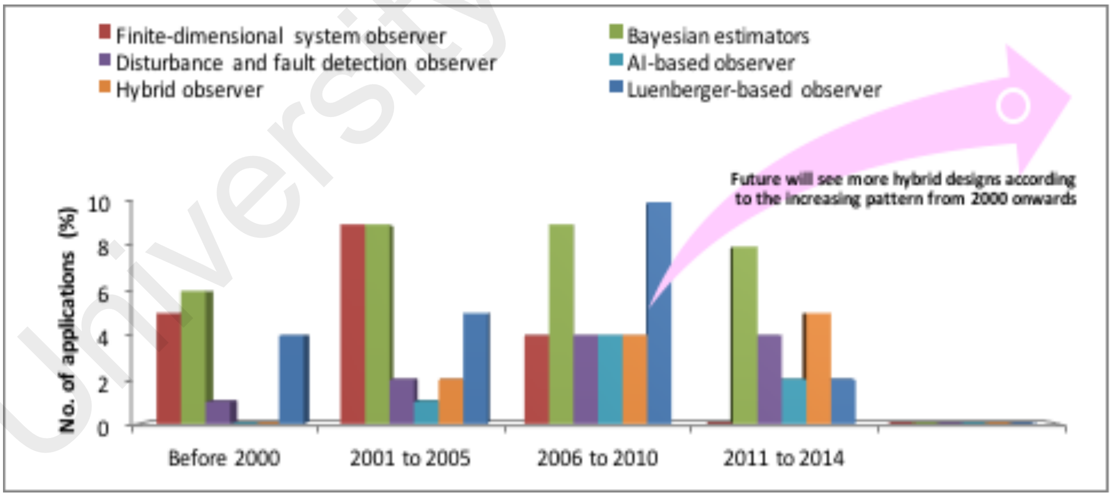


Figure 2.1: Current and future trend of observer in chemical process systems (Mohd Ali, Hussain et al., 2015)

Several single observers that have been combined to establish hybrid observers for parameters estimation in chemical process systems are the extended Luenberger observer (ELO), extended Kalman filter (EKF), reduced-order observer, sliding mode observer (SMO), interval observer and asymptotic observer. The reduced-order observer has been merged three times while ELO, EKF, SMO, continuous and discrete observer two times according to the literature survey. Interval, full-order, adaptive, asymptotic and proportional observers are combined once so far. The number of combinations has been illustrated in Figure 2.2.

Type of observers to be merged depends on the availability information of the plant and the rate of convergence. For example, if kinetics data is not accessible, asymptotic or exponential observer is appropriate, and it may be combined with EKF, interval, sliding mode or adaptive observer for improving the rate of convergence. Apart from that, several observers have never been merged before including the adaptive state observer (ASO), backstepping, specific, generic, geometric, pole-placement, profile positions and disturbance observers. Those observers are also eligible for merging based on their characteristics.

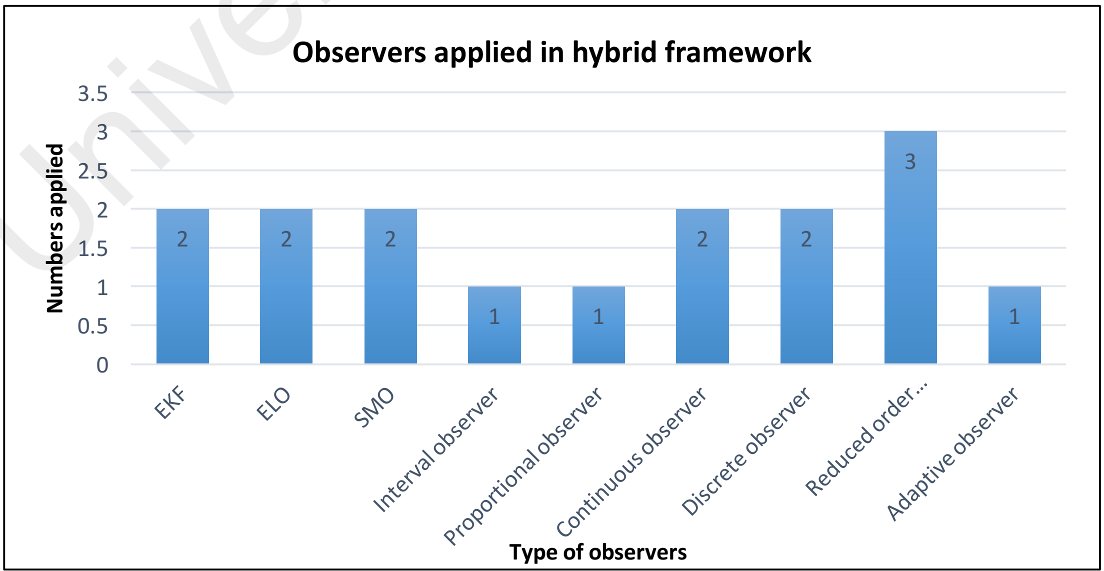


Figure 2.2: Number of times observers applied in hybrid framework

In this research, SMO is combined with fuzzy logic. The combination is chosen based on the outstanding characteristics of the SMO, which provides stable, fast and accurate estimation. Besides that, it does not require precise input assumptions during the design. Meaning that if the initial value of the parameter is wrong, SMO can still recalculate the value until achieving the correct value during the estimation. For simple formulation yet obtaining the best results, SMO is merged with fuzzy logic. SMO has not been combined with another conventional observer to avoid complex formulation during the design and fuzzy logic is a simpler algorithm compared to other AI elements when used with SMO in the hybrid observer design framework.

Then, knowing that the overall control of a system will be enhanced if a controller is coupled with the observer, the MPC controller has been developed in this work. Previous work has also proved that this estimation based control method able to provide better control in the system. For example, KF has been combined with a state feedback controller to maintain the control of drying process by estimating the material moisture content despite disturbances (ambient air temperature, humidity and feed flow rate) in a fluidized bed dryer (Abdel-Jabbar, Jumah, & Al-Haj Ali, 2005).

Then, globally linearized control (GLC) has been added with EKF and ASO to estimate the compositions and flow rates of the top tray as well as distribution coefficients with inadequately known parameters in a distillation column (Amiya Kumar Jana, Nath Samanta, & Ganguly, 2006). Besides that, EnKF and UKF have also been coupled with NMPC for unmeasured disturbances estimation in a hybrid tank system (Prakash, Patwardhan, & Shah, 2010). Nagy et al. have applied proportional integral observer to predict the states in a waste treatment plant (Kiss et al., 2011). Other works include disturbance observer with multivariable controller for estimating disturbances in grinding mill, dissipative observer with on-off controller in non-monotonic reactor for predicting reactor's properties and profile position observer with generic model control (GMC) in debutanizer (Chen et al., 2009; Gupta, Ray, & Samanta, 2009; Schaum, Moreno, Díaz-Salgado, & Alvarez, 2008). Besides that, Yang et al. has also combined MDOB with MPC to stabilize the jacketed stirred tank reactor and to enhance the control performance of a batch distillation column, Murlidhar and Jana have applied ASO with GMC (Murlidhar & Jana, 2007; Yang et al., 2011).

All those works have motivated the coupling of the observer with the MPC controller. Furthermore, an integrator has been added to the MPC to avoid offset while controlling the temperature of the reactor. This embedded integrator MPC has previously been applied in many single-input single-output (SISO) systems and the modifications to suit the multiple-input multiple-output (MIMO) system of the polymerization process for this case are performed. In addition, MPC is chosen since the design also involves the state space model similar with the hybrid observer. Thus, simplicity of the formulation is expected to be achieved.

CHAPTER 3: METHODOLOGY

3.1 Chapter overview

In this third chapter, the general methodologies of the research for developing the proposed hybrid observer and MPC controller are explained. The ethylene polymerization process used to evaluate the performance of the observer and controller is also provided.

3.2 General methodology of research

Information gathering through literature surveys is the initial step in every research project so as to understand the requirements of such research area. Survey will also provide analysis to ensure the project is a novel work and different from the previous works, thus adding new knowledge to the field of study. Once the information has been gathered, they are analyzed in order to decide on the type of observers to be merged and the AI elements to be applied. The early approach is to hybrid two conventional observers and later added the AI element to improve the performances. Upon deciding the type of observers and AI algorithm, the design of observers will begin with the aid of SIMULINK and MATLAB.

The modelling of a polyethylene plant is the next step focusing on the fluidized bed reactor and deciding on the unknown parameters to be estimated by the observer. A test run will be carried out in two different conditions, which are with and without noise to observe the performances. If positive results are obtained, the embedded integrator MPC will be developed based on the previous parameters that have been accurately estimated. The set point tracking and disturbances rejection tests are performed for observing the MPC and overall control performances in the system.

The simulated result will then be validated and compared with the actual pilot plant data for further verification. Once all the results and findings have been completed, they will be analyzed to make conclusions. The workflow of the general methodology is illustrated in Figure 3.1.

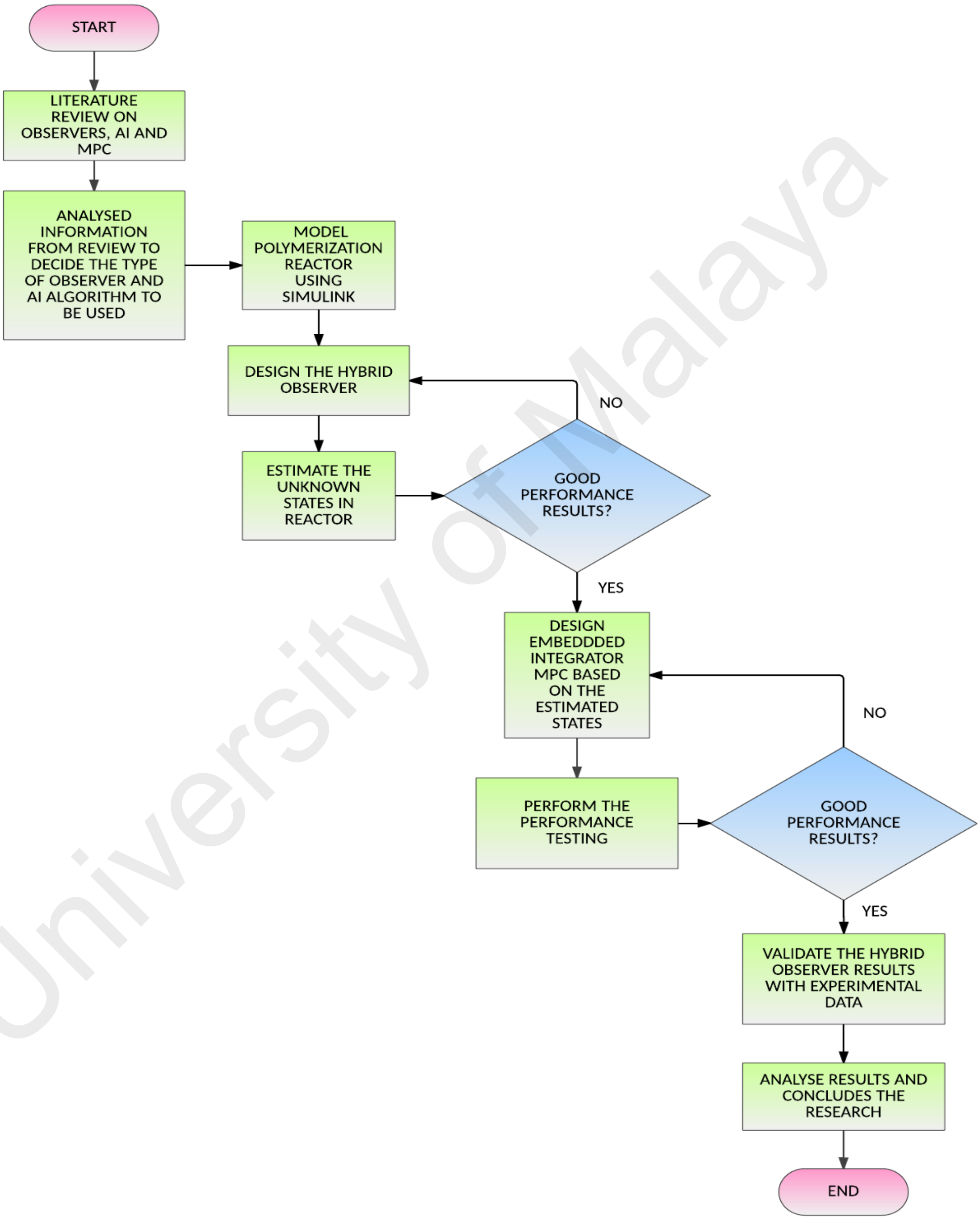


Figure 3.1: General methodology of the research

3.3 Ethylene polymerization process

The polymerization process applied here is based on the well-mixed UNIPOL model designed by McAuley to produce polyethylene in the year of 1990 as illustrated in Figure 3.2 (McAuley, MacGregor, & Hamielec, 1990; McAuley, Talbot, & Harris, 1994). The feed gas is merged with the recycled gas before entering the reactor together with four major components namely the monomer (ethylene), co-monomer (butene), hydrogen (H_2) and nitrogen (N_2).

Those gases act as the fluidization agents and heat transfer media to supply reactants for the growing particles in the reactor. N_2 is also used to transport the catalyst powder and maintain the column pressure at its desired value. On the other hand, the cooling water flowrate is used to control the temperature of the reactor. Ziegler-Natta catalyst is fed continuously into the reactor and the products are withdrawn at a constant bed height.

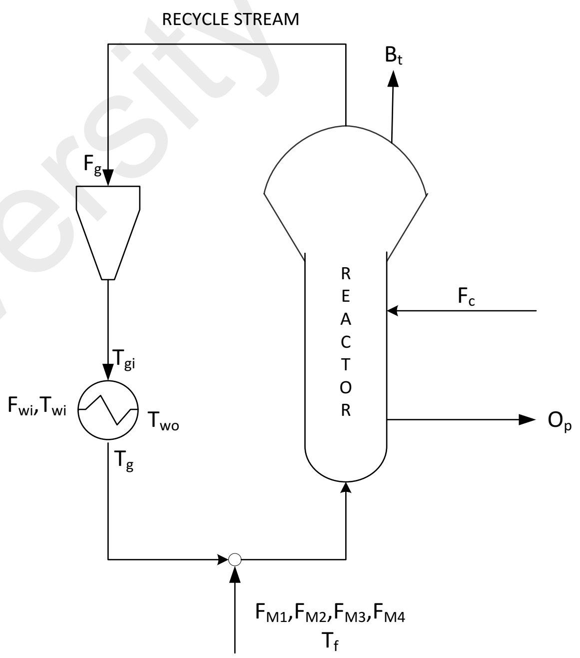


Figure 3.2: Ethylene polymerization reactor

By using M_1 as ethylene, M_2 as butene, M_3 as hydrogen and M_4 as nitrogen, the mole balances are given by (Ali & Ali, 2010):

$$V_g \frac{dC_{M_1}}{dt} = F_{M_1} - x_{M_1} B_t - R_{M_1} \tag{3.1}$$

$$V_g \frac{dC_{M_2}}{dt} = F_{M_2} - x_{M_2} B_t - R_{M_2} \tag{3.2}$$

$$V_g \frac{dC_{M_3}}{dt} = F_{M_3} - x_{M_3} B_t - R \tag{3.3}$$

$$V_g \frac{dC_{M_4}}{dt} = F_{M_4} - x_{M_4} B_t \tag{3.4}$$

With $$R_{M_1} = C_{M_1} Y_c k_{p1} e^{\frac{E}{R}(1/T_r - 1/T_{ref})} \tag{3.5}$$

$$R_{M_2} = C_{M_2} Y_c k_{p2} e^{\frac{E}{R}(1/T_r - 1/T_{ref})} \tag{3.6}$$

Where V_g is the reactor volume, $C_{M_1}, C_{M_2}, C_{M_3}, C_{M_4}$ are the concentration of ethylene, butene, hydrogen and nitrogen. $F_{M_1}, F_{M_2}, F_{M_3}, F_{M_4}$ are the molar flow rates of ethylene, butene, hydrogen and nitrogen. $x_{M_1}, x_{M_2}, x_{M_3}, x_{M_4}$ are the mole fraction of ethylene, butene, hydrogen and nitrogen. B_t is the bleed volumetric flow rate and R_{M_1}, R_{M_2}, R are the gases constant. R_{M_1} depends on the ethylene propagation rate constant (denoted by k_{p_1}), R_{M_2} depends on the butene propagation rate k_{p_2}) 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_r and T_{ref} are the bed/reactor and reference temperature, respectively.

The time variation of number of moles at the catalyst site is given by (Ali & Ali, 2010):

$$\frac{dY_c}{dt} = F_c a_c - k_d Y_c - O_p Y_c / B_w \tag{3.7}$$

With $$O_p = M_{w_1} R_{M_1} + M_{w_2} R_{M_2} \tag{3.8}$$

Here a_c is the active site concentration, F_c is the catalyst flow rate, O_p is the polymer outlet rate, B_w is the mass of polymer, k_d is the deactivation rate constant and M_{w_1}, M_{w_2} are the molecular weight of ethylene and butene respectively.

The equation related to the bed/reactor temperature is given as (Ali & Ali, 2010):

$$(M_r Cp_r + B_w Cp_p)\frac{dT_r}{dt} = HF + HG - HR - HT_r - HP \quad (3.9)$$

While the equation represents the recycle stream temperature is as follows:

$$M_g Cp_w \frac{dT_g}{dt} = F_g Cp_g(T_{gin} - T_g) + F_w Cp_w(T_{win} - T_{wout}) \quad (3.10)$$

Where $HF = F_{M_1}Cp_{M_1} + F_{M_2}Cp_{M_2} + F_{M_3}Cp_{M_3} + F_{M_4}Cp_{M_4}$ (3.11)

$$HG = F_g Cp_g(T_g - T_{ref}) \quad (3.12)$$

$$HT_r = (F_g + B_t)Cp_g(T_r - T_{ref}) \quad (3.13)$$

$$HP = O_p Cp_p(T_r - T_{ref}) \quad (3.14)$$

$$HR = M_{w_1} R_{M_1} \Delta H_r \quad (3.15)$$

The total pressure of the reactor is given by (Ali & Ali, 2010):

$$P_t = (C_{M_1} + C_{M_2} + C_{M_3} + C_{M_4})RT_r \quad (3.16)$$

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

$$F_w Cp_w(T_{win} - T_{wout}) = 0.5UA\left[(T_{wout} + T_{win}) - (T_{gin} + T_g)\right] \quad (3.17)$$

Where $M_r Cp_r$ is the vessel thermal capacitance, Cp_p is the heat capacity of polymer, HF, HG, HT_r, HP are the sensible heat of fresh feed, recycle gas, bed and product accordingly while HR is the enthalpy generated from the polymerization. M_g is water holdup in heat exchanger, whereas Cp_g and Cp_w are the heat capacity of recycle gas and water. Furthermore, F_w , F_g are the cooling water and recycle flow rate respectively, T_{win}, T_{wout} are the cooling water temperature (before and after cooling) while T_{gin}, T_g are the recycle temperatures (before and after cooling). Cp_{M_1},Cp_{M_2}, Cp_{M_3}, Cp_{M_4} are the heat capacity of ethylene, butene, hydrogen and nitrogen respectively. P_t is the total pressure, ΔH_r is the heat of reaction and UA is the overall heat transfer coefficient, (U) multiplied by the heat transfer area, (A).

The melt index equation is represented by Eq. (3.18) below (Ali, Betlem, Weickert, & Roffel, 2007):

$$\frac{dMI}{dt} = \left[r k \left(\frac{C_{M_3}}{C_{M_1}} \right) - MI \right] / 0.9 \tag{3.18}$$

Here, r is a tunable parameter with initial value of 0.88, k is a constant parameter which is 6818.3 and MI is the melt index (Ali et al., 2007).

All the equations are used for the modelling of the ethylene polymerization reactor to obtain the actual value and generate the state space equation for calculating the gain and formulating the equation of the observer.

3.4 Hybrid observer design

In this research, a hybrid observer called the fuzzy-sliding mode observer (fuzzy-SMO) is proposed. It is the combination of the sliding mode observer (SMO) and fuzzy logic for estimating the ethylene and butene concentrations as well as the melt flow index (MFI). SMO is chosen because it offers fast convergence and stable estimation without requiring accurate initial assumption by generating the sliding motion on the measured error and the output error (Spurgeon, 2008). On the other hand, fuzzy logic is an artificial intelligence element that able to simplify the design of the proposed hybrid observer but yet give high accuracy and fast convergence rate.

Fuzzy logic is selected because it is a simpler algorithm to implement when combined with SMO in the hybrid observer design formulation compared to other AI elements such as genetic algorithm (GA) and artificial neural network (ANN). Fuzzy logic consists of rules that are easy to be manipulated without changing the parameters in the fuzzy framework including the membership function and defuzzification types to obtain best results. However, if GA is coupled with the SMO, all the steps including the reproduction, crossover and mutation need to be redefined for obtaining the best generation (output) especially as it totally depends on the random number from the first generation created (Hussain & Ramachandran, 2003). Whereas, if ANN is applied, all the training steps have to be repeated to find the best output and the network may also require changes.

The process model discussed in the section 3.3 will be used as the case study to develop and observe the performances of the hybrid fuzzy-SMO. In general, the first step before designing the observer is to consider the detectability or observability condition of the system because observers have to be designed for a detectable or observable system (Mohd Ali, Hoang, Hussain, & Dochain, 2015). Observability is defined as the condition where all the initial states are visible. For a system to be observable if, for any initial state vectors, its internal states must be inferred by its external states or outputs' knowledge (Evangelisti, 2011; Moreno & Dochain, 2008; Soroush, 1997). On the other hand, detectability is a weaker condition than observability, where the non-observable states may asymptotically decay to zero (Evangelisti, 2011; Moreno & Dochain, 2008). Both concepts will influence the feasibility conditions of the observers (Hoang, Couenne, Le Gorrec, Chen, & Ydstie, 2012; Mohd Ali, Hoang, Hussain, & Dochain, 2015; Moreno & Dochain, 2008).

Two types of observability conditions typically applied for observer designs are the observability matrix and the observability Gramian (Mohd Ali, Hoang, Hussain, & Dochain, 2015). The observability matrix appears with the alteration of the state space models such as conversion to canonical forms, while the observability Gramian arises when considering the operator properties including system reduction and optimal linear quadratic regulators (Curtain & Zwart, 1995; Singh and Hahn, 2005). Both the observability matrix and the observability Gramian provide sufficient conditions for the observability of a system (Mohd Ali, Hoang, Hussain, & Dochain, 2015). The observability matrix however, is related to the differential properties, while the observability Gramian is based on the integral conditions (Tsakalis, 2013). Furthermore, the type of observability used to detect the observable condition will depend on the formulation of the systems (Mohd Ali, Hoang, Hussain, & Dochain, 2015). In this work, we have applied the observability matrix in finding the observable of the system, thus observability Gramian is not discussed in details.

3.4.1 Observability Matrix

The main interest of the observability of a dynamic system is that it allows a priori to come up with an observer which rebuilds the system states with certain rate of convergence (Mohd Ali, Hoang, Hussain, & Dochain, 2015).

Consider a discrete-time system in the form of steady state:

$$x(k+1) = A_d x(k) \tag{3.19}$$

With output measurement given by:

$$y(k) = C_d x(k) \tag{3.20}$$

If $x(0)$ is known then the state variables at every instant of the discrete-time system can also be determined. This is proven for $k = 0,1, \dots, n-1$ as follows based on the substitution of k value into Eq. (3.19) and (3.20).

At $k = 0$:

$$x(1) = A_d x(0) \tag{3.21}$$

$$y(0) = C_d x(0) \tag{3.22}$$

At $k = 1$:

$$x(2) = A_d x(1) \tag{3.23}$$

$$y(1) = C_d x(1) \tag{3.24}$$

Substituting Eq. (3.21) into Eq. (3.22):

$$y(1) = C_d x(1) = C_d A_d x(0) \tag{3.25}$$

At $k = 2$:

$$x(3) = A_d x(2) \tag{3.26}$$

$$y(2) = C_d x(2) \tag{3.27}$$

Substituting Eq. (3.21) and (3.23) into Eq. (3.27):

$$y(2) = C_d x(2) = C_d A_d^2 x(0) \tag{3.28}$$

As a summary, from $k = 0$ until $n - 1$, assuming the n-dimensional vector $x(0)$ has n unknown components, thus give:

$$y(0) = C_d x(0)$$

$$y(1) = C_d x(1) = C_d A_d x(0)$$

$$y(2) = C_d x(2) = C_d A_d^2 x(0)$$

$$\vdots$$

$$y(n-1) = C_d x(n-1) = C_d A_d^{n-1} x(0) \tag{3.29}$$

The matrix blocks C_d, $C_d A_d$, $C_d A_d^2$, ..., $C_d A_d^{n-1}$ each with dimension $p \times n$ will stack on top of each other with overall dimension of the matrix is $np \times n$.

$$\begin{bmatrix} y(0) \\ y(1) \\ y(2) \\ \vdots \\ y(n-1) \end{bmatrix}^{(np)\times 1} = \begin{bmatrix} C_d \\ C_d A_d \\ C_d A_d^2 \\ \vdots \\ C_d A_d^{n-1} \end{bmatrix}^{(np)\times n} \tag{3.30}$$

It will have unique solution provided the system matrix has rank n (order of the system).

$$rank \begin{bmatrix} C_d \\ C_d A_d \\ C_d A_d^2 \\ \vdots \\ C_d A_d^{n-1} \end{bmatrix} = n \tag{3.31}$$

Therefore, the observability matrix, denoted by $\mathcal{O}$, must equal to rank n (i.e. rank $\mathcal{O} = n$) to determine the initial condition, $x(0)$.

$$\mathcal{O}(A_d, C_d) = \begin{bmatrix} C_d \\ C_d A_d \\ C_d A_d^2 \\ \vdots \\ C_d A_d^{n-1} \end{bmatrix}^{(np)\times n} \quad \text{has rank } n \tag{3.32}$$

Now consider the linear continuous-time system:

$$\dot{x}(t) = Ax(t) \tag{3.33}$$

With output measurement given by:

$$y(t) = Cx(t) \tag{3.34}$$

The knowledge of $x(t_0)$ is sufficient to determine $x(t)$ at any time instant. At $t = t_0$:

$$\dot{x}(t_0) = Ax(t_0) \tag{3.35}$$

$$y(t_0) = Cx(t_0) \tag{3.36}$$

By taking the derivative in the continuous-time measurements, for first derivative:

$$\dot{y}(t_0) = C\dot{x}(t_0) \tag{3.37}$$

Substituting Eq. (3.35) into Eq. (3.37):

$$\dot{y}(t_0) = C\dot{x}(t_0) = CAx(t_0) \tag{3.38}$$

For second derivative:

$$\ddot{y}(t_0) = C\ddot{x}(t_0) = CA^2x(t_0) \tag{3.39}$$

For $(n-1)$th derivative:

$$y^{n-1}(t_0) = Cx^{n-1}(t_0) = CA^{n-1}x(t_0) \tag{3.40}$$

As a summary, the following equation is obtained:

$$\begin{gathered} y(t_0) = Cx(t_0) \\ \dot{y}(t_0) = C\dot{x}(t_0) = CAx(t_0) \\ \ddot{y}(t_0) = C\ddot{x}(t_0) = CA^2x(t_0) \\ \vdots \\ y^{n-1}(t_0) = Cx^{n-1}(t_0) = CA^{n-1}x(t_0) \end{gathered} \tag{3.41}$$

Thus $$\begin{bmatrix} y(t_0) \\ \dot{y}(t_0) \\ \ddot{y}(t_0) \\ \vdots \\ y^{n-1}(t_0) \end{bmatrix}^{(np)\times 1} = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{n-1} \end{bmatrix}^{(np)\times n} \times x(t_0) \tag{3.42}$$

It will have unique solution provided the system matrix has rank n (order of the system).

$$rank\begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{n-1} \end{bmatrix} = n \tag{3.43}$$

Therefore, the observability matrix, denoted by $\mathcal{O}$, must equal to rank n (i.e. rank $\mathcal{O} = n$) to determine the initial condition, $x(t_0)$.

$$\mathcal{O}(A, C) = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{n-1} \end{bmatrix}^{(np)\times n} \qquad \text{has rank } n \qquad (3.44)$$

Once the system dynamics have fulfilled the observability or detectability conditions, observers can be designed to estimate the state variables. In this respect, the choice of a suitable observer according to the six classes emphasized in Section 2.2 of Chapter 2 is therefore of great importance (Mohd Ali, Hoang, Hussain, & Dochain, 2015). The flowchart of designing an observer according to those classes is depicted in Figure 3.3. The second step is to define the estimated variables. They are variables which are difficult to be measured and intend to be estimated using the observers.

These variables are also system-dependent and not specific to one parameter for a particular process unit (Liu, 1999) such as solid mass fraction and production rate in a polymerization reactor (Lopez & Alvarez, 2004), the specific growth rate in a bioreactor (Battista et al., 2011) or the reactor concentration in a CSTR (Salehi & Shahrokhi, 2008). Furthermore, the estimated variables decided are usually the crucial or critical parameters that can affect the product quality and potentially lead to uncertainty in the process (Alanis et al., 2010; Fan & Alpay, 2004; Mesbah et al., 2011; Olivier et al., 2012). The parameters should also be updatable for online implementation and able to eliminate bias between the simulation and the on-line estimation (Sandink et al., 2001).

After that, the kinetics information will be identified. Kinetics information will determine the nonlinearity of the system based on its mathematical model (Biagiola & Figueroa, 2004b). This information will aid in selecting the appropriate observers. The

Luenberger-based observer is appropriate for a system where the information is complete and system parameters are known while the Bayesian estimator is suitable for systems where only certain parameters are accessible (Dochain, 2000; Dochain, 2003). Furthermore, for less kinetic information availability, exponential or asymptotic observers may be applied (Dochain, 2000; Assoudi et al., 2002; Sadok & Gouze, 2001; Hoang et al., 2013; Hulhoven et al., 2008) while for systems with incomplete model information, AI-based observers are more appropriate.

Next step is to design the observer equation and compute the gain. The equation is developed to determine the observer structure for the system based on its dynamic knowledge and incorporated with the gain and the error dynamic equation (Bitzer & Zeitz, 2002; Cacace et al., 2010). For a model-based observer, the state space representation is preferably used to represent the formulation of the observer, which also involves the measurement equation (Fuhrmann, 2008; Patwardhan et al., 2006; Patwardhan & Shah, 2005; Senthil et al., 2006). The number of measured variables will also affect the sensitivity of the estimation (Venkateswarlu & Avantika, 2001). Furthermore, the design of the observer structure will require an appropriate gain (Dochain, 2003), and it is usually chosen based on the stability of the error dynamics of the system (Busawon & Kabore, 2001) (Yang et al., 2012). The observer gain can be solved using the Butterworth polynomial or the Ackermann formula (Ruscio, 2009). Additionally, the Riccati equation may also be applied to determine the gain value by considering the error dynamic output (Farza et al., 2011).

The design of the observer is now complete and the performance testing will be carried out to observe the effectiveness of the observer. During the test run, the estimated values are compared to the actual values to determine the performance of the proposed observer (Aamo et al., 2005; Battista et al., 2011; Hajatipour & Farrokhi, 2010; Jana et al., 2006;

Kiss et al., 2011; Salehi & Shahrokhi, 2008). The test is not only important for the design of the single-based observer but also determines whether a hybrid observer is further needed to be developed and implemented (Goffaux et al., 2009; Hulhoven et al., 2006; Othman et al., 2008). If there are huge discrepancies between the actual and estimated values, a hybrid observer may be designed to improve the performances. Furthermore, if the systems are complex and the models are difficult to obtain from the first principles, a hybrid AI-based observer may be a suitable choice (Chairez et al., 2007; Porru et al., 2000; Prakash & Senthil, 2008). Once those design and performance testing have been completed and analyzed in the simulation environment using MATLAB software, the credibility of the observer will be then validated using the experimental data from the real polymerization pilot plant.

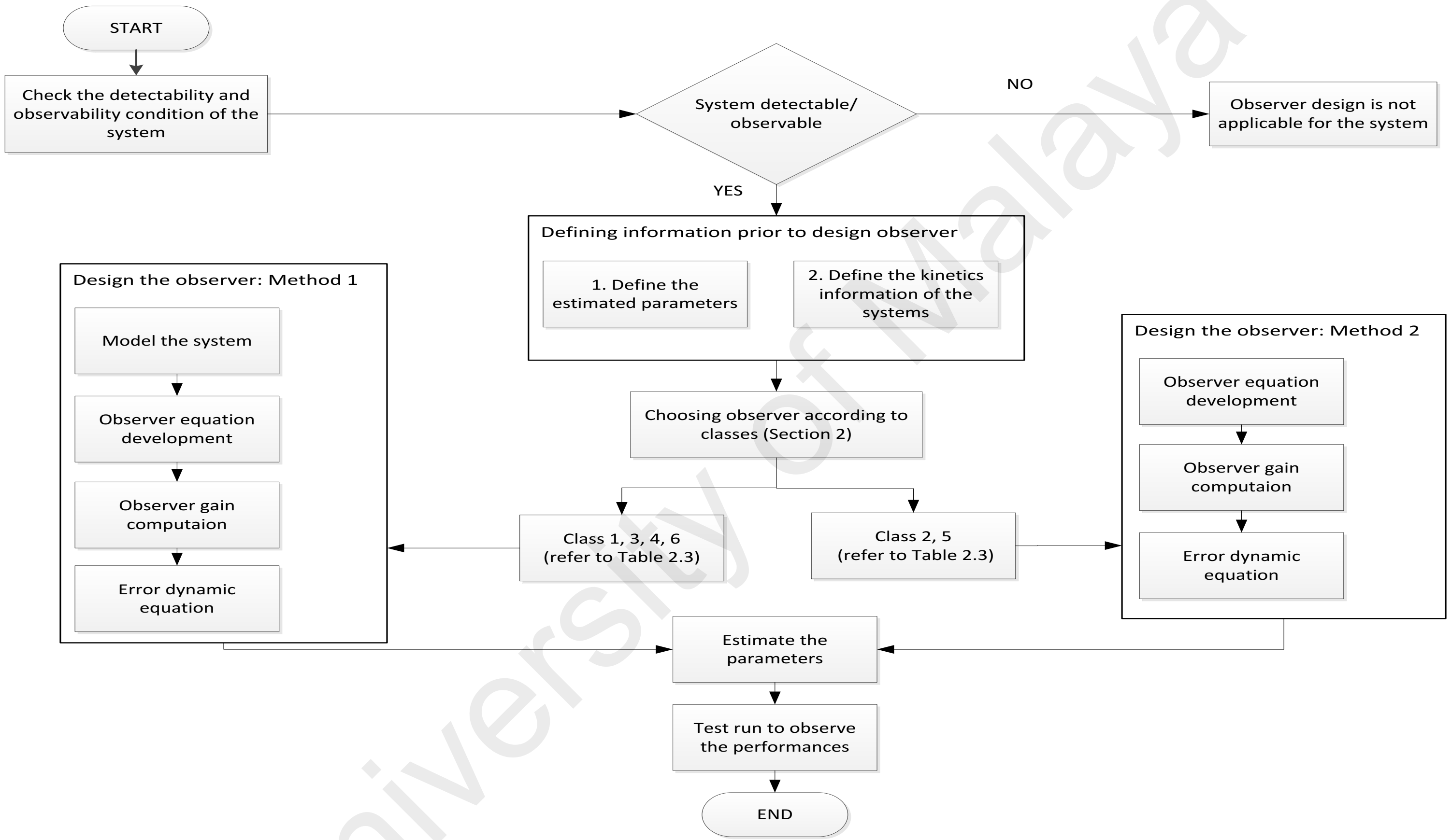


Figure 3.3: The general methodology of observer design according to classes (Mohd Ali, Hussain et al., 2015)

3.5 Model predictive control design

The MPC applied in this research is designed using the state space model as the prediction model. It is modified in such a way as to include an integrator, which is another alternative to guarantee offset-free control results from the controller. The design also considers the measured state estimated from the hybrid fuzzy-SMO as an additional approach to reduce parametric error within the controlled process (Ahn et al., 1999; Hedengren et al., 2007; Mohd Ali, Hoang, Hussain, & Dochain, 2015; Mohd Ali, Hoang, Hussain, & Dochain, 2016; Ramlal et al., 2007).

The observer will aid in improving the implementation of the MPC since it will first estimate the unknown states and deliver the information prior to applying the controller. The proposed MPC is used to control the reactor temperature to maintain the quality of the product. The results also compare the conditions with and without the observer to show the effectiveness of this estimation technique in increasing the performance of the controller, and therefore, of the overall system. The procedure of developing the embedded integrator MPC is illustrated in Figure 3.4.

Similar state space equation from the observer design formulation will be applied in the MPC design since the same process has been considered as the case study. The embedded integrator MPC is developed using the state space as the prediction model and is utilized to control the temperature. It will also be compared to the conventional proportional-integral-derivative (PID) controller and MPC without integrator to highlight its effectiveness that able to outstand the other controllers. The results are then compiled and analyzed.

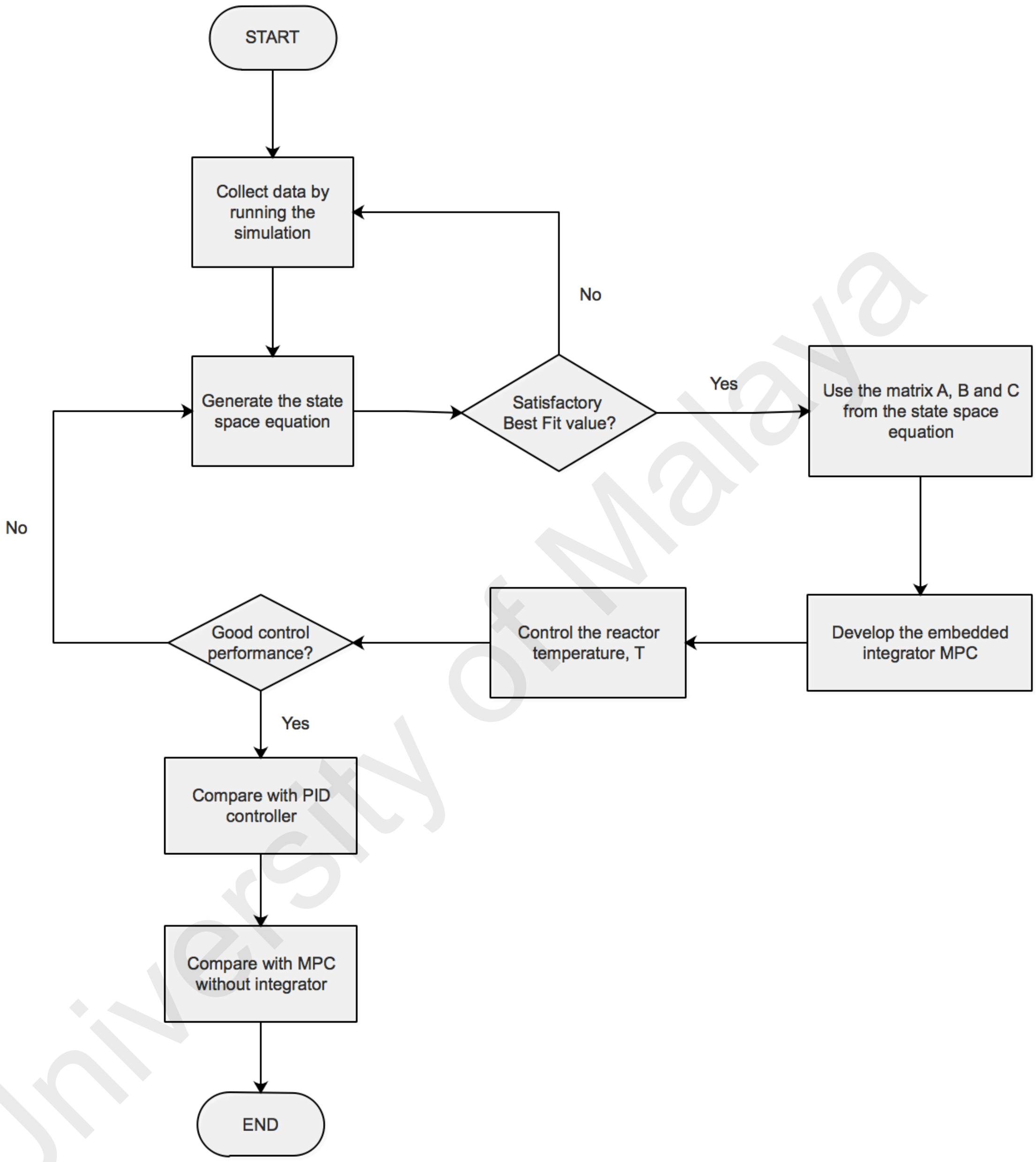


Figure 3.4: Methodology of the MPC design

CHAPTER 4: HYBRID FUZZY-SLIDING MODE OBSERVER

4.1 Chapter overview

The hybrid fuzzy-sliding mode observer design is emphasized in this fourth chapter of the thesis. The formulation is shown step by step accompanied by the necessary explanation. The hybrid observer is used to estimate the ethylene concentration, butene concentration and the melt flow index (MFI) in the ethylene polymerization reactor. Furthermore, the hybrid observer has been compared with the single sliding mode observer, single extended Luenberger observer (ELO), fuzzy logic and hybrid proportional-sliding mode observer (SMO-proportional).

4.2 Design of hybrid fuzzy- sliding mode observer (fuzzy-SMO)

The observer design will begin by identifying the observability conditions of the systems as explained earlier in Section 3.4 of Chapter 3 followed by defining the state (x), input (u) and measured variables (y). After that, the gain of the observer is computed together with the development of the observer's equation ((Mohd Ali, Hoang, Hussain, & Dochain, 2015). In this work, a single sliding mode observer (SMO) is first developed and the performances are evaluated based on the estimation of the parameters namely the ethylene concentration, butene concentration and melt flow index (MFI) in the ethylene polymerization process.

However, due to the unsatisfactory preliminary results obtained, especially in handling noisy conditions, the SMO has been combined with fuzzy logic. The proposed hybrid fuzzy-sliding mode observer (fuzzy-SMO) has been able to improve the estimation for both with and without noise conditions. The methodology is depicted in Figure 4.1. Other observers including the single SMO, single extended Luenberger observer (ELO), fuzzy logic and hybrid proportional-sliding mode observer (SMO-proportional) have been compared with the proposed fuzzy-SMO.

For the formulation development, first considers a general system (Drakunov & Utkin, 1995; Floquet, Edwards, & Spurgeon, 2007):

$$x = Ax + Bu \tag{4.1}$$

$$y = Cx \tag{4.2}$$

Then, define the state variables that need to be estimated, which are the ethylene concentration, C_{M_1}, butene concentration, C_{M_2} and melt flow index, MI for this case. After that, identify the input and measured variables. The process inputs are the input variables, which are the F_{M_1}(molar flow rates of ethylene), F_{M_2} (molar flow rates of butene), molar F_{M_3} (molar flow rates of hydrogen), F_{M_4} (molar flow rates of nitrogen), F_w (cooling water flow rate), F_g (recycle flow rate), F_c (catalyst flow rate) and T_f (feed temperature) while the measured variable is the reactor temperature, T_r . Once those variables have been identified, the observer is formulated by using the state space equation prior to obtain the model (Mäder, 2010) in the form of matrix A, B and C to be applied in Eq. (4.1) and (4.2).

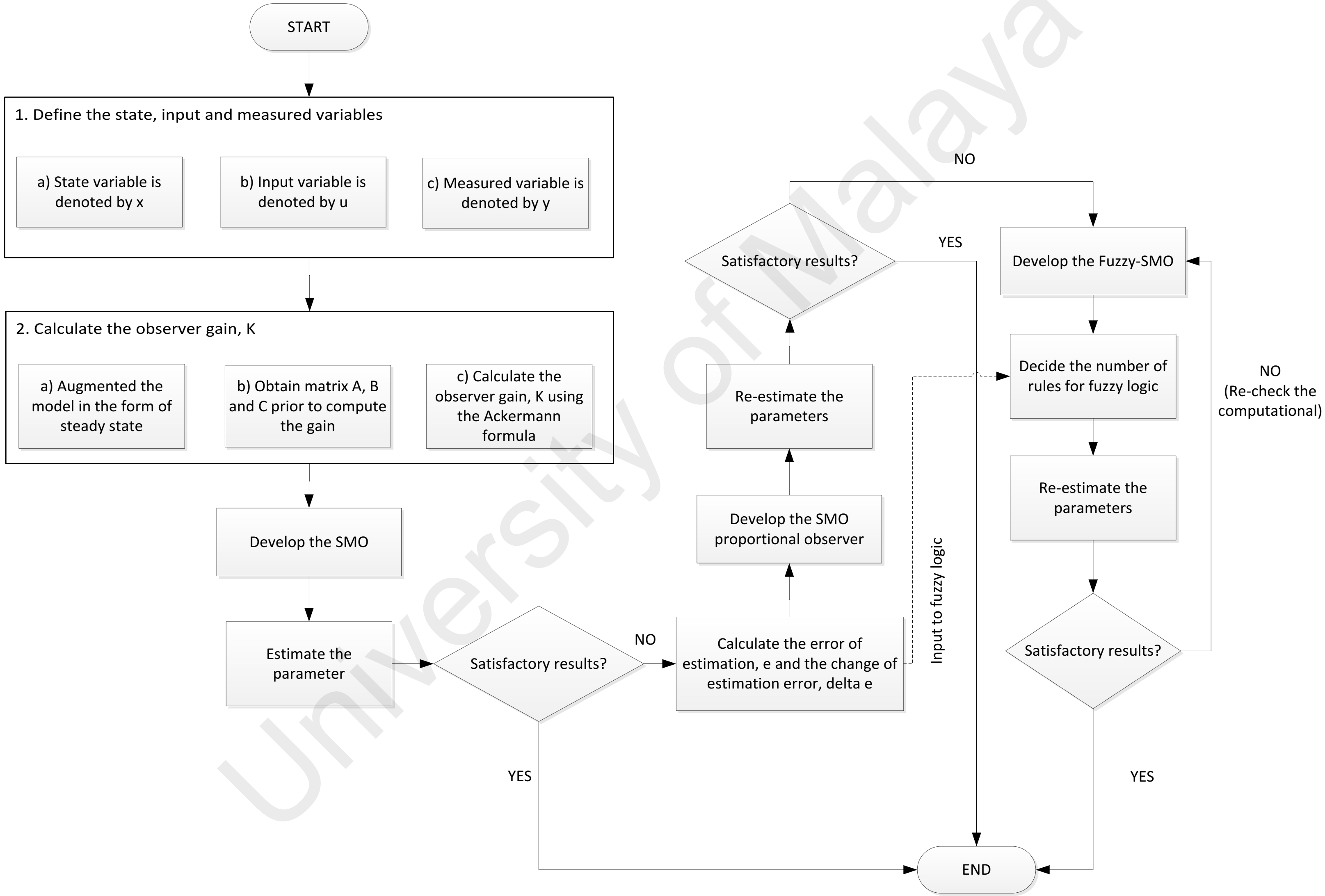


Figure 4.1: The procedure of designing the hybrid fuzzy-SMO

System identification is used for finding the state space model before the observer is developed. The state space model is estimated using the linear parametric model's option by first dividing the input signal data into two parts for estimation and validation. The accurate model can be achieved if both data are matched. For generating the state space model, the subspace N4SID from the MATLAB function is applied and the sampling interval is set as one all the time (Moscinski & Ogonowski, 1995). The highest percentage of the best-fitted value or the model output obtained will determine the final state space model that will be used. Best-fit values describe the balancing between robustness and accuracies. Thus, the fourth order is chosen as the order of the state space model since it provided 100% best-fit value compared to other orders that have been randomly tried as given in Figure 4.2. The parameters of this state space will represent the plant model and will be used in the design procedure (Mohd Ali, Hoang, Hussain, & Dochain, 2016).

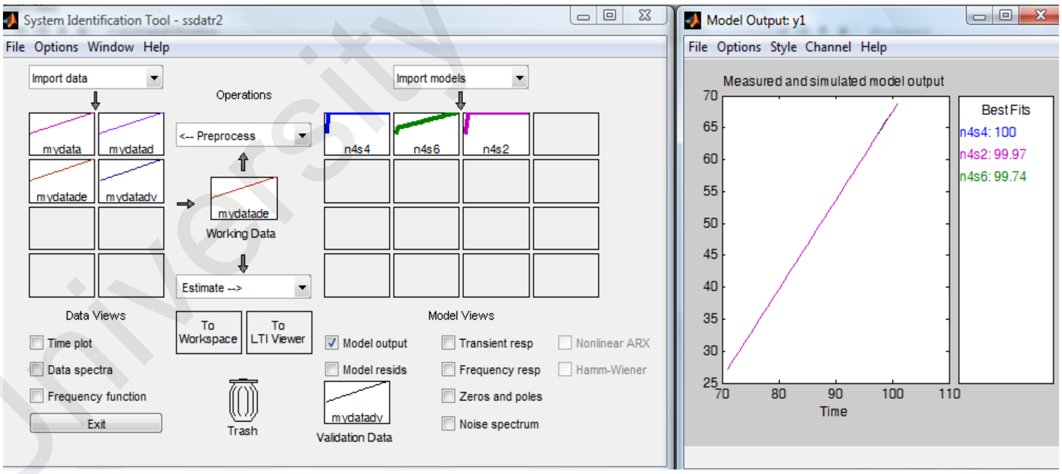


Figure 4.2: The best-fit percentage of state space model

The observability condition must be determined prior to developing the observer to ensure the system is observable. It must have unique solution provided the system matrix has rank n (order of the system) and for this case:

$$rank \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \end{bmatrix} \text{ for } n = 4 \text{ according to the state space order number} \tag{4.3}$$

Therefore, the observability matrix, $\mathcal{O}$ must also has rank n (rank $\mathcal{O} = n$) for the system to be observable (Mohd Ali, Hoang, et al., 2015).

$$\mathcal{O}(A, C) = \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \end{bmatrix}^{(np)\times n} \qquad \text{has rank } n = 4 \tag{4.4}$$

Since both rank from Eq. (4.3) and Eq. (4.4) above is equal to 4, the system is said to be observable and applicable for designing the observer.

After that, the augmented state space model in the form of matrix A_m, B_m and C_m is defined. It is different from the original state space model matrix A, B and C above. The augmented model however, does not change the underlying algorithm conceptually and the properties of the original state space matrix A, B and C are retained. This augmented model will be used throughout the estimation process to add additional dynamics to the original model for increasing the state vector dimension. It is because most model-based estimation algorithms usually assumed that disturbances are noise with zero means, but it is not reliable for many practical applications. In addition, the augmented models can provide simpler method for adjusting the disturbance and noise that acted on the augmented states compared to the original model states (noise colouring). Besides that, augmented models are also able to be applied for online estimation of the system parameters (Mäder, 2010). Because of those advantages, the augmented model is applied for estimating the states.

Using SMO, the equation is defined as follows:

$$\hat{x}_m = A_m x_m + B_m u + K_{ob} sign(y - C_m x_m) \tag{4.5}$$

Where K_{ob} is the observer gain and is calculated based on the pole location using the formula given in Eq. (4.6) and $sign$ is understood as the component wise for the vector argument $z = col(z_1, \dots, z_n)$ and $sign(z) = col(sign(z_1), \dots, sign(z_n))$(Drakunov & Utkin, 1995)

$$K_{ob} = place\ (A_m, C_m, \mathcal{M}) \tag{4.6}$$

From Eq. (4.6), $\mathcal{M}$ is the characteristics equation for the closed loop poles of the system that is the desired location for the error dynamics. On the other hand, the initial value, x_m is assumed with any value in the beginning since SMO can handle any wrong assumptions and help to recalculate them until the desired truth-values are achieved. Then the error of the SMO is defined as in Eq. (3.7), where $\hat{x}_m$ is the estimated value and x_p is the actual plant value. By obtaining the set of error (er) values, the set of change of error (Δer) values are also computed and used as the inputs for the fuzzy logic framework to develop the hybrid observer.

$$er(t) = x_p(t) - \hat{x}_m(t) \tag{4.7}$$

The fuzzy framework is designed using Mamdani inferences and two Gaussians membership functions for the input and a Triangular-shaped membership function for the output. It is a rule-based algorithm consisting of several linguistic variables, which are NV (Negative), ZV (Zero) and PV (Positive). Those variables are combined to form a set of rules with the format of IF (antecedent) and THEN (consequence) as given in in Table

4.1. Four rules have been tested before deciding the best rule to be applied in the fuzzy framework since the generation of the rules are based on trial and error. We named the four different rules as Rule 1, Rule 2, Rule 3 and Rule 4. Each rule consists of different antecedents and consequences.

Table 4.1: The IF and THEN rules for Fuzzy-SMO

	Δer		
er	NV	ZV	PV
NV	PV	ZV	NV
ZV	ZV	ZV	ZV
PV	NV	ZV	PV

The set of rules are given below with the output as the new error to be used in the proposed hybrid observer. As an example, when the error of the sliding mode observer shows a negative value (NV) and the change of error also show a negative value (NV), then the output will be a positive value (PV). This will be recognized by the fuzzy logic framework to generate the output.

$IF\ (er\ is\ NV)\ AND\ (\ \Delta er\ is\ NV)\ THEN\ (the\ output\ is\ PV)$

$IF\ \ (er\ is\ NV)\ AND\ (\ \Delta er\ is\ ZV)\ THEN\ (the\ output\ is\ ZV)$

$IF\ \ (er\ is\ NV)\ AND\ (\ \Delta er\ is\ PV)\ THEN\ (the\ output\ is\ NV)$

$IF\ \ (er\ is\ ZV)\ AND\ (\ \Delta er\ is\ NV)\ THEN\ (the\ output\ is\ ZV)$

$IF\ \ (er\ is\ ZV)\ AND\ (\ \Delta er\ is\ ZV)\ THEN\ (the\ output\ is\ ZV)$

$IF\ \ (er\ is\ ZV)\ AND\ (\ \Delta er\ is\ PV)\ THEN\ (the\ output\ is\ ZV)$

$$IF\ \ (er\ is\ PV)\ AND\ (\ \Delta er\ is\ NV)\ THEN\ (the\ output\ is\ NV)$$

$$IF\ (er\ is\ PV)\ AND\ (\ \Delta er\ is\ ZV)\ THEN\ (the\ output\ is\ ZV)$$

$$IF\ \ (er\ is\ PV)\ AND\ (\ \Delta er\ is\ PV)\ THEN\ (the\ output\ is\ PV) \tag{4.8}$$

Rule 1, which contains 9 antecedents and 9 consequences has been selected as the best rule based on the fastest response with closest to zero error as shown in Figure 4.3 (Castillo, Neyoy, Soria, Melin, & Valdez, 2015; Hušek & Cerman, 2013). Other rules that have been applied during the trial and error process to obtain the best set of rules are Rule 2 which consists of 4 antecedents and 4 consequences, Rule 3 with 25 antecedents and 25 consequences while Rule 4 with 49 antecedents and 49 consequences. The comparisons of the output according to all the rules are also given in the figure when implemented in the hybrid observer formulation. Rule 1 has provided the most accurate output as desired while the other three rules resulted in some errors.

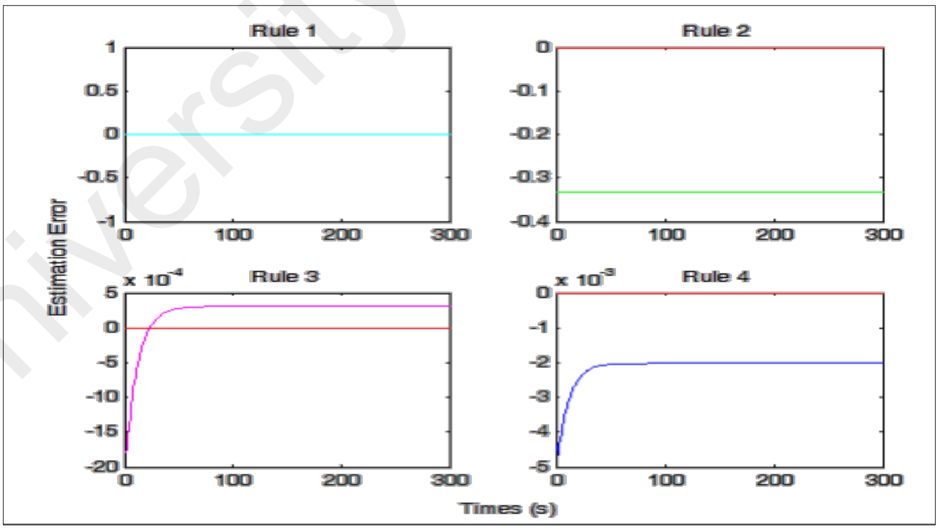


Figure 4.3: Comparisons of output for different fuzzy rules

Then the hybrid fuzzy-SMO for estimating the parameters is given in Eq. (4.9), where e_f is the output from the fuzzy logic based on the rules given in Table 4.1.

$$\hat{x}_{m_f} = A_m x_m + B_m u + K_{ob} sign(e_f) \tag{4.9}$$

where $\hat{x}_{m_f}$ is the notation for the states that are estimated using the hybrid fuzzy-SMO.

Since the polymerization process incorporates many unknown states or variables, the observer is also designed in such a way it can be applied to estimate several parameters without adjusting the whole observer's structure. Therefore, from Eq. (4.5) we formed Eq. (4.10) for the single SMO.

$$\begin{bmatrix} \hat{x}_{m_1} \\ \hat{x}_{m_2} \\ \hat{x}_{m_3} \end{bmatrix} = A_m \begin{bmatrix} x_{m_1} \\ x_{m_2} \\ x_{m_3} \end{bmatrix} + B_m \begin{bmatrix} u \\ u \\ u \end{bmatrix} + \begin{bmatrix} K_{ob_{11}} & K_{ob_{12}} & K_{ob_{13}} \\ K_{ob_{21}} & K_{ob_{22}} & K_{ob_{23}} \\ K_{ob_{31}} & K_{ob_{32}} & K_{ob_{33}} \end{bmatrix} sign\left(\begin{bmatrix} y \\ y \\ y \end{bmatrix} - C_m \begin{bmatrix} x_{m_1} \\ x_{m_2} \\ x_{m_3} \end{bmatrix} \right) \tag{4.10}$$

Here, subscript 1,2,3 represent ethylene, butene concentration and melt index respectively. Whereas for fuzzy-SMO, we define Eq. (4.11) from Eq. 4.9) as follows:

$$\begin{bmatrix} \hat{x}_{m_{f_1}} \\ \hat{x}_{m_{f_2}} \\ \hat{x}_{m_{f_3}} \end{bmatrix} = A_m \begin{bmatrix} x_{m_1} \\ x_{m_2} \\ x_{m_3} \end{bmatrix} + B_m \begin{bmatrix} u \\ u \\ u \end{bmatrix} + \begin{bmatrix} K_{ob_{11}} & K_{ob_{12}} & K_{ob_{13}} \\ K_{ob_{21}} & K_{ob_{22}} & K_{ob_{23}} \\ K_{ob_{31}} & K_{ob_{32}} & K_{ob_{33}} \end{bmatrix} sign\left(\begin{bmatrix} e_{f_1} \\ e_{f_2} \\ e_{f_3} \end{bmatrix} \right) \tag{4.11}$$

Besides that, to imitate a real situation, noise and disturbance are also added to the model. The noise incorporated is a 5% noise variation in the polymerization plant model to illustrate the effectiveness of the proposed approach.

4.3 Ethylene polymerization parameters estimation using fuzzy-SMO

Three parameters have been chosen in order to show the effectiveness of the hybrid observer. The parameters are the difficult-to-measure parameter (MFI) and less difficult-to-measure parameter (ethylene concentration) where the related process model is adapted to the observer's structure. It is difficult to measure the MFI when there are variations in the temperature. Therefore, it must be observed to obtain the accurate MFI values for maintaining the product quality. On the other hand, the ethylene concentration observation in the reactor is important as to determine the amount of the unreacted ethylene for finding accurate overall conversion.

Another parameter, which is butene concentration is estimated to show the uniqueness of the hybrid observer design that allows certain parameters estimation using the same observer structure. Butene concentration is also another favorable parameter to be observed in the polymerization process since it will affect the molecular weight distribution (MWD) of polymer produced. The lower the distribution of the concentration, the higher the MWD of the polymer. This hybrid observer, which allows extension and able to estimate many parameters without redesigning the whole structure is advantageous to be implemented in real plant due to the limitations of the sensors that focus only on estimating specific parameter and are unreliable to estimate unknowns that are due to disturbances and mismatches.

The process is first run in simulation using the initial condition as given in Table 4.2 (Ali & Ali, 2010) to obtain the actual value of the ethylene, butene concentrations and melt flow index for both with and without noise conditions. After that, the hybrid fuzzy-SMO observer is applied to estimate the parameters and compared with the actual value. The error and change of error are also computed to observe the discrepancies between both the actual and the estimated value. Besides that, the hybrid fuzzy-SMO was also compared with the estimation results obtained from the single SMO, fuzzy logic, extended Luenberger observer (ELO) and SMO-proportional observers to highlight the effectiveness of the proposed observer.

Table 4.2: Parameters and variables for the polymerization reactor

Parameter	Values	Parameter	Values
F_{M_1}	131.13 mole/s	F_{M_3}	2.52 mole/s
F_{M_2}	3.51 mole/s	F_{M_4}	1.6 mole/s
F_c	2 kg/h	C_{M_1}	297.06 mole/m^3
C_{M_3}	105.78 mole/m^3	C_{M_4}	166.23 mole/m^3
T_{ref}	360 K	C_{M_2}	116.17 mole/m^3
T_f	293 K	ΔP	3 atm

4.4 Estimation results and discussion

Ethylene concentration result is given in Figure 4.4. Based on the figure, good estimation performances were obtained when the hybrid fuzzy-SMO was applied. It reacted fast towards the actual value to provide accurate estimation in both with and without noise conditions for estimating the ethylene concentrations. In addition, there were no oscillations or offsets found during the estimation, thus giving a smooth and accurate estimation. Regarding the rate of convergence, however, we could not precisely define the exact convergence time since fuzzy logic has been developed based on the 'IF and THEN' rules where the 'IF and THEN' scenario will only take place after SMO has been implemented at certain time, which is a priori unpredictable.

On the other hand, SMO was also able to provide satisfactory estimation when noise is not present in the process. It managed to adjust the estimation value towards the actual value starting from 200 seconds onwards. However, this was not the case once noise has been added. It oscillated and was unable to estimate the ethylene concentration even after running the simulation for 1000 seconds. Similar conditions have been observed when fuzzy logic and SMO-proportional were used respectively. Fuzzy logic has been able to estimate the concentration when the noise was not included in the process, while oscillations are found during noisy conditions. As for SMO-proportional, the oscillations are very high and deviated far from the actual values. Furthermore, when ELO is applied, it was unable to estimate the ethylene concentration for both conditions. Oscillations are observed with high discrepancies found as compared to the actual values.

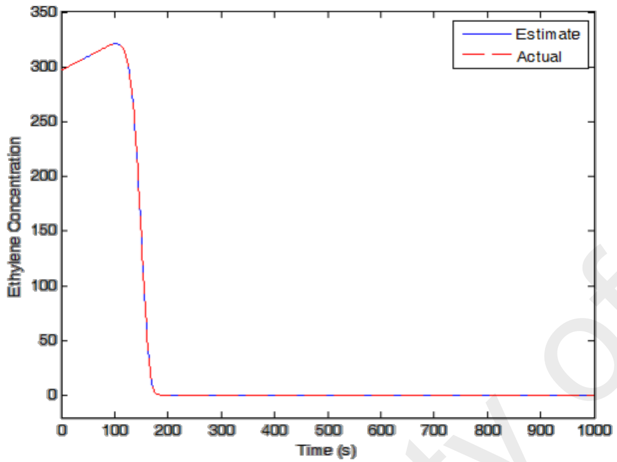
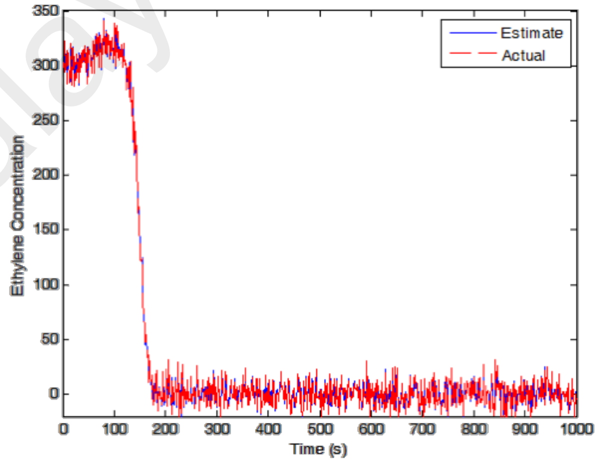
The results of butene concentration estimation are illustrated in Figure 4.5. The proposed hybrid fuzzy-SMO provides better estimation performances compared to other observers. Only fuzzy-SMO has been able to estimate the butene concentration in both with and without noise conditions. It has shown faster estimation and no discrepancies from the actual value were observed. Moreover, there were no oscillations and offsets found during the estimation.

For SMO and fuzzy logic, both were able to estimate the butene concentration when noise has not been included in the polymerization process. However, the estimated values tend to oscillate and deviate from the actual value once the noise was added. This proved that the single observer was unable to handle noise satisfactorily for the ethylene polymerization process. Furthermore, SMO-proportional and ELO were unable to estimate the butene concentration for both the conditions. SMO-proportional has been able to provide close estimation values with minor oscillation for the case without noise and high oscillations pattern are observed during noisy condition. Similarly, ELO has shown oscillations for both cases and was not able in estimating the butene concentration.

In estimating the melt flow index, fuzzy-SMO was again the best observer that was able to provide satisfactory estimation performances regardless of any condition in the ethylene polymerization process. The other observers, unfortunately, did not perform well and were unable to estimate the melt index. SMO, fuzzy logic and SMO-proportional have provided oscillation during the estimation with SMO-proportional showing the worst oscillation patterns. Besides that, offsets are observed when ELO was used as the observer. The results are given in Figure 4.6.

In general, for all the parameters estimated, the hybrid fuzzy-SMO has shown the best results especially in terms of noise handling. There were no discrepancies between the actual and the estimated values when the hybrid fuzzy-SMO had been applied to estimate the three critical parameters in the ethylene polymerization process. In addition, fast and accurate results have been observed during the estimation without any oscillation or offsets. Single SMO or fuzzy logic might be applied as the estimator to the system if noise were not available in the process. However, this is not applicable especially in the practical point of view where the real processes are incorporated with many sorts of disturbances and noise. Therefore, the proposed hybrid fuzzy-SMO is the best approach to be implemented in the ethylene polymerization process specially to cater the noise effect in the process. Furthermore, it is capable to estimate several parameters without significant adjustment in the structure of the observer.

In conclusion, the proposed hybrid fuzzy-SMO has provided accurate, fast and stable estimation despite noisy conditions compared to the single SMO, fuzzy logic, ELO and SMO-proportional observers in predicting three parameters namely ethylene, butene concentrations and melt flow index in an ethylene polymerization process. It is also unique since it can be adjusted to estimate several parameters by only adding the related process model without redesigning the structure of the whole observer. The hybrid fuzzy-SMO is also easy to compute by manipulating the estimation error and the change of error in the fuzzy IF-THEN rules.

<table>
<tr><th>Type of observer</th><th>Condition without noise</th><th>Condition with noise</th></tr>
<tr><td>a) Fuzzy-SMO</td><td>
</td><td>
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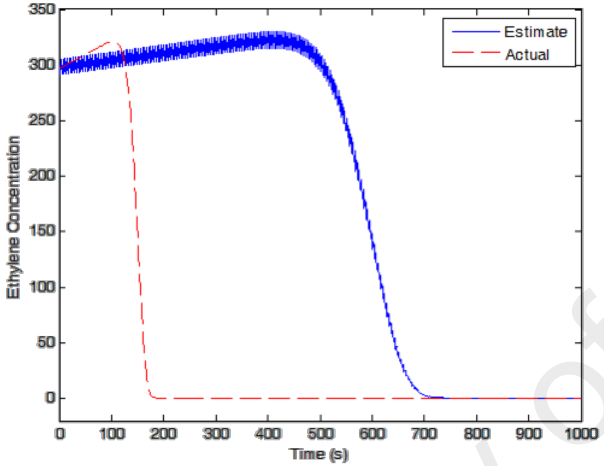
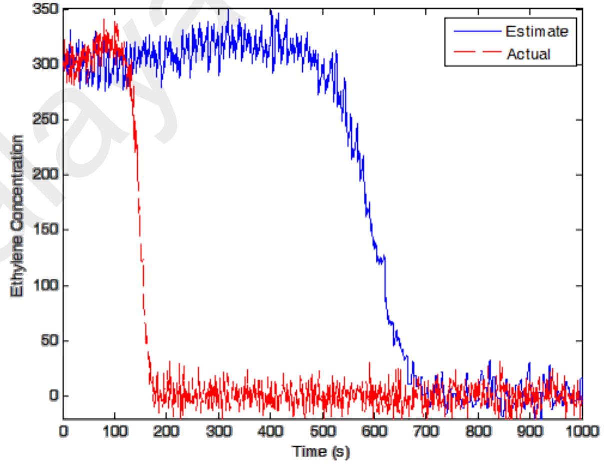
</table>

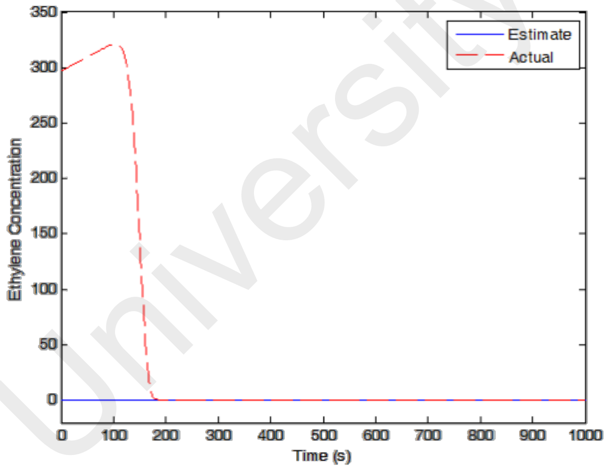
Figure 4.4: Ethylene concentration estimation using various observers namely a) Fuzzy-SMO, b) SMO, c) Fuzzy logic, d) SMO-proportional and e) ELO for both conditions with and without noise in the process

b) SMO





c) Fuzzy Logic



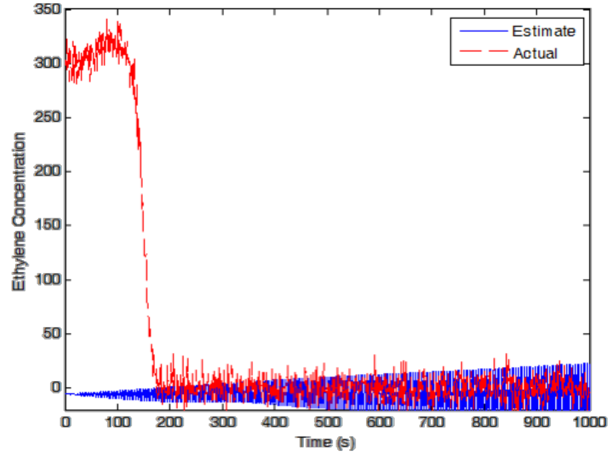


Figure 4.4 (continued)

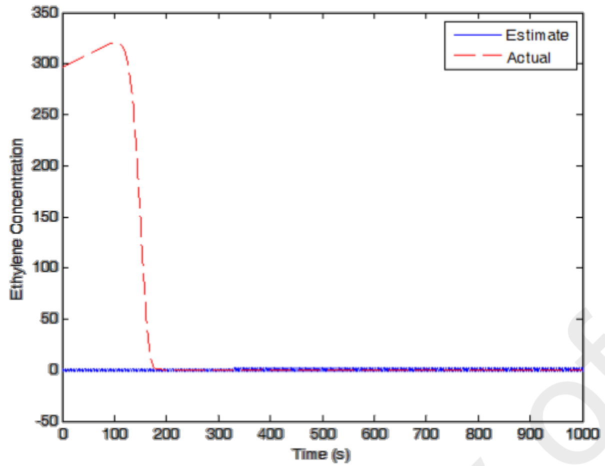
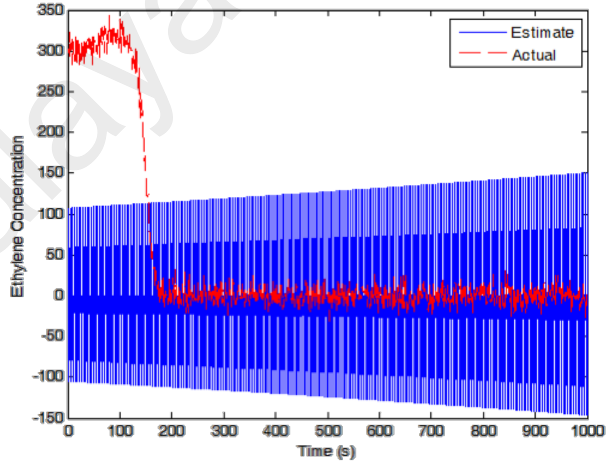
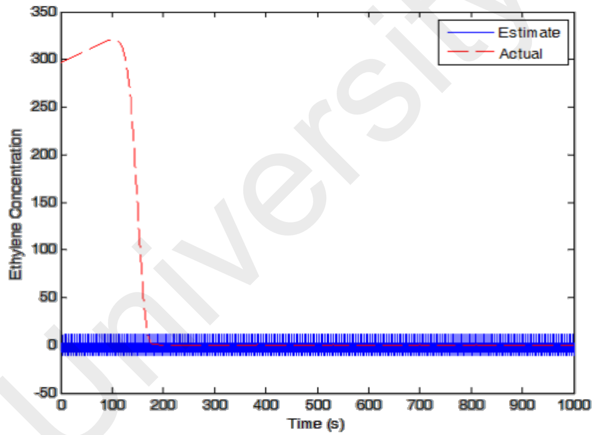
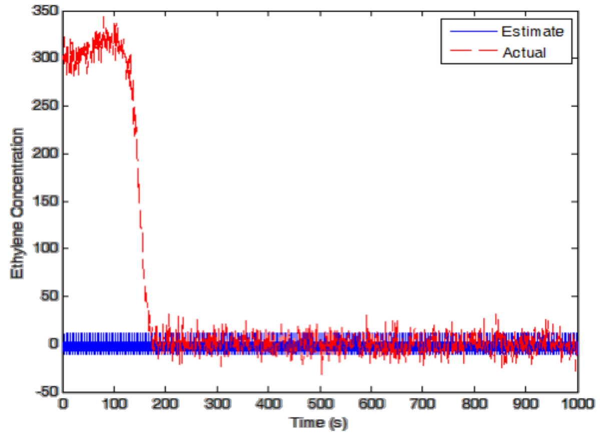
d) SMO-Proportional		
e) ELO		

Figure 4.4 (continued)

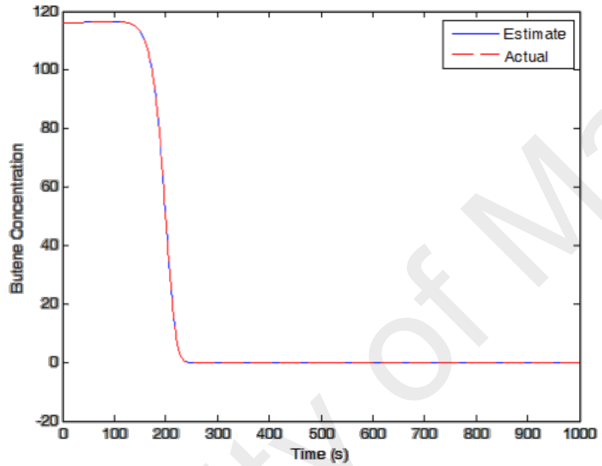
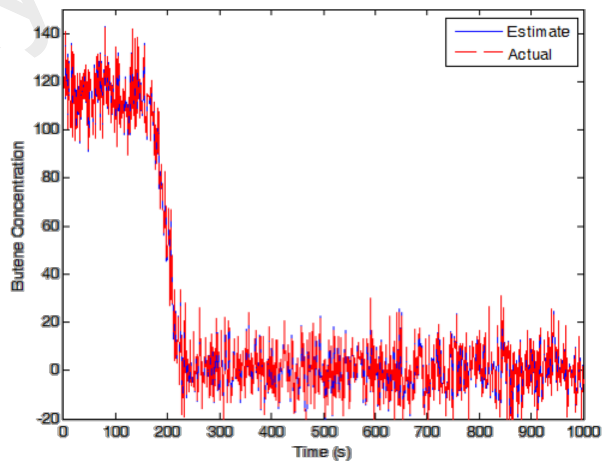
Type of observer	Condition without noise	Condition with noise
a) Fuzzy-SMO		

Figure 4.5: Butene concentration estimation using various observers namely a) Fuzzy-SMO, b) SMO, c) Fuzzy logic, d) SMO-proportional and e) ELO for both conditions with and without noise in the process

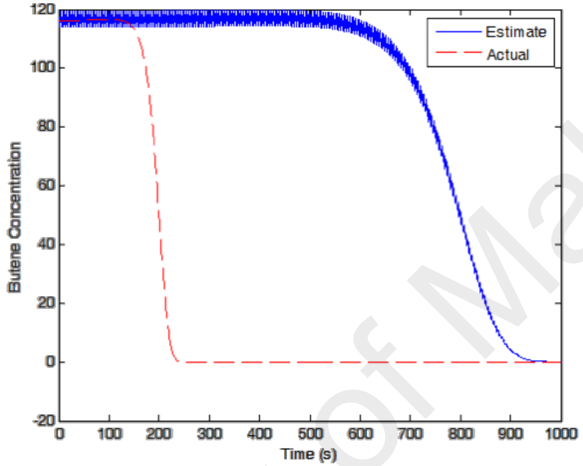
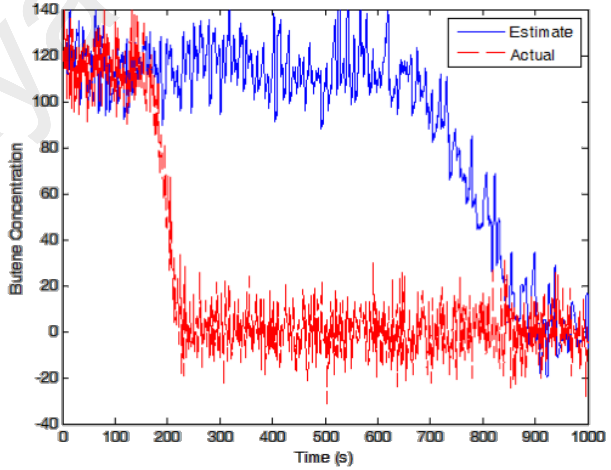
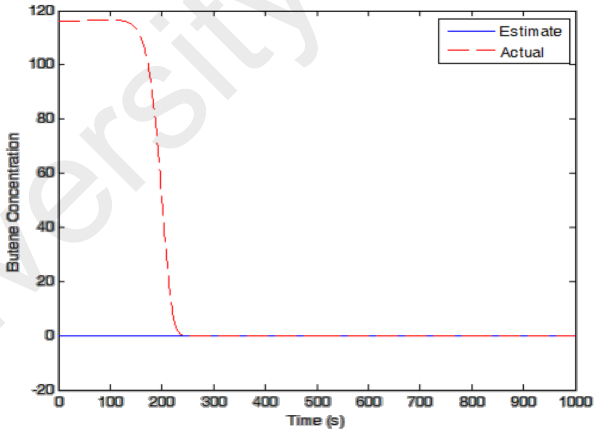
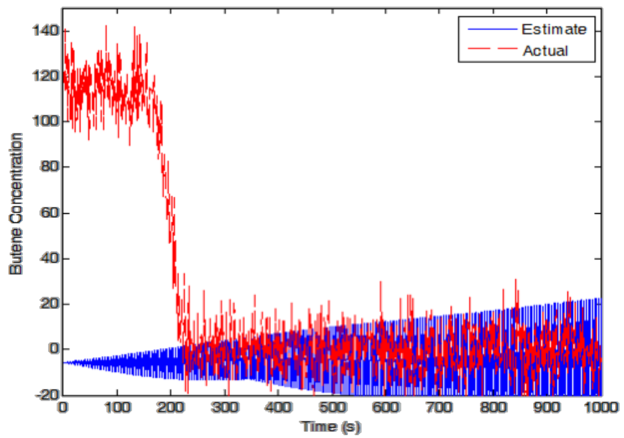
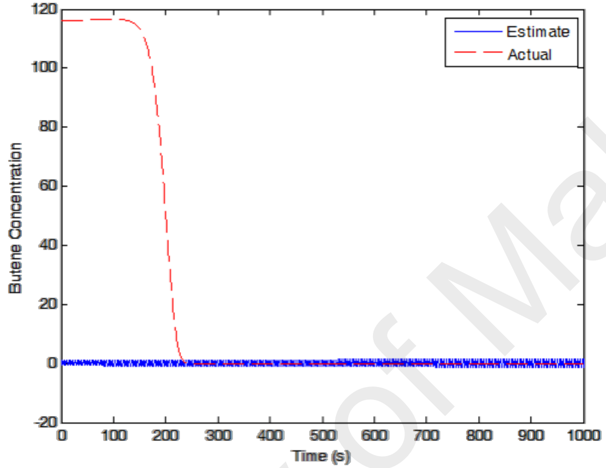
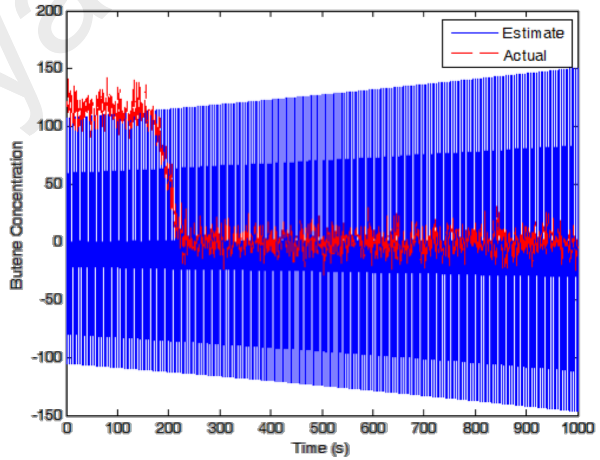
b) SMO	 
c) Fuzzy Logic	 

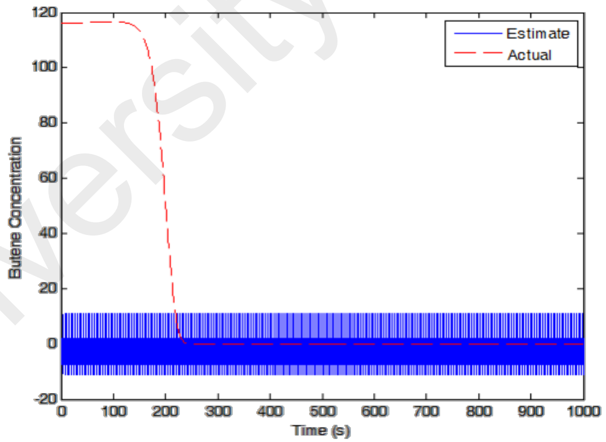
Figure 4.5 (continued)

d) SMO-Proportional





e) ELO



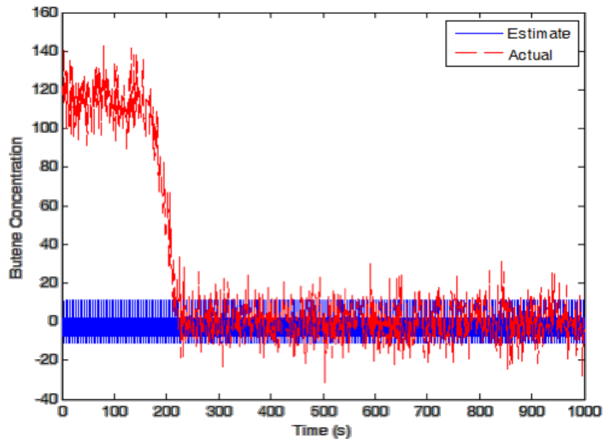


Figure 4.5 (continued)

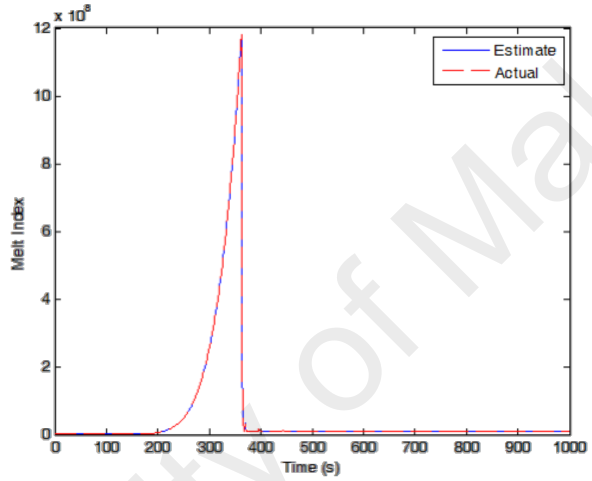
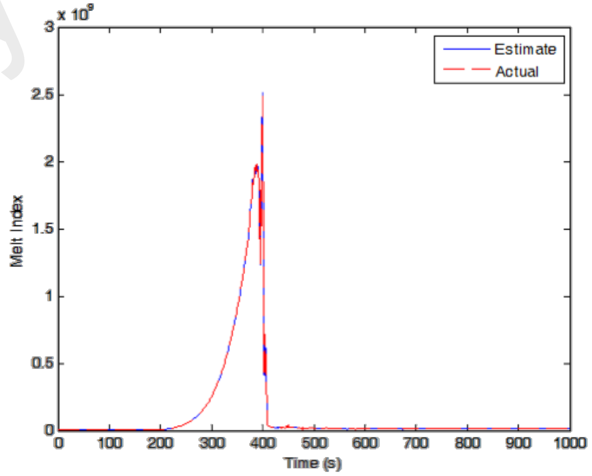
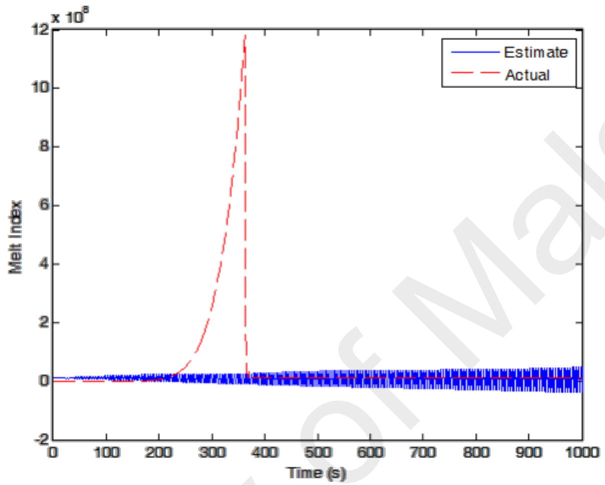
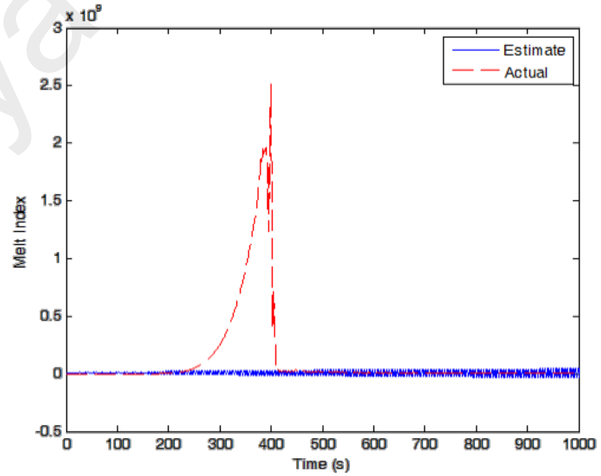
Type of observer	Condition without noise	Condition with noise
a) Fuzzy-SMO		

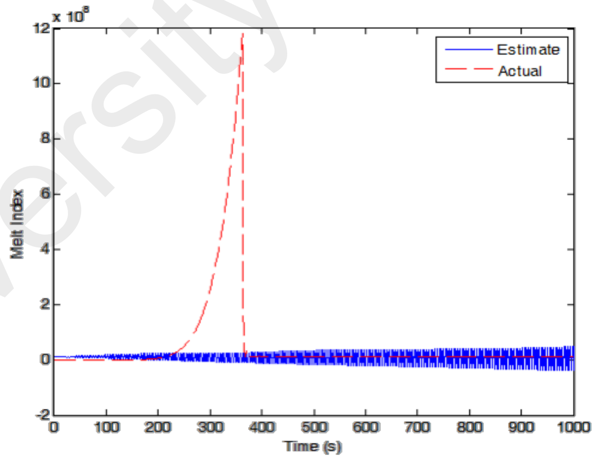
Figure 4.6: Melt index estimation using various observers namely a) Fuzzy-SMO, b) SMO, c) Fuzzy logic, d) SMO-proportional and e) ELO for both conditions with and without noise in the process

b) SMO





c) Fuzzy Logic



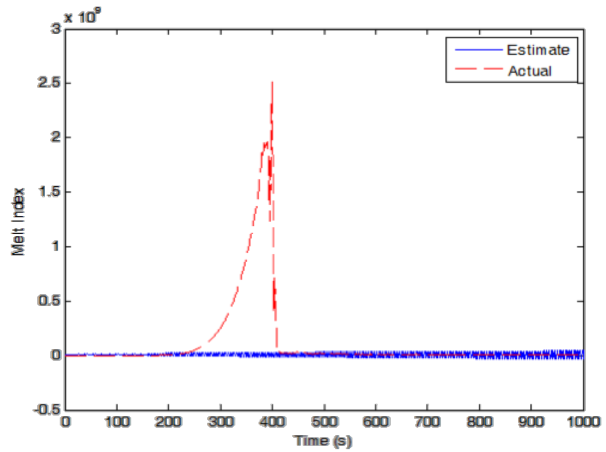


Figure 4.6 (continued)

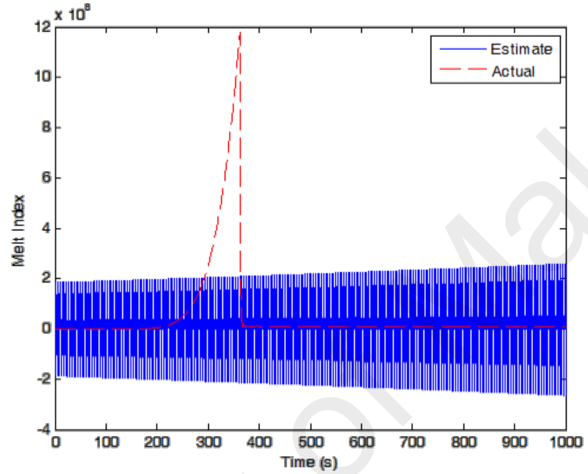
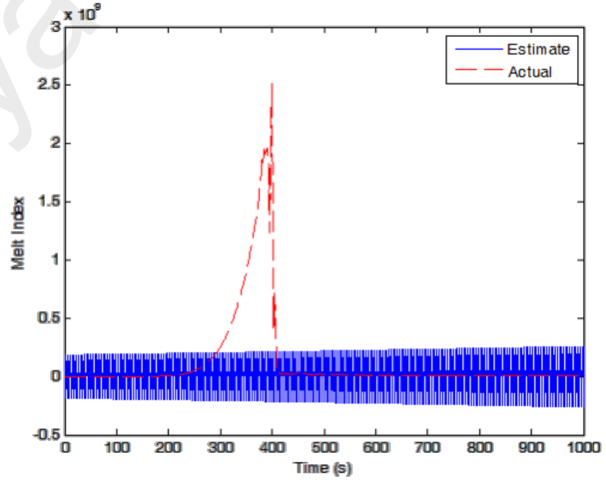
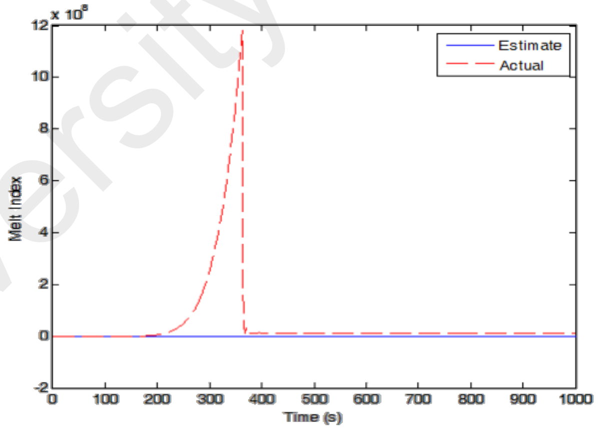
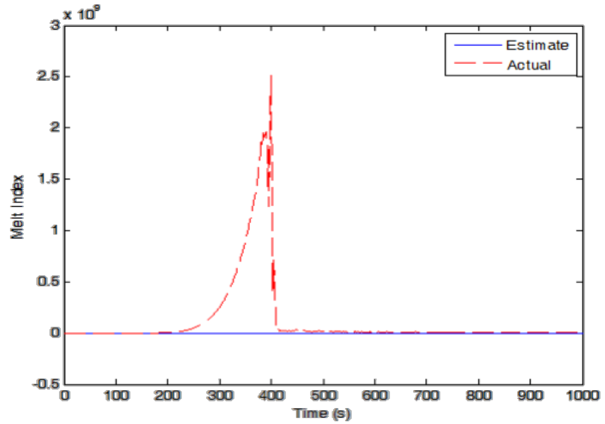
d) SMO-Proportional		
e) ELO		

Figure 4.6 (continued)

CHAPTER 5: EMBEDDED INTEGRATOR MODEL PREDICTIVE CONTROL

5.1 Chapter overview

The design of the embedded integrator model predictive control (MPC) is emphasized in this fifth chapter of the thesis. Three cases of the MPC design will be explained starting from the formulation until the performance testing. It has been coupled with the hybrid observer for enhancing overall control of the system and is compared with the proportional-integral-derivative (PID) controller, MPC without integrator and MPC without observer. All results are compiled and analyzed.

5.2 Design of embedded integrator model predictive control (MPC)

Model predictive control (MPC) in this research is designed in three cases specifically MPC with known initial state without constraints, MPC with unknown initial state without constraints and MPC with unknown initial state with constraints. The first case is an ideal case while the second and third cases are more practical. The difference between the second and third cases is that the second case is practical, but it is limited to the non- existence of constraints.

It is also incorporated with an integrator to ensure offset-free control especially for applying in the multiple-input multiple-output (MIMO) system. This is done by replacing u with Δu in the state space formulation as a new notation to represent the integral factor. Δu acts as the integral effects that enhances the MPC designed by helping in eliminating offsets (Wang, 2009). Therefore, the embedded integrator MPC is better than the ordinary MPC as it can reduce the steady state error, which can decrease the set points deviation closest possible to zero (Perry & Green, 2008).

Besides that, the design considered also the measured state estimated from the hybrid fuzzy-SMO emphasized in Chapter 4. This will help to improve the performance of the MPC since unknown states in the plant tend to disrupt the process and may result in unsatisfactory performances. Besides that, the reason for adding an observer is to directly measure the state variable and as a replacement to a sensor in a control system (Ogata, 1995). The embedded integrator MPC is applied to control the temperature in the ethylene polymerization reactor at its desired setpoint. The schematic design diagram is illustrated in Figure 5.1. The figure can be separated into three elements namely the ethylene polymerization process, the hybrid fuzzy-SMO and the MPC controller. There are many unknowns that can eventually arise from the disturbances and affected the parameters in the reactor thus the hybrid observer will be used to estimate the parameters and convey the information to the controller during the design. The controller, on the other hand, consists of the prediction model that has been modified to add the integral factor for offset-free guaranteed. It is applied to control the reactor temperature at the desired setpoint.

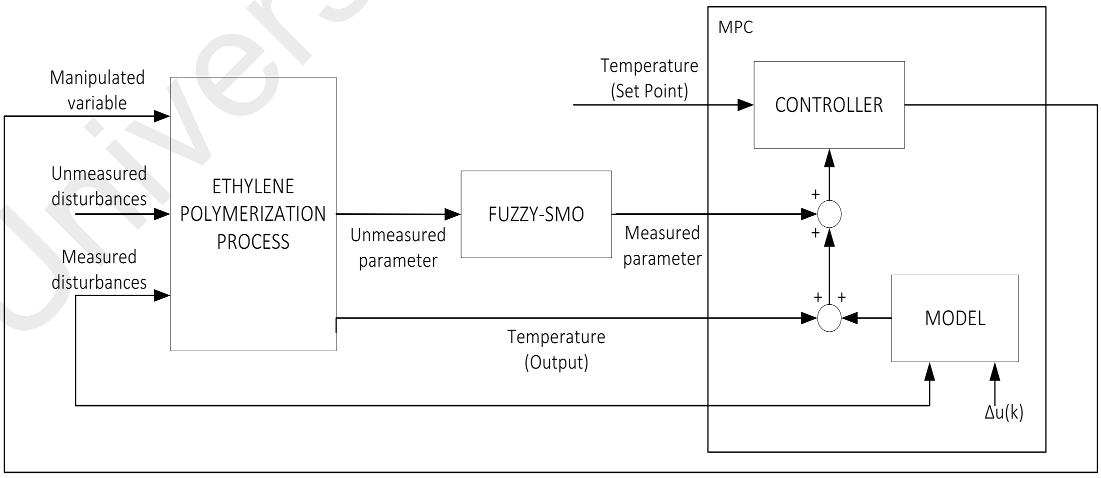


Figure 5.1: The schematic diagram of embedded integrator MPC design

5.2.1 Case 1: MPC with known initial state and without constraint

The MPC with known initial state is the ideal case and has been designed using the state space as the prediction model. This means that the state variable at the current time is always being used for future prediction (Camacho & Bordons, 2004). The state space model is determined using the system identification with details have been explained in section 4.2 of Chapter 4. The augmented state space model will also be used in this MPC, which is in the form of matrix A_m, B_m and C_m. The discrete model components are described in Eq. (5.1) and Eq. (5.2). Here, $u(k)$ is the manipulated or input variable, $y(k)$ is the process output and $x_m(k)$ is the state variable vector (Wang & Young, 2006).

$$x_m(k+1) = A_m x_m(k) + B_m u(k) \tag{5.1}$$

$$y(k) = C_m x_m(k) \tag{5.2}$$

The input $u(k)$ is assumed not to be affected to the output $y(k)$ at the same time based on receding horizon principle where current plant information is needed for the prediction and control. Taking difference equations on both sides of Eq. (5.1) gives Eq. (5.3).

$$x_m(k+1) - x_m(k) = A_m(x_m(k) - x_m(k-1) + B_m(u(k) - u(k-1)) \tag{5.3}$$

With the increment of x_m and $u(k)$, Eq. (5.4), Eq. (5.5) and Eq. (5.6) are achieved (Liuping Wang & Young, 2006).

$$\Delta x_m(k+1) = x_m(k+1) - x_m(k) \tag{5.4}$$

$$\Delta x_m(k) = x_m(k) - x_m(k-1) \tag{5.5}$$

$$\Delta u(k) = u(k) - u(k-1) \tag{5.6}$$

Merging both the Eq. (5.3) and Eq. (5.2), Eq. (5.7) is obtained which is the difference state space equation with integral factor, $\Delta u(k)$ as the input (Wang & Young, 2006).

$$\Delta x_m(k+1) = A_m \Delta x_m(k) - B_m \Delta u(k) \tag{5.7}$$

Then, $\Delta x_m(k)$ is connected to $y(k)$ and a new state variable vector is introduced as Eq. (5.8) and superscript T is a transpose matrix notation (Wang & Young, 2006).

$$x(k) = [\Delta x_m(k)^T \; y(k)]^{\,T} \tag{5.8}$$

Note that,

$$\begin{aligned} y(k+1) - y(k) &= C_m(x_m(k+1) - x_m(k)) \\ &= C_m \Delta x_m(k+1) \\ &= C_m A_m \Delta x_m(k) + C_m B_m \Delta u(k) \end{aligned} \tag{5.9}$$

Both Eq. (5.8) and Eq. (5.9) are combined to form Eq. (5.10) and Eq. (5.11) to be able to apply to MIMO system. $O_m = \overbrace{[0\;0\;...\;0]}^{n_1}$ and I is the identity matrix suited for the system.

$$\overbrace{\begin{bmatrix} \Delta x_m(k+1) \\ y(k+1) \end{bmatrix}}^{x(k+1)} = \overbrace{\begin{bmatrix} A_m & O_m^T \\ C_m A_m & I \end{bmatrix}}^{A_m} \overbrace{\begin{bmatrix} \Delta x_m(k) \\ y(k) \end{bmatrix}}^{x(k)} + \overbrace{\begin{bmatrix} B_m \\ C_m B_m \end{bmatrix}}^{B_m} \Delta u(k) \tag{5.10}$$

$$y(k) = \overbrace{[O_m \quad I]}^{C_m} \begin{bmatrix} \Delta x_m(k) \\ y(k) \end{bmatrix} \tag{5.11}$$

Once the formulation of the new augmented model has been completed, the predictive control system will be designed. It is to predict the output and compute the control signal. Optimization is one of the key factors that must be considered in the MPC design. The sampling instant is assumed to be k_i, where $k_i > 0$ and $x(k_i)$ is the state variable that is available throughout the measurement. The future control trajectory is given in Eq. (5.12) with control horizon, N_c that reflects the number of parameters for the trajectory (Wang & Young, 2006).

$$\Delta u(k_i), \Delta u(k_i + 1), \ldots., \Delta u(k_i + N_c - 1) \tag{5.12}$$

Future state variables are predicted according to number of N_p which is the prediction horizon as shown in Eq. (5.13). Here, $x(k_i + m|k_i)$ is the predicted state variable at $k_i + m$ with known (k_i).

$$x(k_i + 1|k_i), x(k_i + 2|k_i), \ldots, x(k_i + m|k_i), \ldots, x\left(k_i + N_p \middle| k_i\right) \tag{5.13}$$

Based on state space model parameters A_m, B_m and C_m, the future state variables are calculated using the future control parameters as given in Eq. (5.14) (Wang & Young, 2006).

$$x(k_i + 1|k_i) = A_m x(k_i) + B_m \Delta u\,(k_i)$$

$$x(k_i + 2|k_i) = A_m x(k_i + 1|k_i) + B_m \Delta u\,(k_i + 1)$$

$$= {A_m}^2 x(k_i) + A_m B_m \Delta u\,(k_i) + B_m \Delta u(k_i + 1)$$

$$\vdots$$

$$x\left(k_i + N_p \middle| k_i\right) = {A_m}^{N_p} x(k_i) + {A_m}^{N_p-1} B_m \Delta u\,(k_i) + {A_m}^{N_p-2} B_m \Delta u(k_i + 1) + \cdots +$$

$${A_m}^{N_p-N_c} B_m \Delta u(k_i + N_c - 1) \tag{5.14}$$

The predicted output is achieved and given in Eq. (5.15).

$$y(k_i + 1|k_i) = C_m A_m x(k_i) + C_m B_m \Delta u\,(k_i)$$

$$y(k_i + 2|k_i) = C_m {A_m}^2 x(k_i) + C_m A_m B_m \Delta u(k_i) + C_m B_m \Delta u\,(k_i + 1)$$

$$y(k_i + 3|k_i) = C_m {A_m}^3 x(k_i) + C_m {A_m}^2 B_m \Delta u\,(k_i) + C_m A_m B_m \Delta u(k_i + 1) + C_m B_m \Delta u\,(k_i + 2)$$

$$\vdots$$

$$y\left(k_i + N_p \middle| k_i\right) = C_m {A_m}^{N_p} x(k_i) + C_m {A_m}^{N_{p-1}} B_m \Delta u\,(k_i) + C_m {A_m}^{N_{p-2}} B_m \Delta u(k_i + 1) + \cdots + B_m \Delta u(k_i + N_c - 1) \qquad (5.15)$$

All predicted variables are formulated in terms of current state variable information $x(k_i)$ and future control movement $\Delta u(k_i + j)$, where $j = 0, 1, \ldots N_c - 1$. Then, the vectors are defined as Eq. (5.16) and Eq. (5.17).

$$Y = \left[y(k_i + 1|k_i), y(k_i + 2|k_i), \ldots, y(k_i + 3|k_i), \ldots, y\left(k_i + N_p \middle| k_i\right)\right]^T \qquad (5.16)$$

$$\Delta u = [\Delta u(k_i)\ \Delta u(k_i + 1) \Delta u(k_i + 2) \ldots \Delta u(k_i + N_c - 1)]^T \qquad (5.17)$$

Combining both Eq. (5.15) and Eq. (5.16) with (5.17), Eq. (5.18) is obtained.

$$Y = F\, x(k_i) + \Delta u \qquad (5.18)$$

Here,

$$F = \begin{bmatrix} C_m A_m \\ C_m {A_m}^2 \\ C_m {A_m}^3 \\ \vdots \\ C_m {A_m}^{N_p} \end{bmatrix};\ \emptyset =$$

$$\begin{bmatrix} C_m B_m & 0 & 0 & \dots & 0 \\ C_m A_m B_m & C_m B_m & 0 & \dots & 0 \\ C_m {A_m}^2 B_m & C_m A_m B_m & C_m B_m & \dots & 0 \\ & & \vdots & & \\ C_m {A_m}^{N_p - 1} B_m & C_m {A_m}^{N_p - 2} B_m & C_m {A_m}^{N_p - 3} B_m & \dots & C_m {A_m}^{N_p - N_c} \end{bmatrix} \tag{5.19}$$

As it is known, the model predictive control is to predict the output by minimizing the cost function, J to be as close as possible to the desired set point or reference trajectory. The cost function, J given by Eq. (5.20) where the first term is to minimize the errors between predicted output and set points while the second term is the size of the control parameter, Δu when it was minimized (Wang, 2009).

$$J = \overbrace{(R_s - Y)^T (R_s - Y)}^{\text{First}} + \overbrace{\Delta U^T \bar{R}\, \Delta U}^{\text{Second term}} \tag{5.20}$$

Here, $\bar{R} = r_w I_{N_c \times N_c}$ and r_w is the tuning parameters for the desired closed loop performances. Whereas R_s is a vector that content the setpoint information. The optimal control parameter, ΔU can be found by using Eq. (5.17) and the cost function can be denoted by Eq. (5.18).

$$J = (R_s - Fx(k_i))^T (R_s - Fx(k_i)) - 2\Delta U^T \emptyset^T (R_s - Fx(k_i)) + \Delta U^T (\emptyset^T \emptyset + \bar{R}\,)\Delta U \tag{5.21}$$

Then, take $\frac{\partial J}{\partial \Delta u} = 0$, the optimal solution of the cost function is as follows:

$$\Delta U = (\emptyset^T \emptyset + \bar{R})^{-1} \emptyset^T (R_s - Fx(k_i)) \quad (5.22)$$

By connecting Eq. (5.22) to the set point signal, $r(k_i)$ and state variable, $x(k_i)$ the optimal solution for finding the control parameter, Δu is given below:

$$\Delta U = (\emptyset^T \emptyset + \bar{R})^{-1} \emptyset^T (\bar{R}_s r(k_i) - Fx(k_i)) \quad (5.23)$$

5.2.2 Case 2: MPC with unknown initial state and without constraint

The second case of MPC is the unknown initial state without constraints and is designed similarly with case 1, but now the proposed hybrid fuzzy-SMO is included in the design for estimating the unknown states. Therefore, the earlier derivations and steps for the MPC and hybrid observer designs will not be repeated in this section. Similar observer equation is applied with small modification as to couple with the MPC that is given in Eq. (5.24) below.

$$x(k) = A_m x(k-1) + B_m u(k-1) + K_{ob} sign(e_f) \quad (5.24)$$

Then, by comparing both Eq. (5.1) and (5.3) with Eq. (5.24), it is realized that the observer gain, K_{ob} is added here as to include the state estimation framework in the early stage of the MPC formulation. This is to ensure that the MPC will always get the current, or the updated states before proceeding with the control. The performances of this second type of MPC will also be observed based on similar temperature setpoint control as the previous case 1 for comparison.

5.2.3 Case 3: MPC with unknown initial state and with constraint

The third type of the controller design is the MPC with unknown initial state and with inequality constraints. It is similar to the case 2 but with additional of constraints. Therefore, only the equations related to constraints are presented in this section.

$$min \frac{1}{2}\Delta U^T Hx + \ f^T \Delta U \tag{5.25}$$

The value of H and f are found by taking the last two terms of Eq. (5.21) by setting the first term constant, which is denoted in Eq. (5.20) (Wang & Young, 2006).

$$J = \overbrace{-\ 2\Delta U^T \emptyset^T (R_s - Fx(k_i))}^{a} + \overbrace{\Delta U^T (\emptyset^T \emptyset + \bar{R}\ )\Delta U}^{b} \tag{5.26}$$

Note that, Eq. (5.25) is modified to suit Eq. (5.20) by dividing those terms (denoted by a and b) by 2 to obtain Eq. (5.27).

$$J = [-\emptyset^T (R_s - Fx(k_i)]^T \Delta U + \frac{1}{2}\Delta U^T (\emptyset^T \emptyset + \bar{R}\ )\Delta U$$

$$J = \frac{1}{2}\Delta U^T H + \ f^T \Delta U \tag{5.27}$$

Comparing both Eq. (5.25) and (5.27), yields the value of H and f as follows:

$$H = (\emptyset^T \emptyset + \bar{R}\ )\Delta U \tag{5.28}$$

$$f = -\ \emptyset^T (R_s - Fx(k_i)) \tag{5.29}$$

Three types of constraint are taken into account specifically the constraints on the control variable of incremental variations ($\Delta u^{min} \leq \Delta u(k) \leq \Delta u^{max}$), constraints on the amplitude of the control variable ($u^{min} \leq u(k) \leq u^{max}$), and output constraints ($y^{min} \leq y(k) \leq y^{max}$). The output constraints, however, can be defined as the 'soft' constraints. 'Soft' constraints are constraints that are modified with slack variable to avoid constraints conflict occurrence (Liuping Wang & Young, 2006). At time instance, the predictive control scheme predicts the future. The future samples by considering the three first steps, $\Delta u(k_i), \Delta u(k_i + 1), \Delta u(k_i + 2)$ are obtained as Eqs. (5.30), (5.31) and (5.32) (Liuping Wang & Young, 2006).

$$\Delta u^{min} \leq \Delta u((k_i) \leq \Delta u^{max} \tag{5.30}$$

$$\Delta u^{min} \leq \Delta u(k_i + 1) \leq \Delta u^{max} \tag{5.31}$$

$$\Delta u^{min} \leq \Delta u(k_i + 2) \leq \Delta u^{max} \tag{5.32}$$

Now, the three cases of embedded integrator MPC has been completely developed. Tuning is also required to find the optimal control performances (Mahramian, Taheri, & Haeri, 2007; Shridhar & Cooper, 1997). This is done by setting the temperature at a constant value and varying the prediction horizon (N_p), the control horizon (N_c) and the tuning parameters for close loop (r_w) (Ibrehem, 2011; Kiashemshaki, Mostoufi, & Sotudeh-Gharebagh, 2006). The best value of those parameters are N_p= 30, N_c= 10 and r_w= 100 that provides the least oscillation and overshoot.

5.3 Reactor temperature control using the embedded integrator MPC

It is well-known that temperature is one of the standard control variables in the industry that will significantly affect the quality of the product (Ali et al., 2003; Van Brempt et al., 2001). In the polymerization process, the heat removal is limited due to constraints on the cooling water flow rate. The temperature of the reactor will go up high when the cooling water flow rate is saturated; thus the monomer feed has to be reduced manually. The high temperature can cause catalyst degradation and at the same time affect the process (Seki et al., 2001). In addition, the reduction of the monomer will lead to the reduction of the production rate. Therefore, temperature must be controlled precisely to maintain the stability and production rate of the process (Seki et al., 2001).

Furthermore, constraints are added as well in the process since in real situation, all processes are subjected to some form of constraints or another (Camacho & Bordons, 2004). For example, actuators have a limited slew rate and range of action. In practice, the operating points of plants are determined to satisfy economic goals and lie at the intersection of certain constraints. The control system usually operates close to the limits and constraint violations are likely to occur (Bequette, 2003). Therefore, predictive control systems have to anticipate constraint violations and correct them in an appropriate way. A plant that failed to consider constraint on manipulated variables may result in higher values of the objective function and bad performances whereas violating constraints on the controlled variables tend to be costly and dangerous as it could cause damage to equipment and losses in production (Bequette, 2003).

Case 1 has been designed for verification purpose to give insight into the importance of the state observer. This ideal case is developed with known initial state and without specifying any constraint. The value of Δu is calculated and the initial condition is refined. This is a simple simulation case to observe the readiness of the MPC. It will then be extended in case 2 by adding an observer or a state estimator without specifying the initial condition. The observer is applied to estimate the unknown states. It is a replacement of sensors in control systems which are rather expensive in nature. In addition, the observer also helps to measure how well the internal states of a system may react by knowing its external outputs (Ogata, 1995).

Next, I have developed the case 3, which is also a practical case. It was developed without specifying the initial condition and adding inequality constraints. This case is a practical case as all processes are subjected to constraints and the initial state is unknown. In this case, inequality constraints are added and the objective function is formulated using quadratic programming. The cases are then evaluated by changing the temperature setpoint from 45^0C to 55^0C and 75^0C (Ibrehem, 2011; Kiashemshaki et al., 2006) with and without noise as well as disturbance conditions.

The temperature 45^0C is chosen since the reaction will begin from within 45^0C and obtain the optimum production rate at around 60^0C. Therefore, 55^0C that is in the range, has been chosen as the second setpoint (Ibrehem, 2011; Kiashemshaki et al., 2006). In addition, I have also considered the pilot plant of the polymerization reactor that will be used as the validation benchmark, which operates at the temperature ranging from 70^0C to 80^0C. Because of this 75^0C is taken as the final setpoint for the performance testing. Setpoint tracking is important as it may need to be set at different desired condition and if MPC or controller is not able to act towards this changes, then it will disrupt the whole process and can cause problems (Seborg, Mellichamp, Edgar, & Doyle III, 2010).

5.4 MPC performances and discussions

All three cases using the MPC have shown good results by settling to the desired setpoints in a short time even in the presence of noise and disturbances in the process. The results are given in Figures 5.2 and 5.3. Case 1 showed the worst results with higher overshoot but without oscillation since the observer is not included in the design. The unknown states are unable to be estimated thus difficult for the controller to reject the overshoot. As for case 2, when the observer is added, the states are estimated before the control signal value is computed. Therefore, the overshoot is reduced and a better temperature control can be observed compared to the case 1. However, when disturbances are added up to the worst scenario, Case 2 has shown unusual behaviour of the temperature that dropped to -300^{0}C. Therefore, it is not a reliable controller compared to the proposed Case 3. Furthermore, case 3 has the best results, with small overshoot and without oscillation.

The MPC controllers are also compared based on the merit score of error, namely ISE (Integral Squared Error) that penalized large error responses, IAE (Integral Absolute Error) that considered all errors in a uniform manner and ITAE (Integral-Time weighted Absolute Error) that penalize long time errors that occurred in the response. The score is tabulated in Tables 5.1 and 5.2 for with and without noise by considering the temperature setpoint equal to 75^{0}C as an example. We have chosen one out of three setpoints temperature just to show the effectiveness of the controller to handle noise and disturbances.

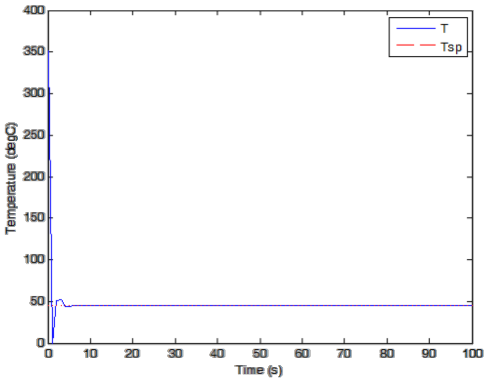
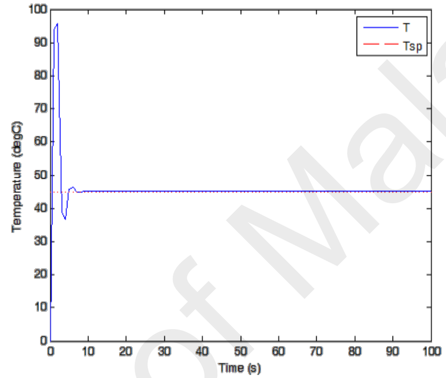
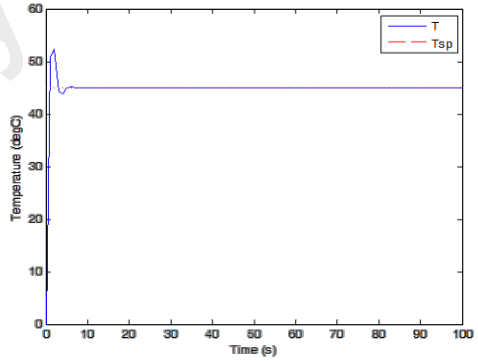
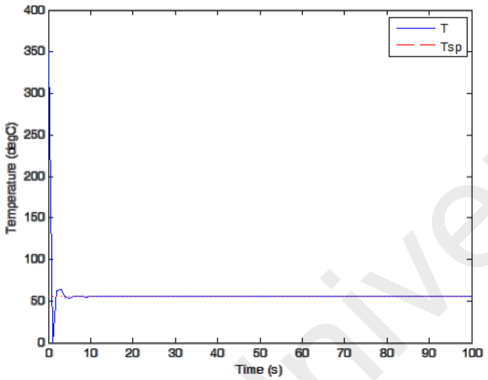
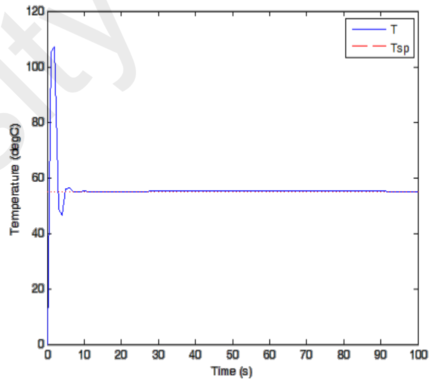
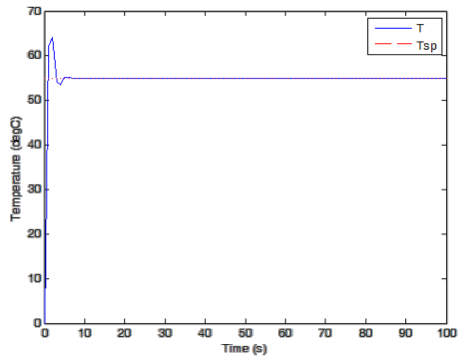
<table>
<tr><th>Set Point</th><th>Case 1 (without observer, no constraint)</th><th>Case 2 (with observer, no constraint)</th><th>Case 3 (with observer and constraints)</th></tr>
<tr><td>$T_{sp} = 45°C$</td><td>
</td><td>
</td><td>
</td></tr>
<tr><td>$T_{sp} = 55°C$</td><td>
</td><td>
</td><td>
</td></tr>
</table>

Figure 5.2: The effect of set points to MPC for without noise/disturbance conditions

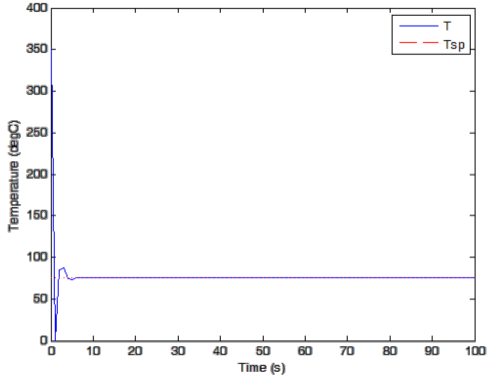
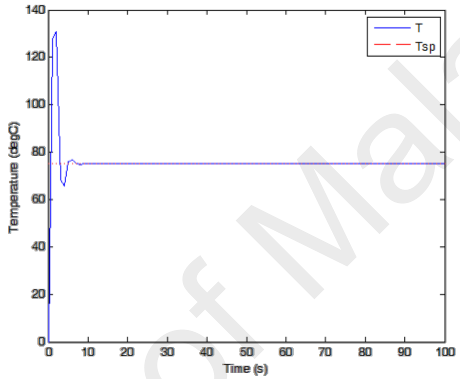
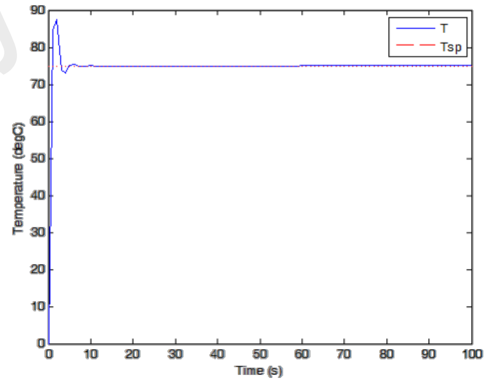
$T_{sp} = 75°C$			

Figure 5.2 (continued)

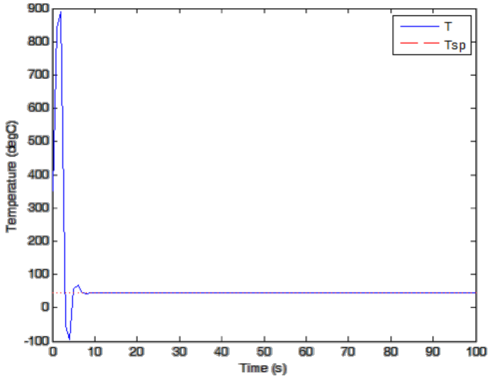
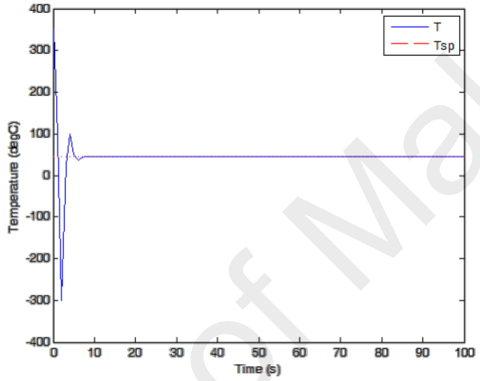
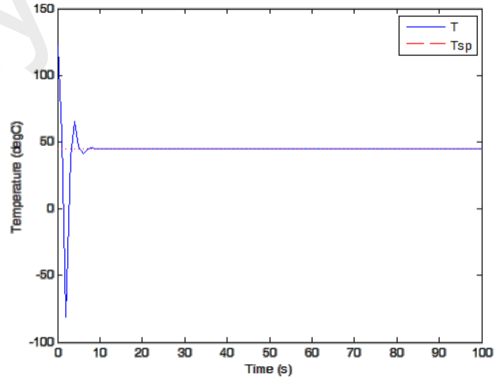
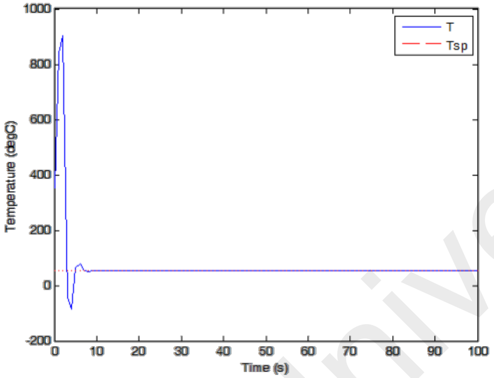
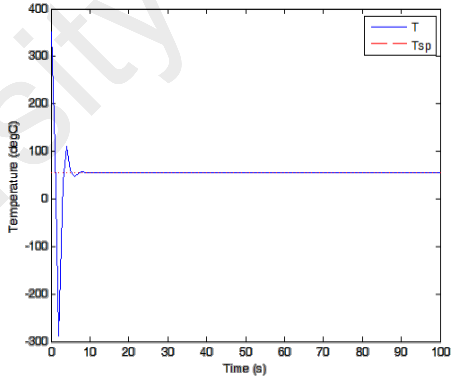
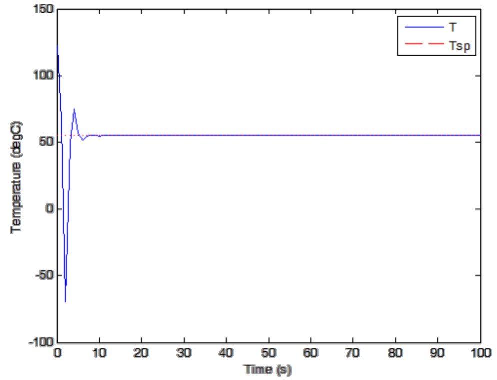
Set Point	Case 1 (without observer, no constraint)	Case 2 (with observer, no constraint)	Case 3 (with observer and constraints)
$T_{sp} = 45°C$			
$T_{sp} = 55°C$			

Figure 5.3: The effect of set points to MPC for with noise/disturbance conditions

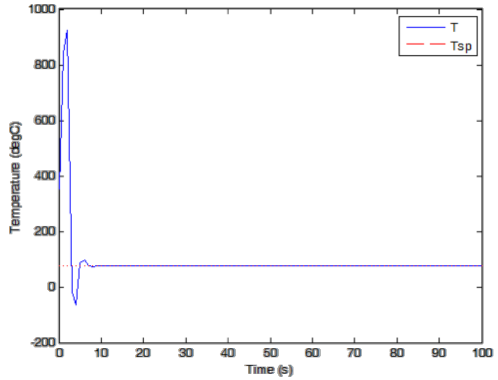
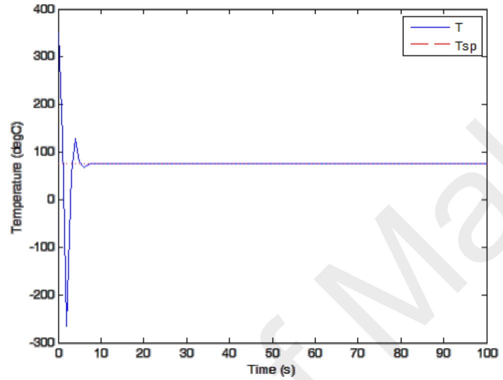
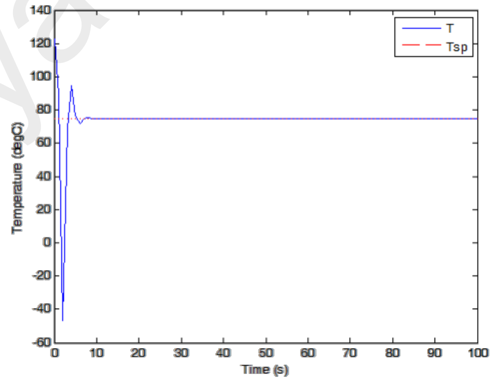
$T_{sp} = 75°C$			

Figure 5.3 (continued)

Table 5.1: The Merit score for the MPC without noise condition

Merit / Controller	ITAE	IAE	ISE
Case 1	8.624e4	1742	3.066e4
Case 2	5069	102.4	105.9
Case 3	943.6	19.06	3.671

Table 5.2: The Merit score for the MPC with noise/ disturbance conditions

Merit / Controller	ITAE	IAE	ISE
Case 1	1.45e4	293	867.3
Case 2	5069	102.4	105.9
Case 3	1356	27.4	7.582

Based on the ITAE, IAE and ISE values tabulated in Table 5.1 and Table 5.2, it is proven that the best controller is the embedded integrator MPC for case 3, which is incorporated with the hybrid observer and constraints. This also revealed that MPC is able to handle constraints efficiently. Besides that, when the observer is combined with the MPC, the observer will estimate the states (including the disturbances and noise) thus giving a smooth temperature control.

In addition, the proposed MPC has also been compared with MPC without both observer and integrator; MPC with observer only; and PID controller to prove its performances. Results are illustrated in Figures 5.4 and 5.5 for various setpoints with and without noise conditions respectively. Based on the figures, PID has shown higher overshoot with no oscillation and the setpoint are achieved at an average of 25s when noise is not available. However, when noise is added to the system, oscillations are observed and the PID controller is unable to handle the conditions and the desired setpoint could not be achieved. As for MPC without both the observer and integrator, large offsets are seen and the controller is unable to reach the setpoint regardless the conditions in the process. Those results are then being improved by adding the observer in the MPC design. The observer will first estimate the unknown states, which include the noise and disturbances and conveys the information to the MPC controller to obtain better performance. Here, we can observe the removal of offsets that due to the integral factor or integrator added in the formulation. Therefore, a guaranteed offset-free control has been accomplished.

When the MPC is equipped with both the observer and integrator, small overshoot with no oscillation have been observed. The setpoints are also achieved faster with an average of 10s for every setpoint tested. The merit scores of error is also given in Tables 5.3 and 5.4. Small merit score can be seen from the proposed MPC compared to the other controllers. Therefore, it can be summarized that for all the setpoints, MPC with embedded integrator performed better than the other controllers by being able to reach the desired setpoints or the steady state conditions faster and more accurate with less overshoot and no oscillation. Besides that, all the results (Figure 5.4 and Figure 5.5) and merit scores (Table 5.3 and Table 5.4) given have proved that the most appropriate controller for controlling the temperature for the ethylene polymerization process, in this case, is the proposed MPC with embedded integrator.

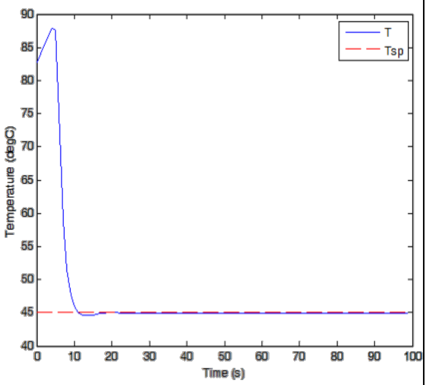
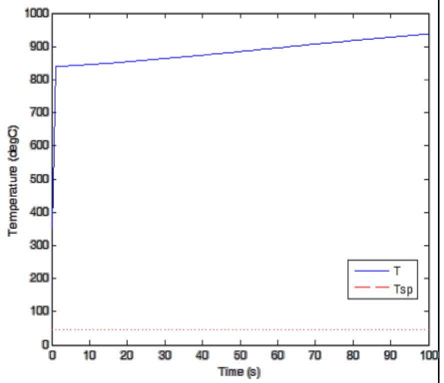
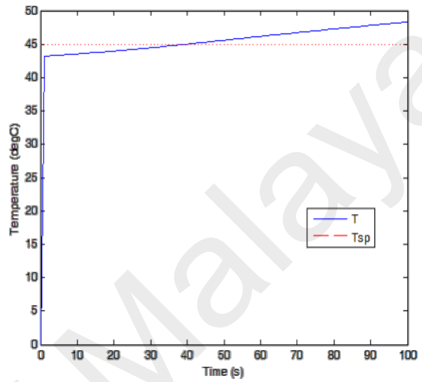
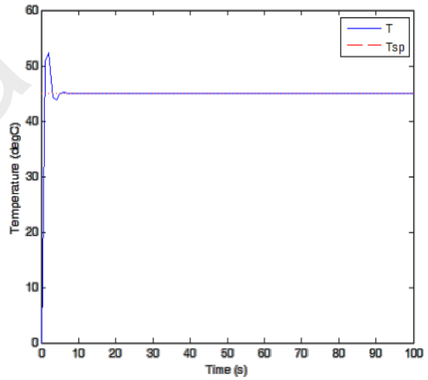
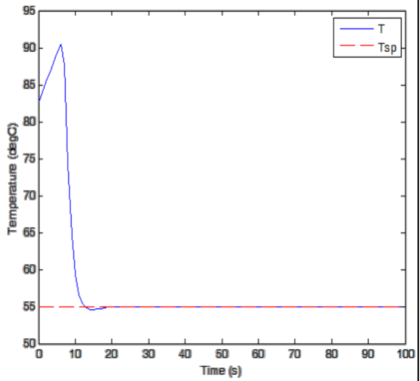
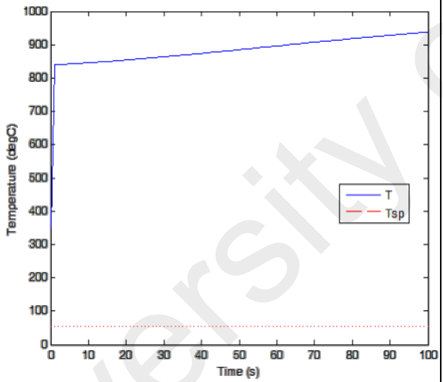
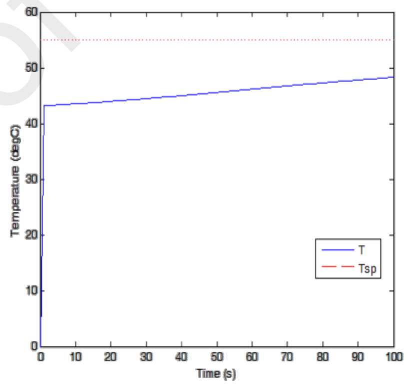
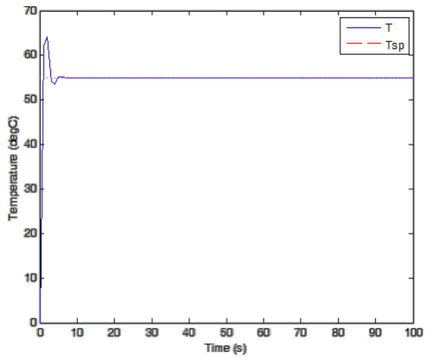
Set point	PID	MPC (without observer and integrator)	MPC (with observer, without integrator)	MPC (with both observer and integrator)
$T_{sp} = 45°C$				
$T_{sp} = 55°C$				

Figure 5.4: Comparison between proposed MPC, MPC without integrator, MPC without observer and integrator as well as PID (without noise condition)

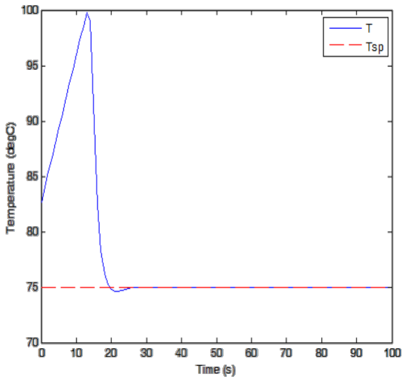
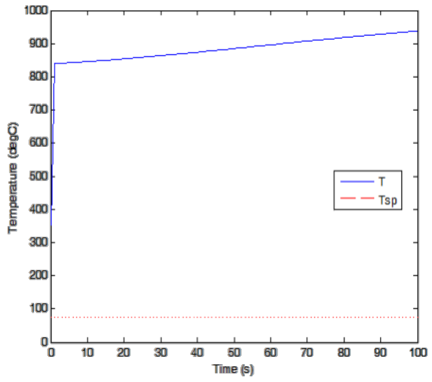
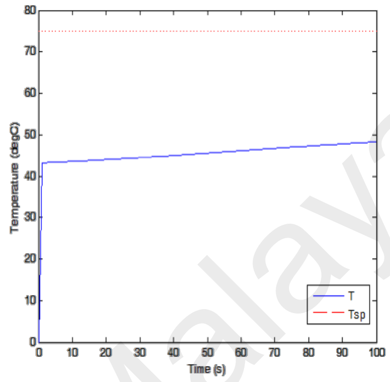
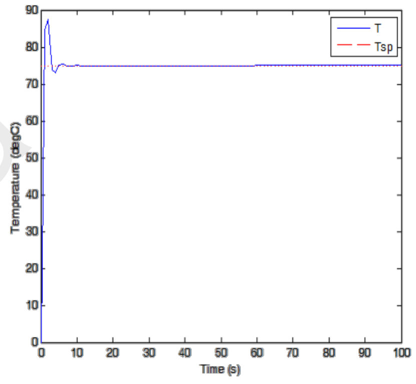
$T_{sp} = 75°C$				

Figure 5.4 (continued)

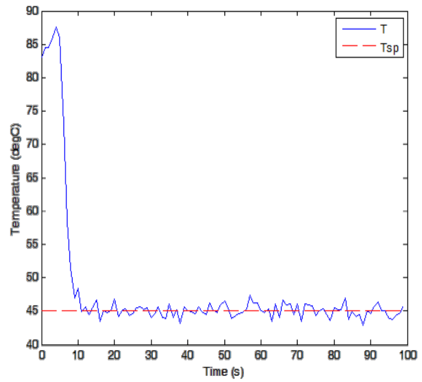
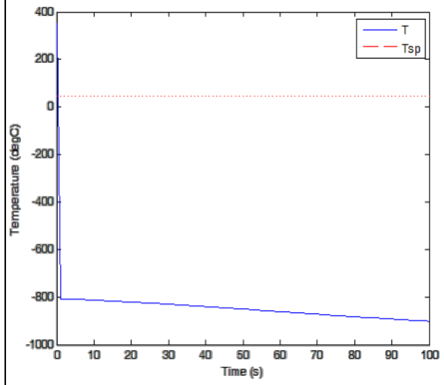
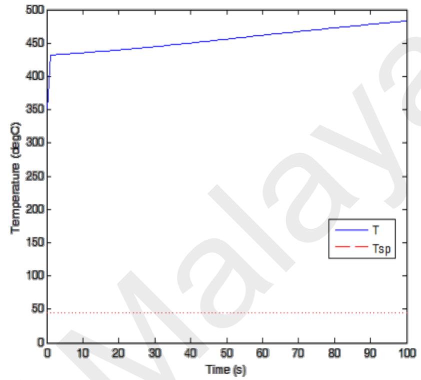
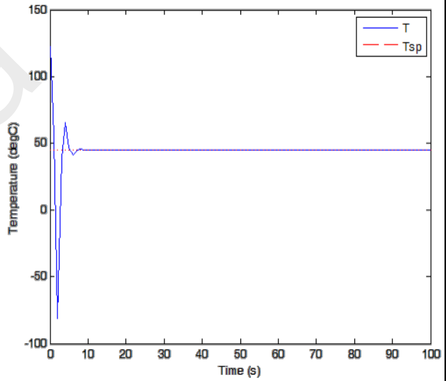
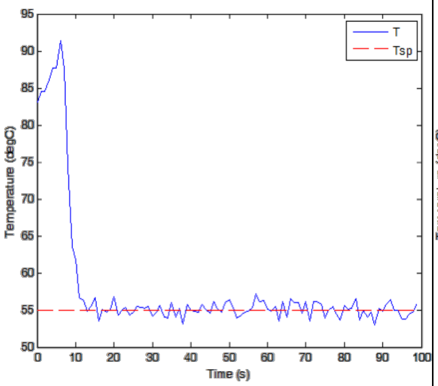
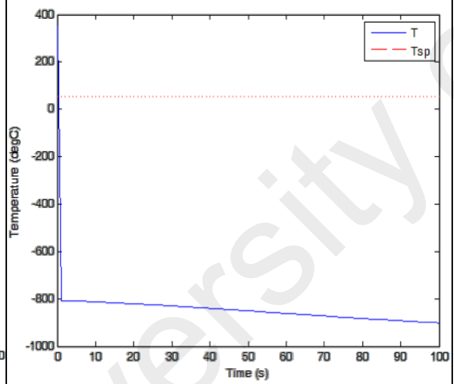
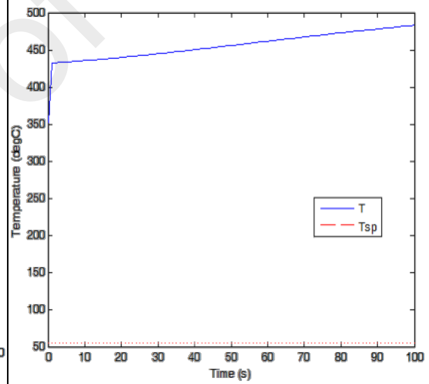
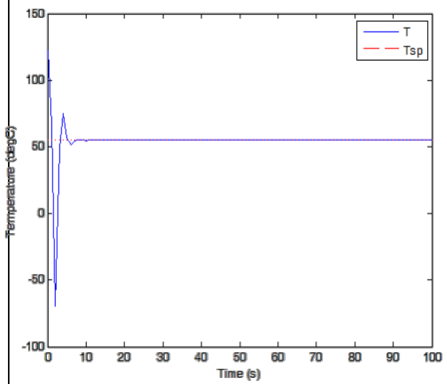
Set point	PID	MPC (without observer and integrator)	MPC (with observer, without integrator)	MPC (with both observer and integrator)
T_{sp} $= 45°C$				
T_{sp} $= 55°C$				

Figure 5.5: Comparison between proposed MPC, MPC without integrator, MPC without observer and integrator as well as PID (with noise condition)

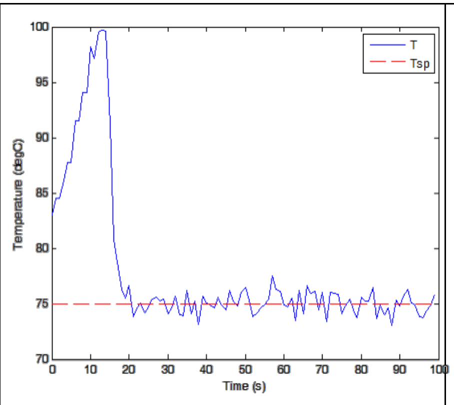
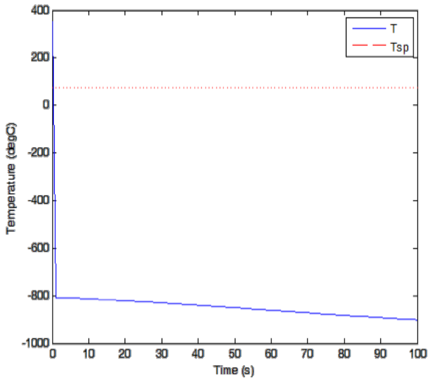
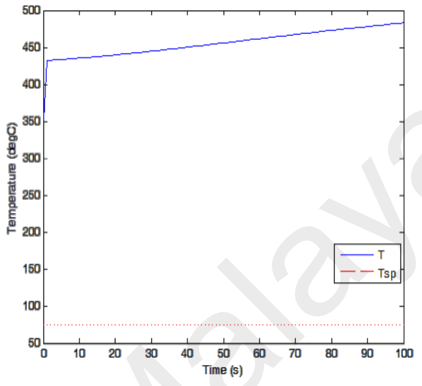
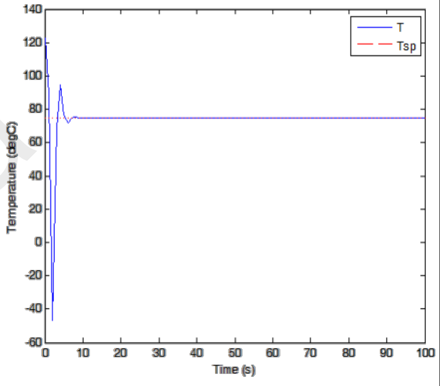
$T_{sp} = 75°C$				

Figure 5.5 (continued)

Table 5.3: The Merit score for the controllers without noise condition

Controller \ Merit	ITAE	IAE	ISE
PID	2897	282.2	4954
MPC (without observer and integrator)	1.358e6	2.743e4	7.602e6
MPC (with observer, without integrator)	1.438e5	2904	8.519e4
MPC (with both observer and integrator)	943.6	19.06	3.671

Table 5.4: The Merit score for the controllers with noise/ disturbance conditions

Controller \ Merit	ITAE	IAE	ISE
PID	6482	341.3	5068
MPC (without observer and integrator)	4.531e6	9.153e4	8.462e7
MPC (with observer, without integrator)	1.888e6	3.813e4	1.469e7
MPC (with both observer and integrator)	1356	27.4	7.582

CHAPTER 6: VALIDATION USING EXPERIMENTAL DATA

6.1 Chapter overview

In this sixth chapter of the thesis, the validation of the hybrid observer is discussed. Experimental data from a real polymerization pilot plant is compared with the simulated plant. The validation benchmark, which is the fluidized bed reactor is introduced and the data are obtained from two experimental runs. All results are compared and analyzed.

6.2 Validation Benchmark

Validation and verification are the terminologies used to describe or to confirm whether the simulation code is adequately representing the process model or algorithms. Validation is a process of deciding that the model accurately represents the conceptual description while verification is a process of determining that the model accurately represents the conceptual based on the real scenario or situation on the perception of the model used (Trucano, Swiler, Igusa, Oberkampf, & Pilch, 2006). Those concepts are often applied in many fields, including process system engineering to verify the precision of a simulation code compared to the pilot or real plant data in order to ensure the capability of the simulation code designed by the researcher. In this work, the similar concept is adapted to define the accuracy of the simulation based hybrid observer design compared to the data obtained from a polymerization pilot plant.

The benchmark considered in this validation procedure is the pilot-scale fluidized bed catalytic reactor for production of polyolefin as depicted in Figure 6.1. This unit consists of the fluidized bed and a disengagement section, where the bed has the height of 150 cm and diameter of 10 cm, while the volume of the disengagement section is 652 cm^3. The reactor contains a specially-fabricated catalyst unit that is located at about 9cm above the metallic mesh plate distributor. Besides that, the polymer powder is retained in the bed for maintaining the good mechanical stability. The temperature of the reactor is kept between 70^0C - 80^0C to allow the reaction and for obtaining best product quality. In addition, a temperature sensor is installed to capture the profile and is located vertically at various points in the pilot plant. If the temperature of the gas mixture is high, the remaining mixture will be directed to the heat exchanger to cool it down. On the other hand, the overall system pressure is stabilized by using an air plunge compressor and the fluctuations of the pressure are balanced by the aid of a buffer container in the form of nitrogen (N_2). A control valve is applied to regulate the inlet gas flow circulation within the reactor. The reactor is designed to tolerate pressure up to 30 bar. Thus, a relief valve is installed to prevent excess pressure buildup.

Figure 6.1: Pilot-scale fluidized bed catalytic reactor

The experiment will begin when the gas is fed at the base reaction zone of the reactor. The feedstock contains nitrogen (N_2), hydrogen (H_2) and the monomer, where the feed gases also act as the heat transferring agent. N_2 acts as the reactant carrier gas while H_2 acts as polymer chain disassembly gas. Then, the catalyst (Ziegler-Natta) is fed near top of the reactor and it will move downwards to start the reaction for producing the product.

A co-catalyst is also added to the reaction mixture for preserving the moisture levels in the reactor to activate the catalyst. The co-catalyst flow could be adjusted between regular and fast speed depending on the amount needed with the help of a control valve. Polymer will grow on the catalyst by increasing its weights and sizes and particle segregation will then occur in the reactor based on the difference in the weight. Next, the polymer particles are continuously withdrawn through the discharge line located at the base of the reactor just close to the distributor. Overall conversion can be as high as 98% provided proper solid fluidization processes are practiced. In order to maintain the proper fluidization, sufficient recycle and make-up gas flowrate must be sustained through the distributor. Finally, the unreacted and unused gases are recycled to a cyclone, which consists of four different filters. The filters are also applied to remove the fine grain particles from the reactor. In addition, contamination is eliminated by keeping the Ziegler-Natta catalyst above the atmospheric pressure level while other gases traces are removed by using purifiers. Furthermore, the separation of the unreacted gases and the solid particles takes place in the disengaging region. The schematic diagram is illustrated in Figure 6.2.

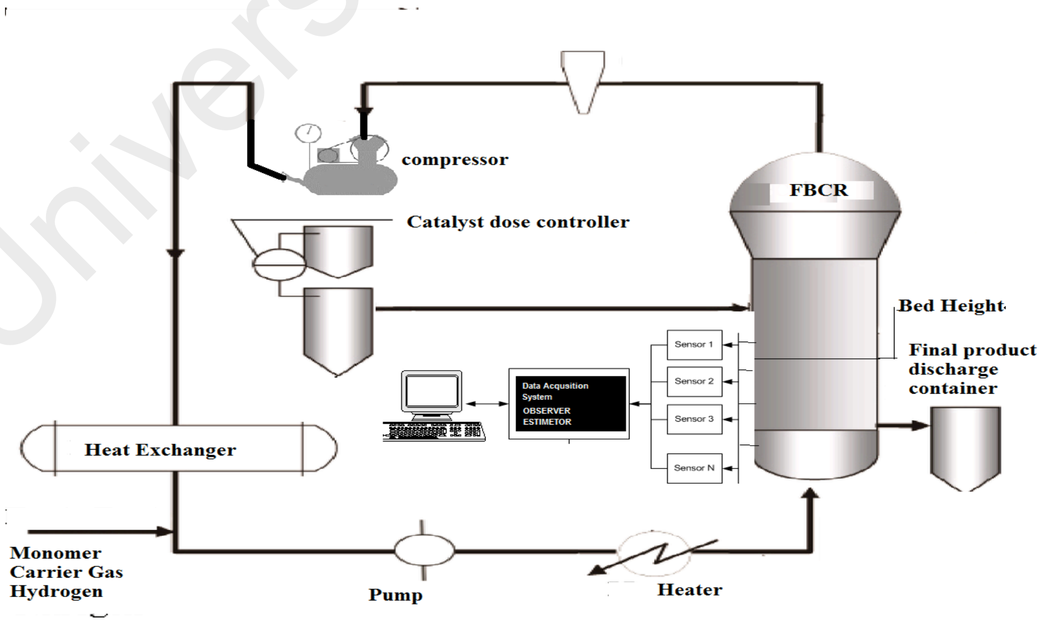


Figure 6.2: Schematic diagram of the pilot-scale fluidized bed catalytic reactor

Data obtained from the experimental will be saved in the data acquisition software system. It is worth to note that due to the complex nature of the pilot plant especially in dealing with the co-catalyst, the process of obtaining reliable sets of data is time consuming and costly. The monomer concentration values are extracted from the data and used to validate the proposed hybrid fuzzy-SMO. In addition, the MPC controller has not been validated since there were no on-line setup for MPC controller in the pilot-scale fluidized bed catalytic reactor.

6.3 Fuzzy-SMO validation

For this validation, the data are obtained from two historical data obtained from the pilot-scale fluidized bed catalytic reactor. The monomer concentration values were taken between 15-30 minutes within 2 hours of experiment as tabulated in Table 6.1 and Table 6.2. The value of the time in the tables are in hour while the concentration is in weight (%) and have been used to compare with the simulated plant. The validation will be performed once the design and analysis of the hybrid fuzzy-SMO observer in the simulation environment have been completed. it is to demonstrate the effectiveness of the proposed observer in estimating the real process parameter. This procedure is given in Figure 6.3. The monomer concentrations that have been extracted from the real pilot plant data will be used as the actual value in the validation. It first value is taken as the reference value and the proposed hybrid fuzzy-SMO is reapplied to estimate the parameter. The new estimated values are then compared with the actual values obtained from the pilot plant.

The validation has also considered the comparison of the fuzzy-SMO with the single SMO and fuzzy logic to highlight its advantages. The results of the validation are observed and discussed. In normal validation procedure, the basic check of the real plant versus the simulation will be performed before validating the observer or the controller.

However, the simulated plant has been modified to meet the characteristics of the validation benchmark provided, thus the basic check is not required (Trucano et al., 2006). In addition, there are no on-line data available for melt flow index (MFI) and the co-monomer concentration therefore the monomer concentration will be used as the indication for validating the proposed hybrid fuzzy-SMO.

Table 6.1: Monomer concentration from first experiment

Time (hour)	Monomer concentration (wt %)
0.0	71.4806
0.4	70.3533
0.6	69.7008
0.7	63.3154
0.9	60.0068
1.0	58.7446
1.2	56.0126
1.3	56.9316
1.5	56.9201
1.7	56.3201
1.9	55.4752
2.3	52.0061

Table 6.2: Monomer concentration from second experiment

Time (hour)	Monomer concentration (wt%)
0.0	64.9458
0.3	64.4089
0.4	64.7252
0.6	63.7534
0.8	60.3486
1.0	52.7796
1.2	43.7147
1.5	37.7083
1.9	33.7533
1.9	33.8104
2.1	31.2704
2.3	30.2726

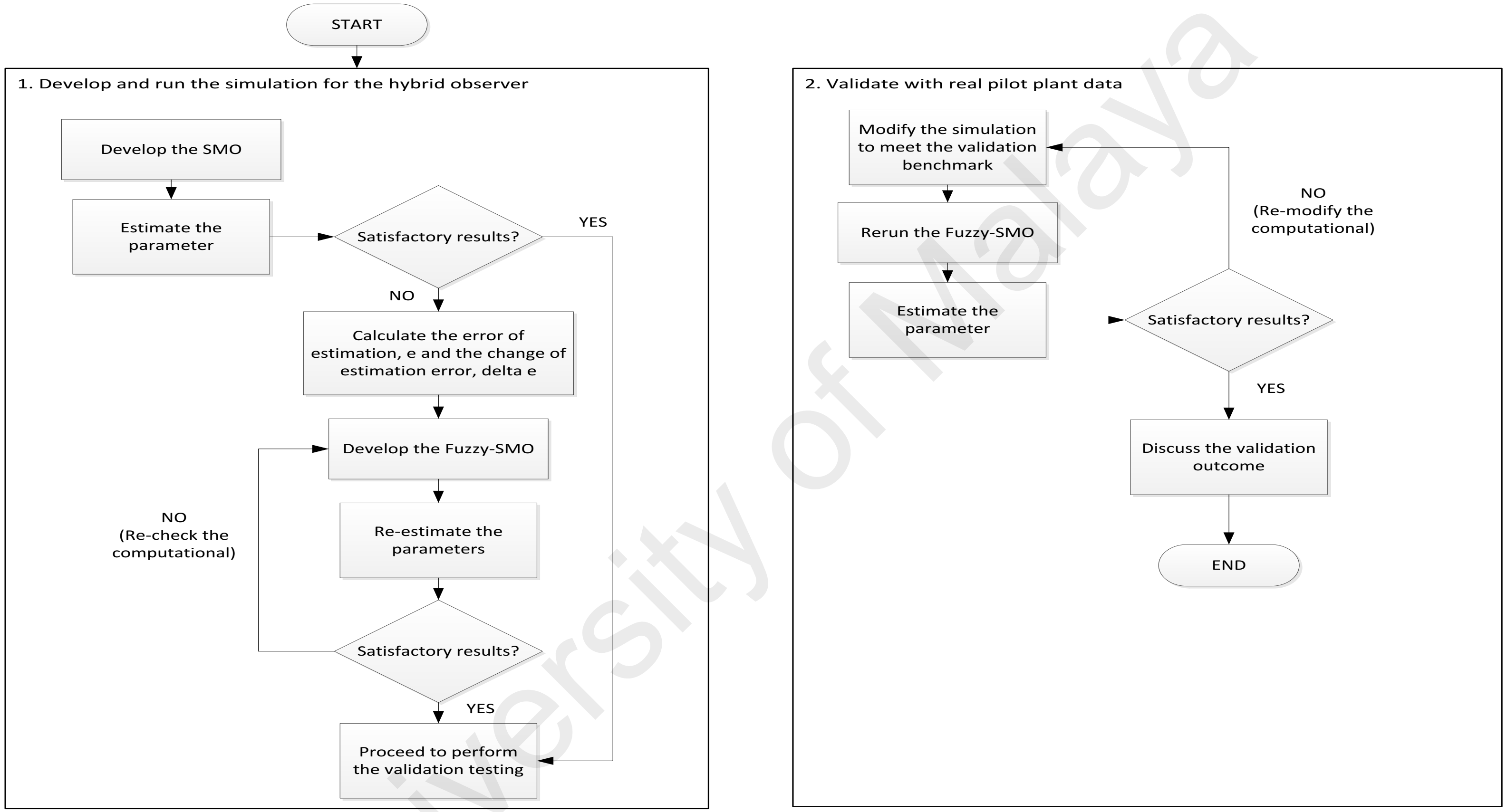


Figure 6.3: The validation procedure of the hybrid fuzzy-SMO

6.4 Validation results and discussions

The validation results are illustrated in Figure 6.4 and 6.5 for the first and second run of the experiments respectively. Based on Figure 6.4, the single sliding mode observer (SMO) and fuzzy logic have not able to estimate the monomer concentration accurately compared to the hybrid fuzzy-SMO. Fuzzy-SMO has estimated the monomer concentration the closest possible to the actual plant value. However, some reading is not able to be accurately estimated due to the modeling discrepancies between the real pilot plant and the simulation framework.

This situation is also related to the choice of the validation benchmark (Trucano et al., 2006). The difference between the benchmark and the simulation will lead to the inaccuracies of the estimation. For this case, the simulated plant is a well-mixed process while the validation benchmark is the two-phase polymerization process. However, to increase the accuracy, the simulated plant has been modified by changing the input parameters as tabulated in Table 6.3. The validation benchmark need not be exactly similar to the simulation model since adjustment can be made to the programming to align the actual and the estimated value (Trucano et al., 2006). Unfortunately, due to this reason, small discrepancies are obtained from the results.

Table 6.3: Input parameters modified for validation purposes

Parameter	Values	Parameter	Values
F_{M_1}	151 mole/s	F_{M_3}	3.92 mole/s
F_{M_2}	4 mole/s	F_{M_4}	1.78 mole/s
F_c	1.08 kg/h	ΔP	20 atm
T_f	348 K		

A similar situation is also observed for the validation using the second experimental data from the pilot plant as in Figure 6.5. Here, the hybrid fuzzy-SMO has managed to estimate the concentration with acceptable result compared to the single SMO and fuzzy logic. Besides that, SMO and Fuzzy logic alone in both Figure 6.4 and 6.5 have shown huge deviations but when it is combined, reasonable results are observed. SMO has the ability to generate the sliding motion on the error between the actual and the estimated value and if the error is big, huge deviations are observed. As for fuzzy logic, the huge deviations exist because of its priori unpredictable IF and THEN rules that unable to ensure the convergence of the estimation. These rules will only take place after certain time and is based on trial and error procedure dependent of the system. Besides that, the combination is based on the errors from the single SMO that have been manipulated as the fuzzy rules and helped to reduce the deviations to give better result. This is the uniqueness of the proposed hybrid observer, which did not require complicated design formulation to obtain good results.

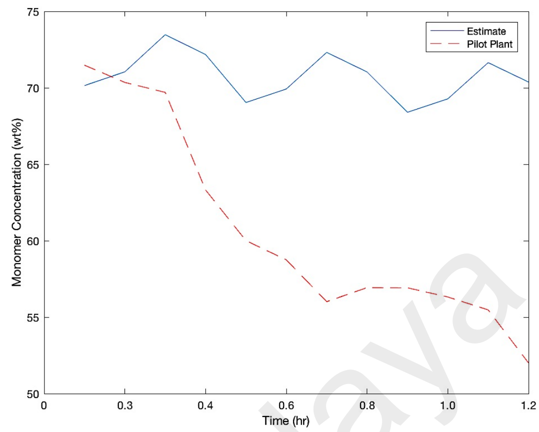
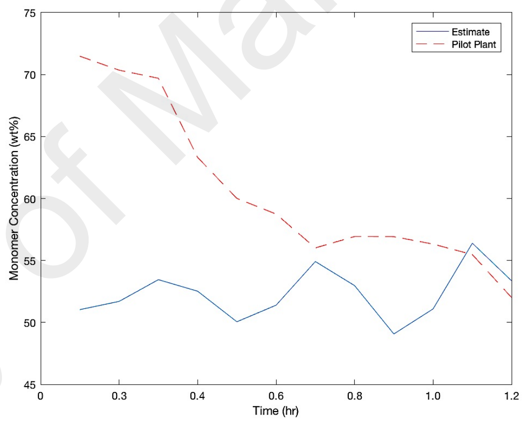
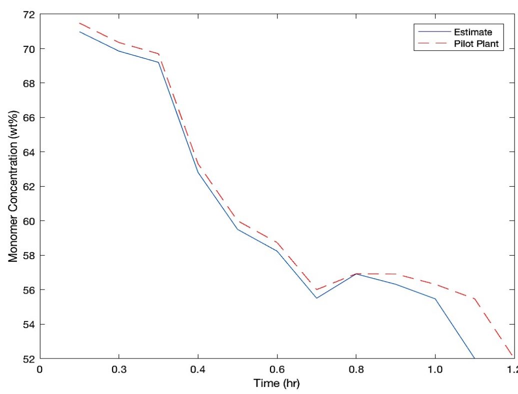
Type of observer	Validation performances
Sliding Mode Observer (SMO)	
Fuzzy Logic	
Fuzzy-SMO	

Figure 6.4: Validation result for the first experiment run

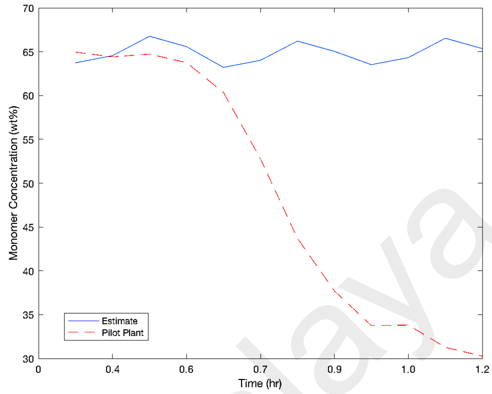
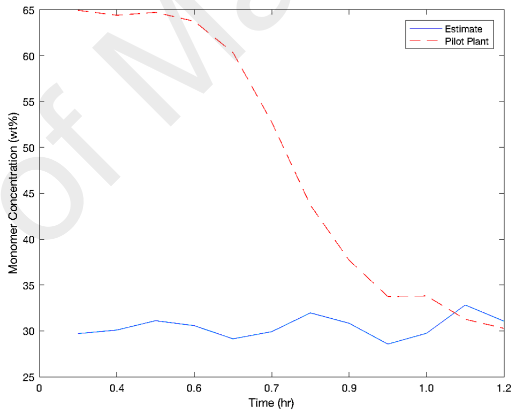
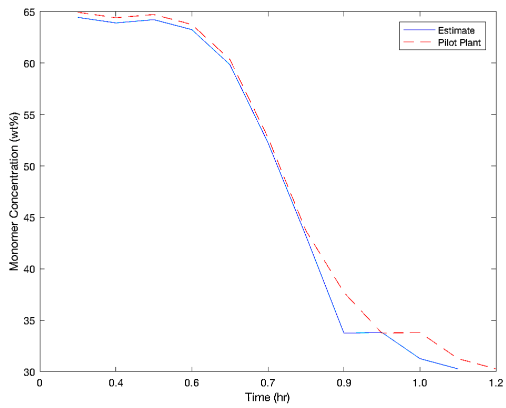
<table>
<tr><th>Type of observer</th><th>Validation performances</th></tr>
<tr><td>Sliding Mode Observer (SMO)</td><td>
</td></tr>
<tr><td>Fuzzy Logic</td><td>
</td></tr>
<tr><td>Fuzzy-SMO</td><td>
</td></tr>
</table>

Figure 6.5: Validation result for the second experiment run

CHAPTER 7: CONCLUSION AND FUTURE WORK

7.1 Chapter overview

In this final chapter of the thesis, the work is summarized and conclusions are given together with the contributions of the research. Several recommendations are also provided for the future work related to the observer and control in the polymerization field.

7.2 Concluding remarks and contributions

In conclusion, a hybrid fuzzy-sliding mode observer (fuzzy-SMO) has been designed to estimate unknown parameters in the ethylene polymerization reactor. It was important to identify the unknowns to avoid disruptions and failures in the process. Sensors have been installed in the plant for measuring the parameters, however they were expensive and unreliable to estimate all the unknowns especially those that have appeared unexpectedly due to disturbances and mismatches as explained in Chapter 1, thus, a better approach such as an observer was introduced. Due to certain limitations of the single and hybrid observers available in the literature at present including low rate of estimation, less accuracy and unable to estimate many parameters at once the hybrid fuzzy-SMO has been proposed. Good performances have been obtained from the proposed observer in estimating the parameters, which provided accurate, fast and stable estimation in the system.

The step by step formulation of the hybrid fuzzy-SMO that combined the conventional observer (SMO) with and artificial intelligence (AI) elements (fuzzy logic) was demonstrated in Chapter 4, all of which satisfied the first objective of this research. It was unique since fuzzy logic has never been combined with SMO before and this type of combination was new in the polymerization process application, thus a novel contribution has emerged. Furthermore, it was also designed in such a way that the formulation could be modified to estimate many parameters without redesigning the whole structure of the observer. Three parameters were estimated namely the ethylene concentration, butene concentration and melt flow index (MFI) by adding only the equation related to the parameter in the observer's formulation. This was another novel contribution since observers available in the literature as emphasized in Chapter 2 have usually being applied to estimate specific parameter and if more parameters are needed to be estimated, the whole structure of the observer must be changed.

Illustrative results were given in supporting and highlighting the effectiveness of the observer in both with and without noise conditions. It was also compared with the single SMO, single extended Luenberger observer (ELO), fuzzy logic and hybrid sliding mode–proportional observer (SMO-proportional), which matched the second objective of the research. The comparisons displayed clearly that the fuzzy-SMO was the best observer to be used in the ethylene polymerization process, where it showed fast, accurate and stable estimation even in the presence of noise in the system.

Further to the use of estimators and to show its usefulness in the control system, a controller was developed to maintain the reactor temperature at it desired setpoint. For this purpose, the MPC as in Chapter 5 was designed considering the measured states estimated by the hybrid fuzzy-SMO earlier, which was also the third objective in this work. The performance of the controller would be enhancing when it was coupled with the observer since the observer would first estimate the states and conveyed the information to the controller.

In addition, an integral factor or integrator was added to the MPC design or better known as the embedded integrator MPC. It was included to add advantage to the MPC controller to guaranty offset-free throughout the application. Three cases of the proposed MPC was developed representing one ideal and two practical cases. The first ideal case (Case 1) was designed intentionally to test the readiness of the programming while the other two cases were more practical to imitate real plant situation. Case 2 was where the hybrid fuzzy-SMO was included as to estimate the unknowns, whereas constraints were introduced in both the inputs and outputs parameters in Case 3. All the MPC performances in controlling the temperature are analyzed to prove the ability of the controller. Case 3 showed the best performances that able to maintain the temperature at any setpoint desired with a small mean of error although disturbances and noises were included in the process, thus suitable to be applied to the ethylene polymerization process. It was also compared with the proportional-integral-derivative (PID) controller, MPC without integrator and MPC without observer for further highlighting its performances and to complete the fourth objective of the research.

The ethylene polymerization process has been incorporated with the hybrid fuzzy-SMO and the embedded integrator MPC, where in general the methodology of the project was explained in Chapter 3. The development and performance testing were carried out in the simulation environment with the aid of MATLAB software. Once the results are compiled and analyzed, they were validated with the experimental data from a polymerization pilot plant. Validation was performed mainly to verify the simulation reliability and to support the ability of the design as well as to achieve the final objective of the research. The validation procedures and outcomes were discussed in Chapter 6 together with the validation benchmark or the pilot plant utilized. Only small discrepancies were observed from the simulated fuzzy-SMO compared to the experimental data and should be able to be improved provided an exact benchmark was available.

The research was completed upon performing the validation, whereby a hybrid observer and the MPC controller have been developed, formulated, tested, analyzed and validated in the ethylene polymerization process. All the objectives were accomplished and the contributions were highlighted. To sum up, a hybrid fuzzy-SMO coupled with the embedded integrator MPC for estimation and advanced control of an ethylene polymerization process has been successfully designed.

7.3 Future works

In future, several works may be performed as follow:

i. Other polymerization parameters such as chain length, molecular weight distribution (MWD) and heat transfer coefficient shall be estimated using the proposed hybrid fuzzy-SMO. It is recommended that those parameters are estimated since they are among others the critical parameters that will affect the product quality in the polymerization process.

ii. The parameters will be used as the known states to implement the embedded integrator MPC controller to control the hydrogen concentration and pressure of the reactor. Hydrogen concentration has the biggest influence in determining the polymer product quality while a maintained pressure value will help in the reaction.

iii. On-line implementation of the hybrid observer and MPC controller will also be scheduled to become the future tasks based on the promising results obtained throughout the research work.

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LIST OF PUBLICATIONS AND PAPERS PRESENTED

Papers published and presented in conferences are listed below:

a) Published (ISI-based)

1. **Mohd Ali, J.,** Ha Hoang, N., Hussain, M.A., & Dochain, D. (2015). Review and classification of recent observers applied in chemical process systems. *Computers & Chemical Engineering*, *76(0)*, 27-41.
2. **Mohd Ali, J.,** Hussain, M.A., Tade, M.O., & Zhang, J. (2015). Artificial Intelligence techniques applied as estimator in chemical process systems – A literature survey. *Expert Systems with Applications, 42*(14), 5915-5931.
3. **Mohd Ali, J.,** Ha Hoang, N., Hussain, M.A., & Dochain, D. (2016). Hybrid observer for parameter estimation in ethylene polymerization reactor: A simulation study. *Applied Soft Computing*, *49*, 687-698.
4. Hussain, M.A., **Mohd Ali, J.,** & Khan, M.J.H. (2014). Neural network inverse model control strategy: Discrete-time stability analysis for relative order two systems. *Abstract and Applied Analysis*, *2014(0)*, 1-11.

b) Published (Scopus-based)

1. **Mohd Ali, J.,** & Hussain, M.A. (2014). Artificial Intelligence Based State Observer in Polymerization Process. *ASEAN Journal of Chemical Engineering*, *2*, 50-56.
2. **Mohd Ali, J.,** & Hussain, M.A. (2016). Hybrid estimation technique for predicting butene concentration in polyethylene reactor. *IOP Conference Series: Materials Science and Engineering*, *121(1)*, 1-8.

c) Under review (ISI-based)

1. **Mohd Ali, J.,** Ha Hoang, N., Hussain, M.A., & Dochain, D. (2016). Hybrid fuzzy-sliding mode observer based model predictive control for controlling reactor temperature of ethylene polymerization process. *Journal of Process Control*, Manuscript under review.
2. **Mohd Ali, J.,** Khan, M.J.H., & Hussain, M.A. (2016). The effectiveness of a hybrid observer based on the experimental data validation from the polymerization pilot plant. *Control Engineering Practice,* Manuscript under review.

d) Conferences

1. **Mohd Ali, J.,** & Hussain, M.A. (2012). *Different Types of Observers Applied in Process Systems*. Paper presented at the 19th Regional Symposium on Chemical Engineering (RSCE2012), 7-8 November 2012, Surabaya, Indonesia.
2. **Mohd Ali, J.,** & Hussain, M.A. (2013). *Observers for Chemical Process Systems*. Paper presented at the 5th Regional Conference on Chemical Engineering (RCCHEE2013), 7-8 February 2013, Pattaya, Thailand.
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4. **Mohd Ali, J.,** & Hussain, M.A. (2013). *Artificial Intelligence Techniques as Estimator in Chemical Process Systems*. Paper presented at the 1st National Colloquium on Process Control (NCPC2013), 1 October 2013, Pulau Pinang, Malaysia.

5. **Mohd Ali, J.,** & Hussain, M.A. (2013). *Fuzzy-Sliding mode observer for monomer concentration estimation in polymerization reactor*. Paper presented at the 20th Regional Symposium on Chemical Engineering (RSCE2013), 12-13 November 2013, Bohol, Philippines.
6. **Mohd Ali, J.,** & Hussain, M.A. (2014). *Parameters Estimation using Hybrid Observer in a Polyethylene Polymerization Process*. Paper presented at the Chemeca2014, 28 September-1 October 2014, Perth, Australia.
7. **Mohd Ali, J.,** & Hussain, M.A. (2015). *State Estimation Based Control in Chemical Process Systems*. Paper presented at the 22nd Regional Symposium on Chemical Engineering (RSCE2015), 24-25 September 2015, Bangkok, Thailand.
8. **Mohd Ali, J.,** & Hussain, M.A. (2015). *Embedded Integrator Model Predictive Control (MPC) Based Hybrid Observer for Polymerization Reactor Control*. Paper presented at the 16th Asian Pacific Confederation of Chemical Congress (APCChe2015, incorporated Chemeca2015), 27 September-1 October 2015, Melbourne, Australia.
9. **Mohd Ali, J.,** & Hussain, M.A. (2015). *Hybrid Estimation Technique for Predicting Butene Concentration in Polyethylene Reactor*. Paper presented at the 2nd Colloquium on Process Control (CPC2015), 1-2 October 2015, Sarawak, Malaysia.
10. **Mohd Ali, J.,** & Hussain, M.A. (2016). *The Comparison of Two Approaches for Designing Observer in Estimating the Monomer Concentration for a Polyethylene Process*. Paper presented at the 7th International Symposium on Design, Operation and Control of Chemical Processes (PSE ASIA 2016), 24-27 July 2016, Tokyo, Japan.

11. **Mohd Ali, J.,** & Hussain, M.A. (2016). *Melt Index Estimation using Two Hybrid Fuzzy-Sliding Mode Observer Methods*. Paper presented at the Chemeca2016, 25-28 September 2016, Adelaide, Australia.