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Hybrid observer for parameters estimation in ethylene polymerization reactor: A simulation study

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ABSTRACT

In this work, we proposed a novel hybrid fuzzy-sliding mode observer designed in such a manner that it can be utilized to estimate various parameters by simply using the related process model, without redesigning the structure of the whole observer. The performances and effectiveness of this hybrid observer are shown through numerical simulation based on a case study involving an ethylene polymerization process to estimate the ethylene and butene concentrations in the reactor as well as the melt flow index. It can be concluded that the proposed hybrid observer provides fast estimation with a high rate of accuracy even in the presence of disturbances and noise in the model. This hybrid observer is also compared with the sliding mode, extended Luenberger and proportional sliding mode observers to highlight its effectiveness and advantages over these observers.

1. Introduction

Estimation of unknown variables in polymerization processes is important for product quality control as well as in avoiding disruption in maintaining this quality [1]. The typical polymerization process is complex with severe nonlinearities, thus applying hardware sensors can be slow in detecting critical parameters and consequently may increase the operating cost [2]. Therefore, software-based observers are developed as alternative sensors since they are cheaper, simple to implement and easy to retune. Researchers have designed several types of observers to predict parameters in polymerization processes such as the monomer concentration, chain length, density, molecular weight distribution (MWD), melt flow index (MFI) and heat transfer coefficient [3]. This development started as early as in 1994 and grew rapidly from the single to the hybrid type observers (including the merging with artificial intelligence (AI) algorithm) [3]. In recent years, artificial intelligence (AI) algorithms have also been applied as estimators to estimate the difficult-to-measure parameters in polymerization processes [4–8].

BenAmor et al. [9] have applied the receeding horizon estimator (RHE) to estimate monomer concentration for methyl methacrylate (MMA) production. Extended Kalman filter (EKF) has also been used to estimate polymer concentration, mass transfer coefficient and specific surface in a reactor producing polyethylene terephthalate (PET) based on the work done by Appelhaus and Engell [10]. In addition, EKF has also been applied in estimating monomer concentration and number of particles per unit volume in a styrene polymerization reactor [11] as well as for predicting melt flow index and density in a polyethylene (PE) production process [12]. In a MMA polymerization reactor, EKF have been applied to estimate several parameters including product conversion, reaction rates, molecular weight distribution (MWD) and heat transfer coefficient based on the work done by Scali et al. [13], Ahn et al. [14], Fan and Alpay [15], Semino and Moretta [16] as well as Crowley and Choi [17] respectively. Besides that, Vasanthi et al. have used the unscented Kalman filter (UKF) to estimate the reaction heat and heat transfer coefficient in a semi-batch polymerization reactor [18] while Jacob and Ramdhane have utilized the UKF to approximate disturbances in a low-density polyethylene (LDPE) process [19]. In addition, the moving horizon estimator has also be applied in the LDPE process to estimate the efficiencies of the initiators and heat transfer coefficient in order to track fouling in the process [20].

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Nomenclature

M_1	Ethylene
M_3	Hydrogen
a_c	Active site concentration
B_t	Bleed flow rate
C_{M_2}	Butene concentration
C_{M_4}	Nitrogen concentration
Cp_{M_2}	Butene heat capacity
Cp_{M_4}	Nitrogen heat capacity
Cp_p	Polymer heat capacity
F_c	Catalyst flow rate
F_g	Recycle gas flow rate
F_{M_2}	Butene flow rate
F_{M_4}	Nitrogen flow rate
M_{w_1}	Molecular weight of ethylene
x_{M_1}	Mole fraction of ethylene
x_{M_3}	Mole fraction of hydrogen
er	Process error
e_f	Error output from fuzzy logic
k_{p1}	Ethylene propagation rate constant
M_g	Eater holdup in heat exchanger
R_{M_1}	gas constant (depends on k_{p1})
R	Ideal gas constant
T_f	Feed temperature
T_{gin}	Recycle stream temperature before cooling
HF	Sensible heat of fresh feed
HT_r	Sensible heat of bed
HR	Enthalpy generated from the polymerization
MI	Melt index
T_{win}	Cooling water temperature before cooling
Y_c	Number of moles of catalyst site
E	Activation energy for propagation
U	Overall heat transfer coefficient
r	Tuneable parameter
x	State variable
y	Measured variables
B	State space matrix
A_m	Augmented state space matrix
C_m	Augmented state space matrix
x_m	Initial assumed value
$\hat{x}_{m_f}$	Estimated value using fuzzy-SMO
NV	Negative
PV	Positive
M_2	Butene
M_4	Nitrogen
B_w	Polymer mass in bed
C_{M_1}	Ethylene concentration
C_{M_3}	Hydrogen concentration
Cp_{M_1}	Ethylene heat capacity
Cp_{M_3}	Hydrogen heat capacity
Cp_g	Recycle gas heat capacity
Cp_w	Water heat capacity
F_w	Cooling water flow rate
F_{M_1}	Ethylene flow rate
F_{M_3}	Hydrogen flow rate
O_p	Polymer outlet rate
M_{w_2}	Molecular weight of butene
x_{M_2}	Mole fraction of butene
x_{M_4}	Mole fraction of nitrogen
Δer	Change of process error
k_d	Deactivation rate constant
k_{p2}	Butene propagation rate constant
k_{p2}	Thermal capacitance of reaction vessel
R_{M_2}	gas constant (depends on k_{p2})
T_r	Bed temperature
T_{ref}	Reference temperature
T_g	Recycle stream temperature after cooling
HG	Sensible heat of recycle gas
HP	Sensible heat of product
$\mathscr{M}$	Characteristics equation for the closed loop poles of the system
P_t	Total pressure
T_{wout}	Cooling water temperature after cooling
ΔH_r	Heat of reaction
V_g	Reactor volume
A	Heat transfer area
k	Constant parameter
u	Input variable
A	State space matrix
C	State space matrix
B_m	Augmented state space matrix
K_{ob}	Observer gain
$\hat{x}_m$	Estimated value
x_p	Actual plant value
ZV	Zero
n	State space order number

Other applications of single observers for estimating parameters in polymerization reactors can be found in several more references [21–30].[1]

Recently to improve the performance of the estimators, hybrid observers [31–39] have been introduced. First, these single observers have been combined with each other where Aguilar-Lopez et al. have combined sliding mode observer (SMO) with a proportional observer to improve the robustness against noise and model uncertainties [40] while Sheibat-Othman et al. have designed a continuous-adaptive observer and high gain continuous-discrete observer for estimating the radical concentration and termination rate coefficient accordingly [38]. Another example of hybrid observer is from the research by Tatiraju et al. [41] where they used the reduced order-Luenberger observer for detecting the initiator concentration and MWD in a polystyrene production process. Then, single observers have been combined with AI algorithms to overcome problems such as offsets and to increase convergence rate [42–45]. Additionally, hybrid neural network (HNN) has been applied to estimate the monomer concentration in a methyl methacrylate (MMA) production process [43] and semi-batch polymerization reactor for producing multi-polymers [45]. Both resulted in accurate and fast convergence rate of the estimations. The conventional observers have also been combined with AI techniques such as the extended Kalman filter with an artificial neural network (EKF-ANN) for estimating the chain length for MMA production [3].

Besides that, AI algorithms have also been used as estimators since their formulation is simpler with higher accuracy and provides faster estimation rate [46]. ANN has been the most popular AI estimator in polymerization processes [4–8]. It has been used in

[1] We refer the readers to [28] D. Dochain, State and parameter estimation in chemical and biochemical processes: a tutorial, Journal of Process Control, 13 (2003) 801–818. [29] C. Kravaris, J. Hahn, Y. Chu, Advances and selected recent developments in state and parameter estimation, Computers & Chemical Engineering, (2012). [30] J. Mohd Ali, N. Ha Hoang, M.A. Hussain, D. Dochain, Review and classification of recent observers applied in chemical process systems, ibid.76 (2015) 27–41. for a comprehensive survey of different types of recent observers in chemical process systems.

estimating the monomer concentration [47] in a styrene polymerization reactor with satisfactory results based only on the operating data. Fuzzy logic, on the other hand, has been applied in predicting the melt flow index in a low-density polyethylene (LDPE) production process [48] and energy efficiencies in a furnace [49].

In this work, we propose a novel hybrid observer that combines the SMO with fuzzy logic for estimating the unknown parameters in a polymerization reactor. SMO is chosen since it provides fast and accurate estimation and suitable for complex nonlinear system without requires further assumptions for the design. On the other hand, fuzzy logic is selected because it is a simple algorithm compared to other algorithms such as neural network and genetic algorithm when combined with the SMO in the hybrid design framework.

Fuzzy logic is simple in comparison with neural network (NN) since it has fuzzy rules that are easy to be manipulated without changing the fuzzy framework parameters including the membership function and defuzzification types to obtain best results whereas if NN is used, all the training steps need to be repeated in order to find the best results and the network may also require changes. Besides that, if GA is coupled with the SMO, all the reproduction, crossover and mutation steps are also needed to be redefined to obtain the best generation (output) especially since it depends on the random number of first generation [50].

The purpose of the hybrid observer is to overcome the limitations showed by the single sliding mode observer to handle situations when there is modeling error and mismatches. The proposed fuzzy-SMO observer will reduce the estimation time, eliminate offsets and provides a simple and systematic approach in the design since the estimation error could be reduced by applying the fuzzy rules. The inputs to the fuzzy logic framework are the estimation error and the change of error from the estimation results obtained from the single SMO.

It is worth noting that combining SMO with other types of observers such as the proportional observer, called the proportional-SMO may be tedious as the overall dynamics must be considered to cater for the estimation of specific parameters [40]. Besides that, the proposed hybrid observer is designed in such a way that it can estimate several parameters without redesigning the structure of the whole observer. Whereas, many available observers in the literature considered the dynamics of the process model once again and redesigned the whole observer if it requires to be applied for another estimation purpose even in the same process [30]. This is one of the major contributions and novelty of this hybrid observer and makes it different from the other observers available in the literature [30]. The performances of the proposed fuzzy-SMO are shown through simulation studies in estimating ethylene concentration, butene concentration and melt flow index in the polymerization reactor.

This paper is organized as follows. Section 2 discusses on the well-mixed single-phase ethylene polymerization process while Section 3 introduces the hybrid fuzzy-SMO with its general formulation. Later, in Section 4 the effectiveness of the proposed observer is illustrated based on ethylene concentration, butene concentration, and melt flow index (MFI) estimations. Comparisons with the single SMO, extended Luenberger observer (ELO) and proportional SMO are also simulated to show the advantages and efficacy of the approach. Future work and conclusions are given in Section 5.

2. Polymerization process

2.1. Process description

The polymerization process applied here is based on the well-mixed UNIPOL model for the polymerization process developed by McAuley [51,52]. The reactor used for producing polyethylene is illustrated in Fig. 1. The feed gas is merged with the recycled gas and enters the fluidized bed reactor with four major components namely the monomer (ethylene), co-monomer (butene), hydrogen (H_2) and nitrogen (N_2). These gases act as the fluidization agents, heat transfer media and supply reactants for the growing particles in the reactor. Besides that, N_2 is used to transport the catalyst powder and maintain the column pressure at its desired value. Ziegler-Natta catalyst is fed continuously into the reactor and the products are withdrawn at a certain rate while the bed height is held constant. The process models used for modeling and developing the proposed hybrid observer for the estimation are given in Section 2.2.

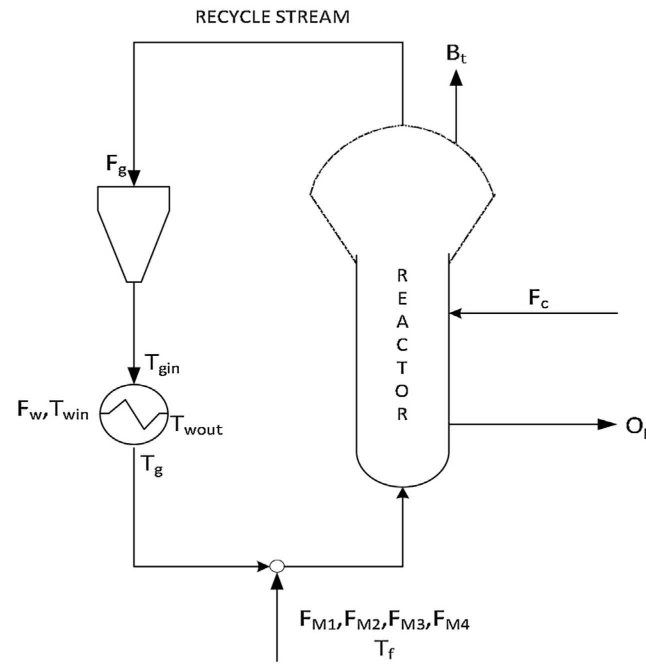


Fig. 1. Ethylene polymerization reactor.

2.2. Process model for parameter estimations

By taking M_1 as ethylene, M_2 as butene, M_3 as hydrogen and M_4 as nitrogen, the mole balances are given by [53]:

$$V_g \frac{dC_{M_1}}{dt} = F_{M_1} - x_{M_1} B_t - R_{M_1} \tag{2.1}$$

$$V_g \frac{dC_{M_2}}{dt} = F_{M_2} - x_{M_2} B_t - R_{M_2} \tag{2.2}$$

$$V_g \frac{dC_{M_3}}{dt} = F_{M_3} - x_{M_3} B_t - R \tag{2.3}$$

$$V_g \frac{dC_{M_4}}{dt} = F_{M_4} - x_{M_4} B_t \tag{2.4}$$

$$\text{With} R_{M_1} = C_{M_1} Y_c k_{p1} e^{\frac{E}{R}(1/T_r - 1/T_{ref})} \tag{2.5}$$

$$R_{M_2} = C_{M_2} Y_c k_{p2} e^{\frac{E}{R}(1/T_r - 1/T_{ref})} \tag{2.6}$$

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 [53]:

$$\frac{dY_c}{dt} = F_c a_c - k_d Y_c - O_p Y_c / B_w \quad (2.7)$$

$$\text{With} O_p = M_{w_1} R_{M_1} + M_{w_2} R_{M_2} \quad (2.8)$$

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 [53]:

$$(M_r Cp_r + B_w Cp_p)\frac{dT_r}{dt} = HF + HG - HR - HT_r - HP \quad (2.9)$$

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

$$M_g Cp_w \frac{dT_g}{dt} = F_g Cp_g (T_{gin} - T_g) + F_w Cp_w (T_{win} - T_{wout}) \quad (2.10)$$

$$\text{Where} HF = F_{M_1} Cp_{M_1} + F_{M_2} Cp_{M_2} + F_{M_3} Cp_{M_3} + F_{M_4} Cp_{M_4} \quad (2.11)$$

$$HG = F_g Cp_g (T_g - T_{ref}) \quad (2.12)$$

$$HT_r = (F_g + B_t) Cp_g (T_r - T_{ref}) \quad (2.13)$$

$$HP = O_p Cp_p (T_r - T_{ref}) \quad (2.14)$$

$$HR = M_{w_1} R_{M_1} \Delta H_r \quad (2.15)$$

The total pressure of the reactor is given by [53]:

$$P_t = (C_{M_1} + C_{M_2} + C_{M_3} + C_{M_4}) R T_r \quad (2.16)$$

And the relation of cooling water with the temperature is given by [53]:

$$F_w Cp_w (T_{win} - T_{wout}) = 0.5 UA[(T_{wout} + T_{win}) - (T_{gin} + T_g)] \quad (2.17)$$

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. (2.18) below [54]:

$$\frac{dMI}{dt} = [rk(\frac{C_{M_3}}{C_{M_1}}) - MI]/0.9 \quad (2.18)$$

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 [54]. All the equations are used for the modelling of the reactor to generate the actual plant value as well as the state space representation for calculating the observer's gain and designing the observer's equation. The details of the methodology will be explained in Section 3.

3. Methodology of hybrid fuzzy-sliding mode observer (fuzzy-SMO)

In this paper, we propose a hybrid observer called fuzzy-sliding mode observer (fuzzy-SMO) that combines sliding mode observer with fuzzy logic to estimate the ethylene and butene concentrations as well as the melt flow index (MFI). SMO is chosen because it offers fast convergence and stable estimation while having the ability to generate the sliding motion or signal on the measured error and the output error. This will ensure the estimated values are in good agreement with the actual values [55,56]. On the other hand, fuzzy logic is an artificial intelligence element [57,58] with simple computational method that simplify the design of the proposed hybrid observer but yet give high accuracy and fast convergence rate. The process model discussed in the previous section will be used to develop the hybrid fuzzy-SMO.

The design methodology is depicted in Fig. 2. Based on the figure, the observer design starts by identifying the observability conditions of the system 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 [30]. In this work, we have initially developed a single SMO and the performances are evaluated based on the estimation of the parameters namely ethylene, butene concentrations and melt index in the polymerization process. However, due to the unsatisfactory preliminary results obtained especially in handling noisy conditions, we have combined SMO with fuzzy logic. The proposed hybrid fuzzy-SMO has been able to improve the estimation for both situations including noise and without noise.

For the formulation development, first let us consider a general system [59,60]:

$$\dot{x} = Ax + Bu \quad (3.1)$$

$$y = Cx \quad (3.2)$$

Now, after defining the state variables or the states we intend to estimate, which are the ethylene concentration, C_{M1}, butene concentration, C_{M2} and melt flow index, MI, we identify the input variables that are the process inputs namely 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). The measured variable is the bed/reactor temperature, T_r.

Then the observer is formulated by using the state space equation first to obtain the model [61] in the form of matrix A–C to be applied in Eqs. (3.1) and (3.2). The state space model is estimated using the linear parametric models option by first dividing the input signal data into two parts for estimation and validation. The model can be generated accurately if both data are matched. Altogether 100 data are generated from running the polymerization model explained in Section 2. These data will be used for the estimation and validation of the state space model. Final state space model to be applied is determined by the best-fitted value that is the highest percentage based on the model output obtained. Best-fit value defined the balance between robustness and accuracy. The parameters of this state space are taken as the plant model and the overall observer design procedure will start from this plant model.

However, before developing the observer, the observability condition is examined to ensure the system is observable. It must have unique solution provided the system matrix has rank n (order of

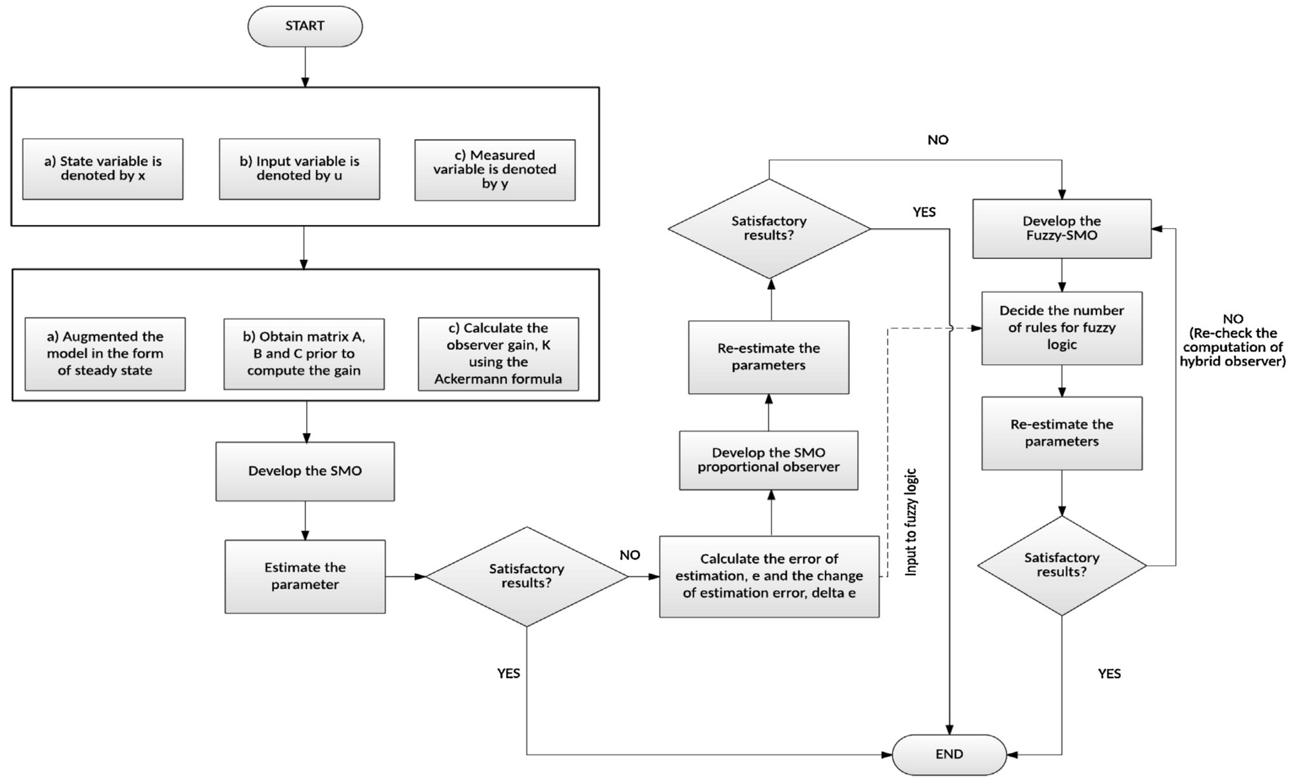


Fig. 2. The methodology of the hybrid observer design.

the system) [30].

$$rank \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \end{bmatrix} \text{ for } n = 4 \text{ in this case according to the state space order number} \quad (3.3)$$

Therefore, observability matrix, $\mathcal{O}$ must has rank n (rank $\mathcal{O} = n$) for the system to be observable.

$$\mathcal{O}(A, C) = \begin{bmatrix} C \\ CA \\ CA^2 \\ CA^3 \end{bmatrix}^{(np)\times n} \quad \text{has rank } n = 4 \quad (3.4)$$

Let us define the augmented state space model in the form of matrix A_m, B_m and C_m which are different from the original state space model matrix A–C above. The augmented model, however do not change the underlying algorithm conceptually and the properties of the original state space matrix A–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 normally assumed that disturbances are noise with zero mean, which is not reliable for many practical applications. In addition, augmented models can provide simpler method for adjusting the disturbance and noise that acts 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 system parameters [61]. Note also that the selection of the sliding mode observer design will be determine by the uncertainty distribution of the matrix A_m–C_m, which is capable of rejecting the uncertainty hidden in the system inputs [55]. Thus, in this case the existence condition lies within the properties of the matrix A_m–C_m.

The augmented model applied for estimating the states and use in the SMO design is defined as:

$$\dot{\hat{x}}_m = A_m x_m + B_m u + K_{ob} sign(y - C_m x_m) \quad (3.5)$$

Where K_{ob} is the observer gain and is calculated based on the pole location using the formula given in Eq. (3.6) and *sign* is understood componentwise [59] for vector argument $z = col(z_1, \ldots, z_n)$ and $sign(z) = col(sign(z_1), \ldots, sign(z_n))$.

$$K_{ob} = place(A_m, C_m, \mathcal{M}) \quad (3.6)$$

Where $\mathcal{M}$ is the characteristics equation for the closed loop poles of the system that is the desired location for the error dynamics.

The x_m value is initially assumed with any values since SMO will help to recalculate the estimated values until the desired truth-values have been 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.

$$er(t) = x_p(t) - \hat{x}_m(t) \quad (3.7)$$

The set of values of *er* and the change of error, Δer are used as the inputs for the fuzzy logic framework.

The fuzzy framework will first involve the fuzzification step which will change the input into the fuzzy sets. Then, the fuzzy inference mechanism will be developed using the Mamdani inference system and consists of two Gaussians membership functions for the input and 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 Table 1. Four rules have been tested before deciding the best rule to be applied in the fuzzy framework. We named the four different rules as Rule

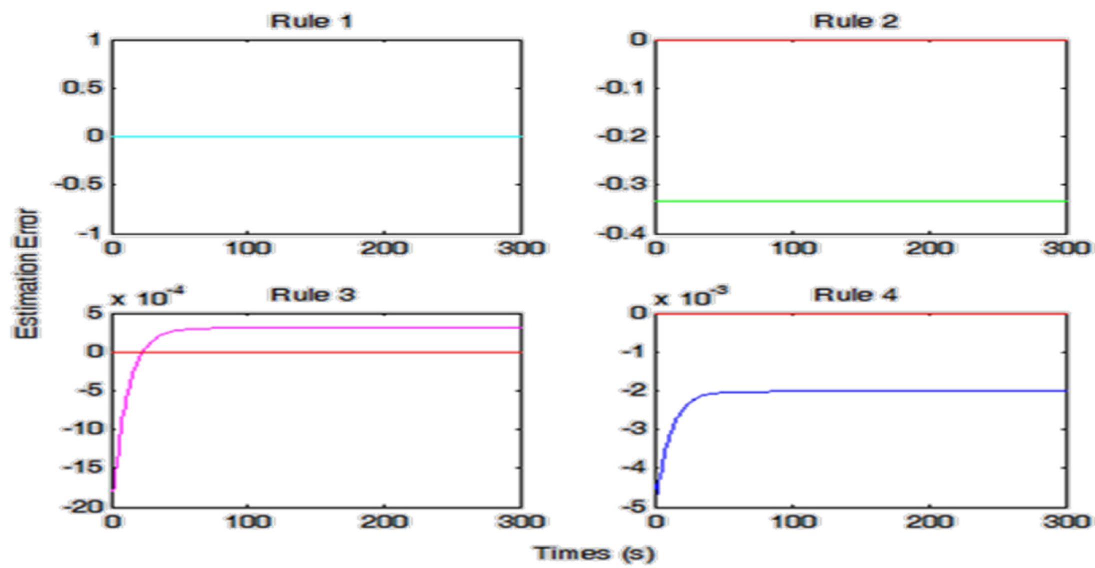


Fig. 3. Comparisons of output for different fuzzy rules.

Table 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

1–Rule 4. Each rule consists of different antecedents and consequences. Rule 1, which contains 9 antecedents and 9 consequences has been selected as the best rules based on the fastest response with closest to zero error shown [62,63].

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.

$$\begin{aligned}
&IF\ (er\ is\ NV)\ AND\ (\Delta er\ is\ NV)\ THEN\ (the\ output\ is\ PV)\\
&IF\ (er\ is\ NV)\ AND\ (\Delta er\ is\ ZV)\ THEN\ (the\ output\ is\ ZV)\\
&IF\ (er\ is\ NV)\ AND\ (\Delta er\ is\ PV)\ THEN\ (the\ output\ is\ NV)\\
&IF\ (er\ is\ ZV)\ AND\ (\Delta er\ is\ NV)\ THEN\ (the\ out\ put\ is\ ZV)\\
&IF\ (er\ is\ ZV)\ AND\ (\Delta er\ is\ ZV)\ THEN\ (the\ out\ put\ is\ ZV)\\
&IF\ (er\ is\ ZV)\ AND\ (\Delta er\ is\ PV)\ THEN\ (the\ output\ is\ ZV)\\
&IF\ (er\ is\ PV)\ AND\ (\Delta er\ is\ NV)\ THEN\ (the\ output\ is\ NV)\\
&IF\ (er\ is\ PV)\ AND\ (\Delta er\ is\ ZV)\ THEN\ (the\ output\ is\ ZV)\\
&IF\ (er\ is\ PV)\ AND\ (\Delta er\ is\ PV)\ THEN\ (the\ output\ is\ PV)
\end{aligned} \tag{3.8}$$

Other rule 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 given in Fig. 3 when implemented in the hybrid observer formulation. Rule 1 has provided the most accurate output as desired while the other three rules resulted with some errors.

After the rules have been decided, the defuzzification step will be performed to convert the chosen fuzzy set into the real data or value. Defuzzification used here is the centroid method using the center of gravity approach to obtain the best crisp value to be applied to the process.

Then the hybrid fuzzy-SMO for estimating the parameters is given in Eq. (3.9) where e_f is the output from fuzzy logic based on the rules in Table 1.

$$\hat{x}_{m_f} = A_m x_m + B_m u + K_{ob} sign(e_f) \tag{3.9}$$

where $\hat{x}_{m_f}$ is 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. (3.5) we formed Eq. (3.10) for the single SMO.

$$\begin{bmatrix}\hat{x}_{m_1}\\ \hat{x}_{m_2}\\ \hat{x}_{m_3}\end{bmatrix} = A_m\begin{bmatrix}x_{m_1}\\ x_{m_2}\\ x_{m_3}\end{bmatrix} + B_m\begin{bmatrix}u\\ u\end{bmatrix} + \begin{bmatrix}K_{ob11} & K_{ob12} & K_{ob13}\\ K_{ob21} & K_{ob22} & K_{ob23}\\ K_{ob31} & K_{ob32} & K_{ob33}\end{bmatrix} sign\left(\begin{bmatrix}y\\ y\end{bmatrix} - C_m\begin{bmatrix}x_{m_1}\\ x_{m_2}\\ x_{m_3}\end{bmatrix}\right) \tag{3.10}$$

Here, subscript 1–3 represent ethylene, butene concentration and melt index respectively. We have chosen to estimate those parameters that show the effectiveness of the hybrid observer in estimating a difficult-to-measure parameter (MFI) and less difficult-to-measure parameter (ethylene) where the related process model is adapted to the observer's structure. The MFI is difficult to measure when there are variations of temperature thus the accurate value of MFI must be obtained for higher product quality while the unreacted ethylene concentration in the reactor is important to predict the amount of recycle ethylene for getting the accurate overall conversion. As for butene, it is estimated to show the uniqueness of the hybrid observer design that allow other parameter estimation using the same observer structure. For the fuzzy-SMO, we define Eq. (3.11) from Eq. (3.9) as follows:

$$\begin{bmatrix}\hat{x}_{m_{f_1}}\\ \hat{x}_{m_{f_2}}\\ \hat{x}_{m_{f_3}}\end{bmatrix} = A_m\begin{bmatrix}x_{m_1}\\ x_{m_2}\\ x_{m_3}\end{bmatrix} + B_m\begin{bmatrix}u\\ u\end{bmatrix} + \begin{bmatrix}K_{ob11} & K_{ob12} & K_{ob13}\\ K_{ob21} & K_{ob22} & K_{ob23}\\ K_{ob31} & K_{ob32} & K_{ob33}\end{bmatrix} sign\left(\begin{bmatrix}e_{f1}\\ e_{f2}\\ e_{f3}\end{bmatrix}\right) \tag{3.11}$$

Besides that, to imitate the real situation, noise and disturbance are also added to the model. The noise incorporated is a 5% Gaussian

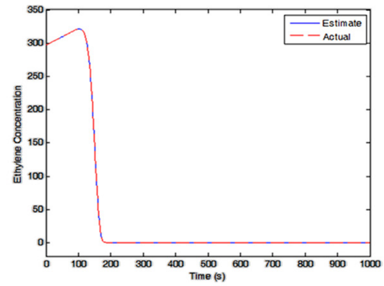
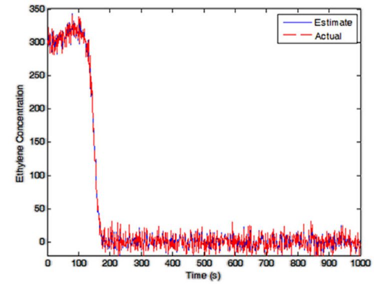
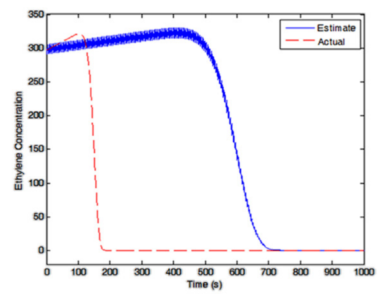
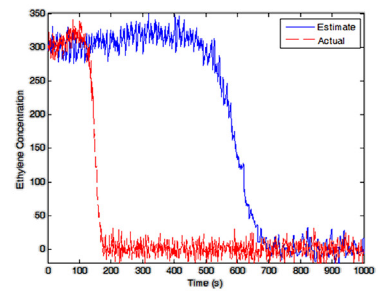
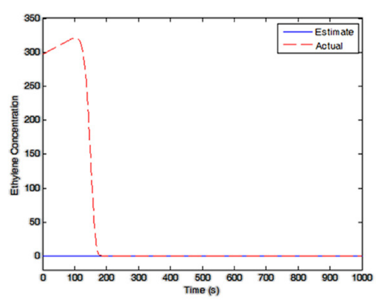
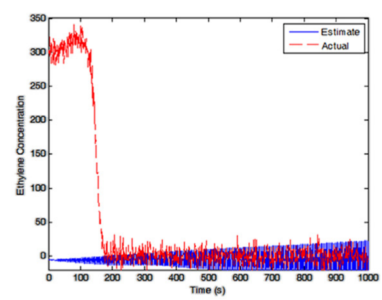
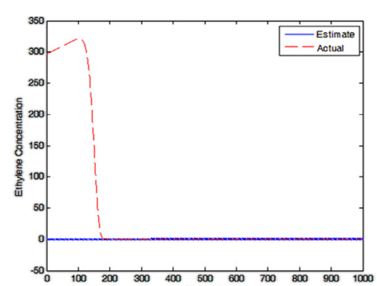
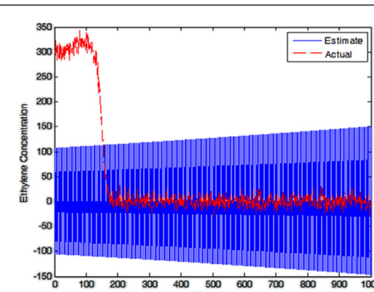
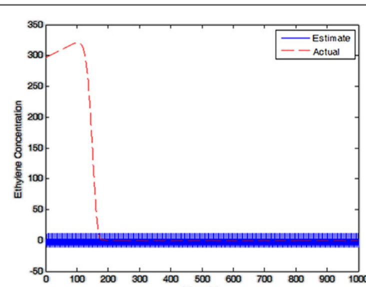
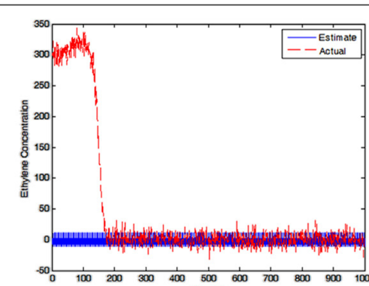
Type of observer	Condition without noise	Condition with noise
a) Fuzzy-SMO		
b) SMO		
c) Fuzzy Logic		
d) SMO-Proportional		
e) ELO		

Fig. 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.

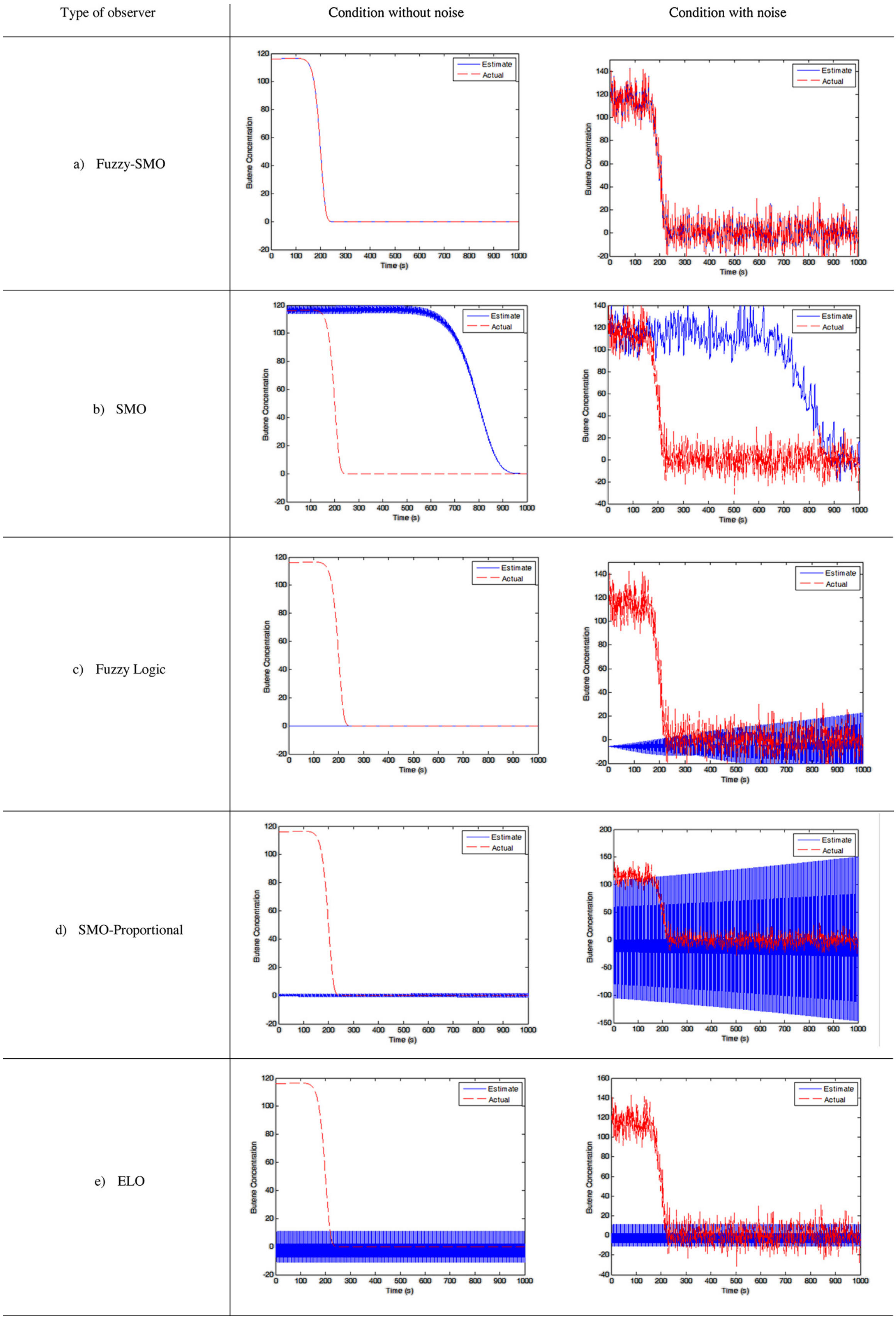


Fig. 5. Butene concentration estimation using various observers namely (a) Fuzzy-SMO, (b) SMO, (c) Fuzzy logic, (d) SMO-proportional and (e) ELO for both conditions with and without noise in the process.

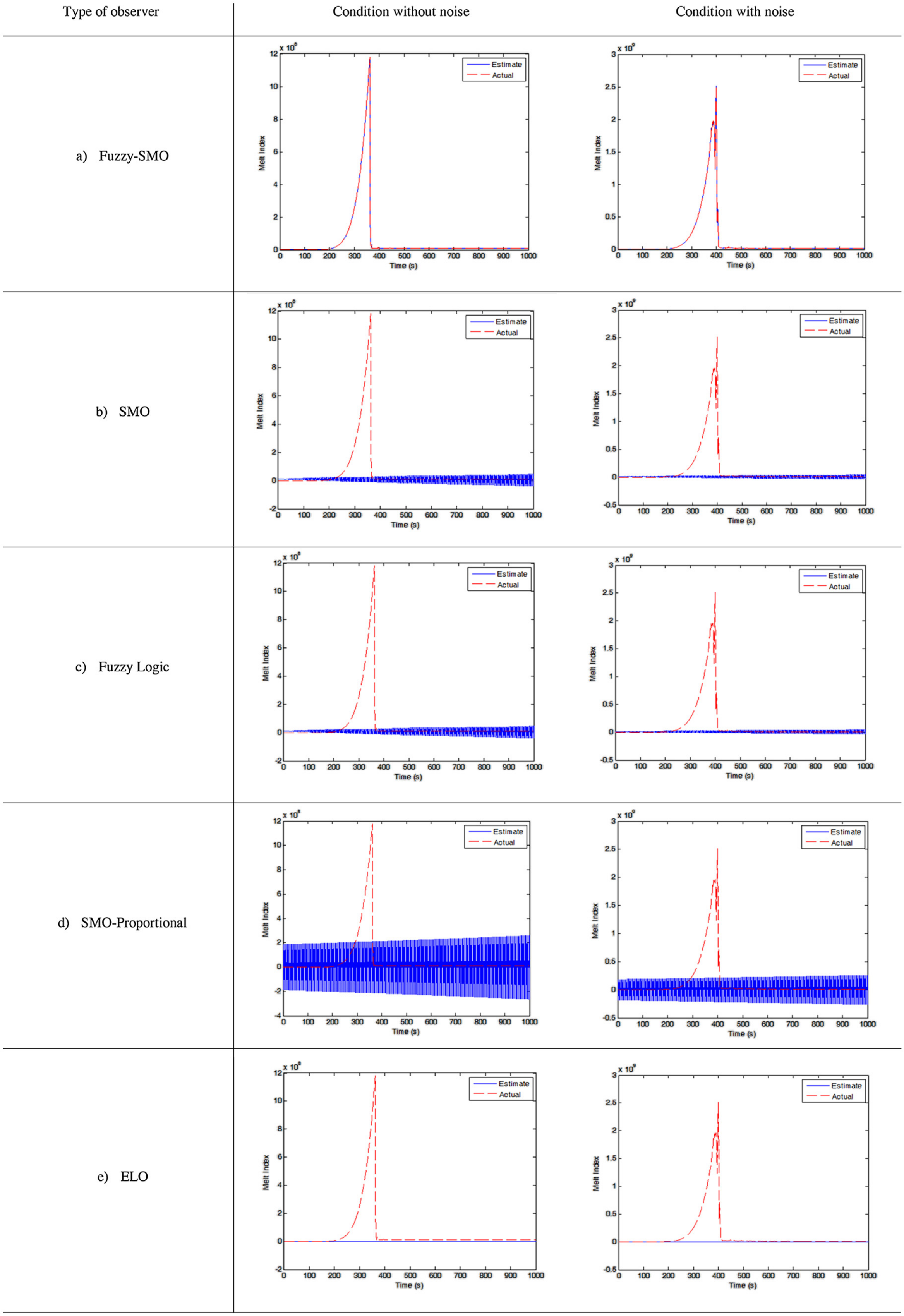


Fig. 6. Melt index estimation using various observers namely (a) Fuzzy-SMO, (b) SMO, (c) Fuzzy logic, (d) SMO-proportional and (e) ELO for both conditions with and without noise in the process.

Table 2
Parameters and variables for the polymerization reactor.

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

noise variation in the polymerization plant model to illustrate the effectiveness of the proposed approach.

4. Simulation results

The process is first run in simulation using the initial condition as given in Table 2 [53] 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 that has been discussed in Section 3 will be applied to estimate the parameters and compared with the actual value. To do this, we simulated Eq. (3.5) first and calculated the error and change of error for the single SMO, which will show the discrepancies between both the actual and the estimated value. Then, we combined the single SMO with fuzzy logic using the error and changed of error as inputs to the fuzzy framework where the rule is defined in Table 1. After that, we simulated using Eq. (3.9) for our system, which is the proposed hybrid observer formulation and compared the result with the single SMO, fuzzy logic, extended Luenberger observer (ELO) and SMO-proportional observers to highlight the advantages of the proposed observer over the other observers. Later, to highlight on a major advantage of this method, which allow several parameters to be estimated without changing the structure of the observer, we applied the hybrid observer using Eq. (3.11).

Based on Fig. 4, better estimation performances were found when the hybrid fuzzy-SMO was applied. It reacted fast towards the actual value to provide accurate estimation under both conditions of with and without noise for estimating the ethylene concentrations. In addition, there were no oscillations or offsets found during the estimation, thus giving smooth and accurate estimations. In terms of 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 a particular time, which is a priori unpredictable.

The SMO was only 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 s onwards. However, this was not the case once noise has been added. It resulted in oscillations and was unable to estimate the ethylene concentration even after running the simulation for 1000 s. Similar conditions were observed when fuzzy logic and SMO-proportional were used. Fuzzy logic was able to estimate the concentration when noise was not included in the process but gave oscillations during noisy conditions. As for SMO-proportional, the oscillations were very high and deviated far from the actual values when noise were added. On the other hand, ELO was unable to estimate the ethylene concentration for both conditions where oscillations were observed.

The results of butene concentration estimation are illustrated in Fig. 5. The proposed hybrid fuzzy-SMO provided better estimation performances compared to the other observers. Only fuzzy-SMO has been able to estimate the butene concentration for both with and without noise conditions. It showed 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 but the estimated values gave oscillations and deviated from the actual value once noise was added. This proved that these single observer designs were unable to handle noise satisfactorily for the ethylene polymerization process. However, the SMO-proportional and ELO were not able to estimate the butene concentration under all conditions where the SMO-proportional has gave small oscillations for the case without noise and high oscillations from the noisy condition. When the ELO was applied, severe oscillation patterns were observed for both cases.

As shown in Fig. 6, in estimating the melt flow index, fuzzy-SMO was again the best observer that was able to provide good estimation performances regardless of any condition in the ethylene polymerization process. The other observers, did not perform well and were unable to estimate the melt index. The SMO, fuzzy logic and SMO-proportional provided oscillations during the estimation with SMO-proportional giving the worst oscillation patterns and large offsets were observed when ELO was used as the observer.

In general, for all the parameters estimated, the hybrid fuzzy-SMO showed the best results even under noisy conditions. There were no discrepancies between the actual and the estimated values when the hybrid fuzzy-SMO was 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. The single SMO, fuzzy logic and SMO-proportional can only be applied as estimator when noise was not present whereas ELO is not suitable to be implemented in the ethylene polymerization process since it failed to estimate all the parameters. Hence these observers are not suitable in the real processes, which always contain a variety of disturbance and noise. Therefore, the proposed hybrid fuzzy-SMO has been found to be the best to implement in the ethylene polymerization process even under noise and disturbance effects in the process. Furthermore, it is able to estimate several parameters without major adjustment in the structure of the observer, which is a major advantage of this approach.

5. Conclusion and future work

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.

As for the future work, other critical polymerization parameters such as chain length, molecular weight distribution (MWD) and heat transfer coefficient will be estimated using the proposed hybrid fuzzy-SMO. The estimated parameters will then be used to develop a controller based on model predictive control strategy to regulate the polymerization reactor temperature and hydrogen concentration since it will has bigger influence on the melt flow index that determines the quality of the polyethylene. Furthermore, the online testing in the pilot plant will also be carried out to observe the performance for both the estimator and controller.

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