Hybrid estimation technique for predicting butene concentration in polyethylene reactor

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Abstract. A component of artificial intelligence (AI), which is fuzzy logic, is combined with the so-called conventional sliding mode observer (SMO) to establish a hybrid type estimator to predict the butene concentration in the polyethylene production reactor. Butene or co-monomer concentration is another significant parameter in the polymerization process since it will affect the molecular weight distribution of the polymer produced. The hybrid estimator offers straightforward formulation of SMO and its combination with the fuzzy logic rules. The error resulted from the SMO estimation will be manipulated using the fuzzy rules to enhance the performance, thus improved on the convergence rate. This hybrid estimation is able to estimate the butene concentration satisfactorily despite the present of noise in the process.

1. Introduction
Butene or co-monomer concentration is also another favorable parameter besides monomer concentration in polymerization process since it tends to affect the molecular weight distribution (MWD) of the polymer produced. The lower the distribution of the co-monomer the higher the MWD of the polymer [1]. Therefore, it is also crucial to monitor the distribution of this co-monomer. So far, there is no effort in estimating this parameter in the polymerization reactor since many researchers are focusing on the estimation of monomer and other parameters including reaction rate and chain length, which will give higher impact to the process. Concentrations are estimated using estimators prior to implement the control procedure in a polymerization reactor [2] [3, 4] [5] [6] [7].

Estimator will estimate the unknown variables better than the so-called expensive sensors especially in terms of accuracy and estimation time [8]. In certain cases, the conventional estimator will be merged with other estimator to avoid offsets and improved the convergence rate. The combination can be either between two or more conventional estimators or with artificial intelligence (AI). AI has also been applied by several researchers as estimators and in some cases they are better than the conventional estimator and are easier to be formulated [9].

For this work, we combined the conventional sliding mode observer (SMO) with fuzzy logic to estimate the co-monomer concentration in an ethylene polymerization reactor. SMO is and extended
version of extended Luenberger observer that have been proven to provide fast estimation and is also a stable estimator without require any input assumption during the estimation process [10]. On the other hand, fuzzy logic is the simplest algorithm of AI, suitable to be combined with those conventional estimators by manipulating only the IF and THEN rules for enhancing the estimation performances and overcoming the limitations of the single SMO. Fuzzy rules are applied based on the estimation error, and the change of error to obtain desired results faster with minimal efforts.

Introduction is given in this section follow by the ethylene polymerization reactor model in section 2. The hybrid estimator design according to a case study is discussed in section 3 while conclusion is in section 4.

2. Ethylene polymerization reactor model

The ethylene polymerization reactor model for this work is based on the well-mixed UNIPOL model developed by McAuley (1990) [11, 12]. The reactor is illustrated in figure 1 where the feed gas is combined with the recycled gas before entering at the bottom of the fluidized bed reactor. Another input stream is the feed gas containing the Ziegler-Natta catalyst. Butene is one of the four major components entering the reactor. The other components are the monomer (ethylene), hydrogen (H2) and nitrogen (N2). The reactor temperature is controlled by manipulating both the cooling water and the feed temperature.

![Figure 1. Polymerization reactor for producing polyethylene.](image)

The mole balances of the process taking $M_1$ as ethylene, $M_2$ as butene, $M_3$ as hydrogen and $M_4$ as nitrogen are as follow:

\[
V_g \frac{dC_{M_1}}{dt} = F_{M_1} - x_{M_1} B_t - R_{M_1} \tag{1}
\]

\[
V_g \frac{dC_{M_2}}{dt} = F_{M_2} - x_{M_2} B_t - R_{M_2} \tag{2}
\]

\[
V_g \frac{dC_{M_3}}{dt} = F_{M_3} - x_{M_3} B_t - R \tag{3}
\]

\[
V_g \frac{dC_{M_4}}{dt} = F_{M_4} - x_{M_4} B_t \tag{4}
\]

With \[ R_{M_1} = C_{M_1} Y_c k_{p1} \left( \frac{E}{T - 1/T_{ref}} \right) \tag{5} \]
Number of moles at the catalyst site is given by:

\[ R_{M_2} = C_{M_2} Y_c e^{\frac{E}{R_1/T - 1/T_{ref}}} \]  

(6)

With outlet rate as:

\[ \frac{dy_c}{dt} = F_c a_c - k_d Y_c - O_p Y_c / B_w \]  

(7)

The total pressure of the reactor is given by:

\[ P_t = (C_{M_1} + C_{M_2} + C_{M_3} + C_{M_4})RT \]  

(9)

\[ F_w C_{p_w}(T_{wi} - T_{wo}) = 0.5UA\left[(T_{wo} + T_{wi}) - (T_{g} + T_{g})\right] \]  

(10)

Bed temperature and recycle stream temperature are described as follows:

\[ (M_r C_{p_r} + B_w C_{p_r}) \frac{dT}{dt} = HF + HG - HR - HT - HP \]  

(11)

\[ M_g C_{p_g} \frac{dT_g}{dt} = F_g C_{p_g}(T_{g} - T_{g}) + F_w C_{p_w}(T_{wi} - T_{wo}) \]  

(12)

Where

\[ HF = FM_1 C_{p_1} + FM_2 C_{p_2} + FM_3 C_{p_3} + FM_4 C_{p_4} \]  

(13)

\[ HG = F_g C_{p_g}(T_{g} - T_{ref}) \]  

(14)

\[ HT = (F_g + B_t)C_{p_g}(T - T_{ref}) \]  

(15)

\[ HP = O_p C_{p_r}(T - T_{ref}) \]  

(16)

\[ HR = M_{w_1} R_{M_1} \Delta H_r \]  

(17)

The above equations are applied to develop the polymerization model in SIMULINK/MATLAB to obtain the actual value that will be compared with the value from the proposed hybrid estimator. They are also used to develop the estimator’s equation that we will show in section 3.

3. Hybrid estimator design

SMO is first developed and the error of estimation (e) as well as the change of error (Δe) is recorded and being used as the input to the fuzzy logic framework for developing the hybrid fuzzy-SMO estimator. The schematic diagram is given in figure 2.
In order to estimate butene concentration, the SMO equation is given below:

$$\hat{C}_{M_2} = z_2 + K_{11} \text{sgn}(T) + K_{12} \text{sgn}(T_g)$$  \hspace{1cm} (18)

Where $z_2$ is as follow:

$$[z_2] = [a] - [K_{11} \ K_{12}] \begin{bmatrix} f \\ g \end{bmatrix}$$  \hspace{1cm} (19)

Where  
$$a = \frac{1}{V_g} (F_{M_2} - \mathcal{C}_{M_2} B_t - R_{M_2})$$  \hspace{1cm} (20)

$$f = \frac{1}{(M_f C_{P_f} + B_w C_{P_p})} (HF + HG - HR - HT - HP)$$  \hspace{1cm} (21)

$$g = \frac{1}{M_g C_{P_g}} [F_g C_{P_g} (T_{gi} - T_g) + F_w C_{P_w} (T_{wi} - T_{wo})]$$  \hspace{1cm} (22)

Where $a$ is taken from the process model specifically Eq. (2) while $f$ and $g$ represented the measured reactor temperature ($T$) and recycle stream temperature ($T_g$) from Eq. (11) and (12) respectively.

Then the hybrid fuzzy-SMO is designed as given in Eq. (16) where $e_f$ is the output from fuzzy logic. The input of the fuzzy logic is the error ($e$) and the change of error ($\Delta e$) obtained from the estimation results using the single SMO. The fuzzy logic rules are tabulated in Table 1 with $e = \text{error}$, $\Delta e = \text{change of error}$, NS = negative small, NL = negative large, ZO = zero, PS = positive small and PL = positive large.

$$\hat{C}_{M_2} = z_2 + K_{21} \text{sgn}(e_f) + K_{22} \text{sgn}(e_f)$$  \hspace{1cm} (23)

| $e$   | NS | NL | ZO | PS | PL |
|-------|----|----|----|----|----|
| NS    | PL | PL | ZO | ZO | ZO |
| NL    | PL | PL | ZO | ZO | ZO |
| ZO    | PS | PS | ZO | ZO | ZO |
| PS    | ZO | ZO | NS | NL | NL |
| PL    | ZO | ZO | NS | NL | NL |
The results are given in figure 3 and figure 4 based on with and without noise conditions. Based on the figures, we observed that Fuzzy-SMO showed immediate convergence (0s) compared to SMO (20s) and able to estimate accurately despite the noise. Therefore, the proposed hybrid estimator is able to estimate the butene concentration by eliminating the offset and slow estimation time obtained using the single SMO. The hybrid Fuzzy-SMO is also in good agreement with the actual concentration during noisy condition.

This similar observer has been also applied in estimating monomer concentration and melt index with satisfactory results. It is also being compared with hybrid extended Luenberger observer (ELO) and fuzzy logic or Fuzzy-ELO [13, 14].

![Figure 3. Butene concentration estimation (without noise/disturbance)](image)
4. Conclusion
Fuzzy-SMO is the best approached in predicting the butene or co monomer concentration in an ethylene polymerization reactor and able to handle noise as well as provide fast convergence compared to the single SMO. In future, the estimator will be applied to predict several other key features in a polymerization process such as melt index, heat transfer coefficient, molecular weight distribution (MWD) and reaction rate using the hybrid estimator.

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Nomenclature

- $B_t$: Bleed flow rate
- $B_w$: Polymer mass in bed
- $C_{M_2}$: Co-monomer concentration
- $C_{M_1}$: Monomer concentration
- $C_{M_4}$: Nitrogen concentration
- $C_{M_3}$: Hydrogen concentration
- $C_{pM_2}$: Co-monomer heat capacity
- $C_{pM_3}$: Hydrogen heat capacity
- $C_{pM_4}$: Nitrogen heat capacity
- $C_{p_R}$: Recycle gas heat capacity
- $C_{p_p}$: Polymer heat capacity
- $C_{p_r}$: Recycle water heat capacity
- $F_c$: Catalyst flow rate
- $F_w$: Cooling water flow rate
- $F_g$: Recycle gas flow rate
- $F_{M_1}$: Monomer flow rate
- $F_{M_2}$: Co-monomer flow rate
- $F_{M_3}$: Hydrogen flow rate
- $F_{M_4}$: Nitrogen flow rate
- $O_p$: Polymer outlet rate
- $e$: Process error
- $\Delta e$: Change of process error
- $k_d$: Deactivation rate constant
- $k_{p_1}$: Monomer propagation rate constant
- $k_{p_2}$: Co-monomer propagation rate constant
- $M_rC_{p_r}$: Thermal capacitance of reaction vessel
- $P_t$: Total pressure
- $T$: Bed temperature
- $T_f$: Feed temperature
- $T_{wo}$: Cooling water temperature after cooling
- $T_g$: Recycle stream temperature after cooling
- $P_{M_1}$: Monomer partial pressure
\[ P_{M2} \] Co-monomer partial pressure
\[ P_{M3} \] Hydrogen partial pressure
\[ P_{M4} \] Nitrogen partial pressure
\[ T_{wi} \] Cooling water temperature before cooling
\[ T_{ref} \] Reference temperature
\[ T_{gi} \] Recycle stream temperature before cooling

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