Temperature control of low density polyethylene (LDPE) tubular reactor using Model Predictive Control (MPC)

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Abstract. Application of advanced process control has become demanding in order to save energy and reduce operating cost, while attaining excellent controllability of the process. This situation can be achieved via better controller action performance compared to conventional control scheme such as PID controller. Model Predictive Control (MPC) has a wide application in the industry due to its ability to handle multivariable control and optimized process performance. In this study, a linear based MPC was implemented to control Low Density Polyethylene (LDPE) tubular reactor temperature. The control of LDPE tubular reactor is challenging due to the complexity of the polymerization process and the nature of the reactor itself. The steady state polymerization reactor model was simulated using Aspen Plus software. The validated steady state reactor model was then exported to Aspen Dynamic software for dynamic simulation. In order to implement online control of the process, the dynamic model was linked with Matlab Simulink environment. The linear model of the process was estimated using State-space model identification technique. Sequential Quadratic programming (SQP) method was adopted by the MPC to calculate the controller action. The performance of MPC was compared to a PID controller. Based on the results, MPC had overcome PID performance in set point tracking and disturbance rejection test despite its low accuracy process model. The linear model low accuracy drawback was compensated by proper tuning of the MPC. In overall, MPC had demonstrated its capability to control the process with optimized control action, which can lead to production cost saving in the long run.

1. Introduction
One of the well-known commodity polymers in the industry is Low density polyethylene (LDPE) [1]. LDPE is widely used in packaging, adhesives, coatings, and films. LDPE is mainly produced through free radical polymerization of ethylene gas using tubular or autoclave reactor in high temperature and pressure environment. LDPE polymerization process is known to exhibit dynamic nonlinear behaviors [2, 3]. Nonlinear behavior such as multiple steady state, parametric sensitivity, thermal runaway, and autonomous oscillation are usually associated with exothermic polymerization process (e.g., LDPE) especially in continuous stirred tank reactor [4]. Furthermore, heat from the polymerization process needs to be regulated appropriately to maintain stable and safe reactor operations. Reactor temperature distribution was also reported able to affect polymer quality parameters such as density and molecular weight [5]. These quality attributes need to be closely monitored as they will eventually influence the polymer end-use properties.
such as melt flow index and gloss index [6]. Thus, a control scheme that can properly control the reactor temperature is needed.

Conventionally, Proportional Integral Derivative (PID) controller had been applied to control the reactor temperature. Although the controller had widely accepted by the industry due to its straightforward application, the controller still needs some improvement in term of optimal process output tracking and minimizing the controller action. Application of adaptive control such pole placement technique has been reported to show better servo control performance with less overshoot and abrupt changes than PID [7]. Apart from that, advanced process control such as Model predictive control (MPC), has been gaining popularity in the industry [8]. MPC is known for its capability in handling constrained multivariable control problems optimally. MPC has been tested in controlling industrial autoclave LDPE reactor temperature [9]. In their study, the controller has managed to improve the performance of previous PI controller with shorter settling time and smaller overshoot in set point tracking. However, the controller had performed a bit worse than PI controller in rejecting disturbance at feed temperature. In a combination of set point tracking and disturbance rejection test, MPC again displayed superior performance than PI controller. Moreover, MPC with adaptive capability has also been used to control the polymer quality properties along with the reactor temperature in LDPE tubular reactor [10]. In their study, MPC had outperformed PID in both SISO and MIMO cases. Most of the MPC reported in the literature was based on first principle modeling (FPM) [11]. Although, FPM has the advantage of accurate process representation, the development effort, cost and time are high. Thus, application of chemical process simulator such as Aspen Plus, ProSIM and gPROMS can facilitate this by providing an extensive framework for the rigorous model development. These models can be developed with less time and complexity and can be further used for control or optimization study.

In this study, linear based MPC was developed to control industrial LDPE tubular reactor model. The tubular reactor model was simulated using Aspen Dynamic linked with MPC controller inside the Matlab Simulink platform. This setup provides an online MPC control scheme of the dynamic tubular reactor model. A linear model of the process was estimated using State-space model identification technique. The linear model was used as MPC process model. Sequential Quadratic programming (SQP) method was used as the MPC optimizer. This paper is arranged as follows; First, the reactor steady state and dynamic modeling work are detailed out. Second, the model identification technique and controller development are briefly explained. Third, the results of the reactor sensitivity analysis, linear model identification, and MPC performance tests are presented and discussed. Finally, some conclusions and future study are proposed at the end of the paper.

2. Reactor modeling

2.1. Tubular reactor

The reactor considered in this work is adapted from [12] work which resembles a standard industrial reactor with a length to diameter ratio of over 20000. The reactor operates at a high temperature around 300°C, pressure around 2200 bar, and axial velocity around 11 m/s. These severe conditions are needed for the free radical polymerization to take place inside the reactor. The feed to the reactor contains ethylene gas (monomer), oxygen and traces of hydrocarbons (or inerts). In addition, telogen or chain transfer agent (CTA) is also added at the feed stage. The addition of CTA will control the production of prohibitively large polymer molecules which can increase the polymer mixture viscosity. Thus, CTA is typically used to control the final grade of the polymer, which relates to the Melt Flow Index (MFI). The reactor is divided into five zones. The first two zones are used for preheating the reactor mixture to the optimal temperature for the first peroxide (or initiator) injection. In the third zone, an initiator is injected to generate free radicals that will react with ethylene monomer to produce long growing chains of ethylene molecules (or polyethylene). At the same time, oxygen also decomposes to produce free radicals. The polymerization reaction will be stopped after the initiator is depleted. The fourth zone is regarded as a cooling zone. Since
ethylene polymerization is an exothermic process, the excess heat needs to be removed to match the second initiator activation temperature. In the fifth and final zone, the second initiator is introduced and the polymerization reaction resumed. The amount of initiator corresponds to the polyethylene final conversion rate. Typically, the conversion rate for using the tubular reactor is 20-30%. However, uncontrolled amount of initiator injection can lead to a dangerous reactor runaway situation. Further properties and configuration of the reactor can be referred to [13] work.

2.2. Steady state simulation

The steady state model of LDPE tubular reactor is developed using Aspen Plus software, as shown in figure 1. Here, five RPLUG models with counter current jacket flow are used to simulate the whole reactor zones. Initiator injection is added before reactor zone 3 and zone 5 as mentioned before. In order to simulate thermodynamic properties and phase behavior of the process, Perturbed-chain statistical fluid theory (PC-SAFT) is chosen as the model property method. PC-SAFT is known as one of the best equation of state (EOS) to represent the polymerization process [14]. The heat of polymerization of the process is calculated by adjusting the heat of formation (DHFVK) of the ethylene segment so that the calculated heat of polymerization matches the literature data in [12]. The DHFVK value used in this study is -2.669 x 10^7 J/kmol. The pressure drop along the reactor is estimated to be approximately 10% of the reactor inlet pressure as observed in industrial practice [14].

![Tubular reactor model flowsheet in Aspen Plus.](image)

2.3. Kinetic model and parameters

In this process, LDPE is produced via free radical polymerization of ethylene gas. There are many reaction steps involved in the mentioned polymerization process leading to the complex polymer structure with short and long chain branches. [15] and [16] study has been referred to obtain the reaction mechanisms and kinetic parameters for this work. The complete polymerization reaction mechanisms and kinetic parameters used in this is available in [17] work. In order to achieve the desired reactor temperature profile and polymer conversion, some tuning was made to initiators and beta scission activation energy. These small adjustments...
are required due to the difference in modeling techniques used in Aspen Plus simulation compared to the original work. Aspen Data Fitting technique is used to retune the initiator’s kinetic activation energy to meet the reactor temperature profile, while Aspen Design Spec is used to achieve preferred number average of molecular weight (MWN) by beta scission kinetic activation energy modification.

2.4. Dynamic simulation

In order to obtain a dynamic model that can be applied in an online control scheme, the current steady state Aspen Plus model is exported to Aspen Dynamic for dynamic simulation. Flow-driven simulation option was selected during the model export process. Then, Aspen Dynamic model was linked to Matlab Simulink so it can be used as a model block from within the Simulink environment. The development of the controller was carried out within the Matlab Simulink platform.

3. Control scheme development

3.1. Input-Output selection

Based on Muhammad and Aziz [18] review, most of the control objective on LDPE tubular reactor study reported in the literature are focusing on product quality variables (i.e. Melt Flow Index or Gloss Index) and reactor temperature. In practice, temperature control is utilized by manipulating either initiator and/or jacket feed flow rates to maintain the reactor’s temperature and prevent temperature runaway. In this study, initiator 1 and initiator 2 feed flow rates are selected as manipulated variables (MV1 and MV2) to control maximum reactor temperature in Zone 3 and Zone 5 (CV1 and CV2). These zones are needs more attention since initiator points are located here and thus, polymerization process occurred. The disturbance variables considered were -10% in feed composition and -5% in feed flowrate. These variables are typically more exposed to disturbances since they are originated from outside of the system and not controlled by the reactor controller per se [19]. Furthermore, sensitivity and open loop analysis among the variables are performed to provide a deeper understanding of the system behavior.

3.2. Linear model identification

In general, a linear model can be obtained from the nonlinear process using identification technique. Identification technique requires input-output data of the process in order to identify its parameters based on the desired model type. For this study identification purpose, a set of train and validation data was generated from Aspen Dynamic model by using excitation signals from Matlab Simulink. Here, initiator 1 and initiator 2 flowrates are excited with ±10% of changes from their steady state value based on generalized multiple level noise (GMN) sequences. The dataset was generated for 500 minutes using 0.1 minutes sampling time. Based on the input-output data, the state-space model was estimated using Subspace method. The identification method was carried out using Matlab System Identification. The linear model was later used as a process model in MPC and as a base model in PID tuning.

3.3. MPC control scheme

In this study, MPC was developed to control the maximum reactor temperature inside the tubular reactor. MPC works by solving an optimization problem (or objective function) at each control interval. The solution to the problem will determine the optimal manipulated variables to be used in the plant until the next control interval. Sequential Quadratic Programming (SQP) algorithm was implemented to solve the objective function. The objective function used in this study is presented below where; \( p \) is prediction horizon, \( J_y \) is the objective function for output reference tracking, \( J_u \) is the objective function for manipulated variable tracking, \( z_k \) is the optimal MV solution, \( n_y \) is the number of control variable (CV), \( n_u \) is the number of MV, \( W_y \) is tuning weight for CV, \( W_u \) is the tuning weight for
MV, \( r \) is the reference signal, \( y \) is the predicted CV, and \( \Delta u \) is the deviation of MV from steady state. \( \Delta u_{\text{target}} \) was set to zero since the linear model is in deviation form.

\[
J_y J_u(z_k) = \sum_{j=1}^{n_y} \sum_{i=1}^{p} \left[ W_y [r(k + 1) - y(k + 1)] \right]^2 + \sum_{j=1}^{n_u} \left[ W_u [\Delta u(k + 1) - \Delta u_{\text{target}}(k + 1)] \right]^2
\]

where \( z_k = [\Delta u(k)^T \Delta u(k + 1)^T \ldots \Delta u(k + p - 1)^T \ \varepsilon_k] \)  

In order to evaluate MPC controller performance, PID controller was developed as a comparison in set point tracking and disturbance rejection test.

4. Results and discussion

4.1. Model validation and sensitivity analysis

Aspen model temperature profile and validation results are shown in figure 2. Based on the figure, Aspen model has managed to simulate the reactor temperature profile close to the industrial data with R-squared value of 0.981. Simulation result from [16] is also shown as comparison. Table 1 displays the simulation results for polymer properties. From the table, polymer properties from Aspen model are within acceptable accuracy with the industrial data.

![Validation for Aspen model temperature profile compared with industry data](image)

Figure 2. Validation for Aspen model temperature profile compared with industry data [12] and Agrawal model [16].
Table 1. LDPE process conversion and property validation

| Properties       | Industrial data | Agrawal model | Aspen model |
|------------------|-----------------|---------------|-------------|
| Conversion       | 0.300           | 0.297         | 0.295       |
| MWN (g/mol)      | 21900           | 21901         | 22070       |
| Density (gm/cc)  | 0.530           | -             | 0.565       |

The sensitivity analysis of initiator feed flowrate effect on maximum reactor temperature profile in Zone 3 and Zone 5 are presented in figure 3. Based on the figures, the linear region for maximum reactor temperature in Zone 3 and Zone 5 is under 3% and 5% respectively. Thus, initiator feed flow rate that is greater than these values will produce nonlinear (asymmetrical) profile as presented in the figure for initiator with ± 10% change. The interaction between the variables is investigated in Figure 4. Based on the figure, significant responses only occurred within the primary pairing of MV1-CV1 and MV2-CV2. The cross pairing of MV1-CV2 had displayed a small interaction. The pairing of MV2-CV1 does not affect due to the injection point has passed over CV location. Based on Relative Gain Array (RGA) calculation, the significant interaction between the variables had occurred to the main pairing only (lambda below than 1). In addition, the Conditional Number (CN) obtained for the system is 3.9129, which indicate a well-conditioned system and has a small effect on process/model mismatch (PMM). Thus, based on the RGA calculation and moderate CN results, it can be appropriately justified that the effect of loop interaction in this process can be neglected.

Figure 3. Sensitivity analysis for maximum reactor temperature profile (in deviation) for Zone 3 (left) and Zone 5 (right).
4.2. Linear model results

The linear model estimation and validation results are presented in figure 5. In the CV1 estimation result, it shows that the linear model was unable to estimate specific regions of the validation data accurately. This due to the inability of the linear model identification technique to estimate higher order process variable sufficiently. Based on normalized root mean square error (NRMSE), the linear model accuracy is at 0.7670 (1.0 equals to a perfect fit). In the CV2 estimation results, the model has managed to simulate the profile successfully with NRMSE equals to 0.9435. In overall, CV1 profile has proven to have higher nonlinearity behavior than CV2. Thus, controlling CV1 profile will be challenging to MPC since it depends solely on the accuracy of its process model to make error estimation of the current process.

Figure 4. Open-loop step response profiles between the variables.
4.3. Control scheme performance

In this part, the controller performance of both MPC and PID is evaluated. The tuning parameters for MPC and PID are presented in table 2. The MPC prediction and control horizon is determined based on the recommendation by Seborg [20] and further re-tuned during the online simulation. The MPC tuning weights were acquired by simulating the linear model with Matlab MPC Designer apps. The weights obtained from the app served as the initial tuning weights for MPC in controlling the nonlinear tubular reactor model online. Based on the controller performance results, further retuning was made manually. The PID controller parameters are obtained by using Matlab PID Tuner apps. The PID was tuned for tighter control of outputs and more aggressive control moves. The summary of both controller performance tests is shown in table 3. Integral square error (ISE) was applied to analyze the controller performance.

Table 2. MPC and PID final tuning parameters.

|                     | MPC (2-by-2) | PID            |
|---------------------|--------------|----------------|
|                     |              | MV1-CV1    | MV2-CV2    |
| Prediction Horizon  | 20           | 0.023439319 | 0.011884008|
| Control Horizon     | 5            | 0.150897631 | 0.060246602|
| CV Tuning Weight    | [10,10]      | 0.000910222 | 0.000586048|
| MV rate Tuning Weight| [0.1,0.1]   |               |             |
4.3.1. **Set point Tracking.** In this test, both controllers are required to follow the designated temperature set point. MPC had shown a superior set point tracking ability on CV1, as displayed in figure 6. On the CV2 profile, MPC and PID have almost comparable performance. MPC had able to reach the set point less than 5 minutes on both profiles. The MPC fast response can be further examined by observing the controller’s MV profile. The MPC controller had employed a more aggressive control action than PID. This performance proves MPC ability to optimize the process in order to find the most optimal MV action in order to reach the target faster.

![CV1 profile](image1)
![CV2 profile](image2)
![MV1 profile](image3)
![MV2 profile](image4)

**Figure 6.** Set point tracking test CV and MV profiles.

4.3.2. **Disturbance Rejection.** Both controllers ability to reject disturbances in the feed flow rate and feed composition are presented in figure 7 and figure 8. In figure 7, the overall performance of MPC was better than PID. In CV1 profile, MPC had accomplished a small output deviation due to its faster controller action than PID. MPC had exercised a more assertive control move on CV2 profile, which made it able to reject the disturbance faster than PID. In figure 8, MPC had attained better disturbance rejection performance than PID in CV1 profile. In CV2 profile, MPC had presented a smaller performance divergence compared to PID. All this is due to MPC ability to calculate and implement optimal MV profile contrasted to PID feedback error method.

Based on table 3, MPC has shown superior performance than PID in all aspect. Although the linear model accuracy of CV1 profile is low, MPC can be still able to compensate the model mismatch through proper tuning. The application of optimizer had benefited MPC in searching for the optimal solution in order to achieve the target and minimizing the effort as well. In many cases, MPC had produced a more efficient control move than PID and thus able to reach the target as fast. The ability of MPC prediction horizon had made the control aware of the disturbance situation faster and thus, finding an optimal way to counter it. Therefore, MPC ability to reduce production cost while achieving good control of the temperature was demonstrated.
Figure 7. Disturbance rejection performance for minus 5% disturbance in feed flowrate.

Figure 8. Disturbance rejection performance for minus 10% disturbance in ethylene feed composition.
Table 3. Controller performance summary based on ISE.

| Performance Test           | CV1  |     | CV2  |     |
|----------------------------|------|-----|------|-----|
|                            | MPC  | PID | MPC  | PID |
| Set point Tracking         | 4.9105| 15.0314| 4.6426| 7.1054|
| Disturbance Rejection 1    | 0.2878| 1.1901| 0.1943| 0.3192|
| Disturbance Rejection 2    | 0.7380| 3.4810| 0.0025| 0.0053|

5. Conclusion
In this study, MPC controller was developed to control LDPE tubular reactor maximum temperature in Zone 3 and Zone 5. The reactor model as developed using Aspen Plus for steady-state modeling and Aspen Dynamic for dynamic modeling. In order to implement MPC control scheme, a linear model of the process was developed based on input-output data of the reactor model using State-space model identification technique. The linear model was adopted later in MPC as a process model, and Sequential Quadratic programming (SQP) was utilized in MPC optimizer. The performance of MPC was evaluated together with PID controller. The results, in general, demonstrated MPC outstanding capability in tracking set point and rejecting disturbance. Application of process model to give estimates of the current and future process and optimizer to calculate an optimized solution of the control objective, have assisted MPC in performing its task. The model lower accuracy in CV1 profile was compensated by using MPC tuning weights. For the same reason, the prediction and control horizon in this case, was also selected to be larger than normal (based on the rule of thumb). MPC capability in reducing production cost was proven by in achieving good reactor temperature control with minimal initiator usage. The future research should be focusing on controlling the product end-use quality such as Melt Flow Index (MFI), which is the biggest priority in the polymerization reactor.

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References
[1] Azmi A and Aziz N 2016 Int. J. Appl. Eng. Res. 11(19) 9906-9913
[2] Häfele M, Kienle A, Boll M, and Schmidt C U 2006 Comp. Chem. Eng. 31(2) 51-65
[3] Russo L.P. and B.W. Bequette 1998 Chem. Eng. Sci. 53(1) 27-45
[4] Kiparissides C, Verros G, Pertsinidis A, and Goossens I 1996 AIChE J. 42(2) 440-454
[5] Cao L, Li D, Zhang C, and Wu H 2007 Comput. Chem. Eng. 31(11) 1516-1524
[6] Yoon W J, Kim Y S, Kim I S, and Choi K Y 2004 Korean J. Chem. Eng. 21(1) 147-167
[7] Ham J Y and Rhee H K 1996 J. Process Cont. 6(4) 241-246
[8] Qin S J and Badgwell T A 2003 Cont. Eng. Pract. 11(7) 733-764
[9] Berber R. and Coşkun S 1996 Comput. Chem. Eng. 20 S799-S804
[10] Anghelea M and De Keyser R 2001 European Control Conference (ECC) 2267-2272
[11] Muhammad D and Aziz N 2017 Chem. Eng. Trans. 56 769-774
[12] Asteasuain M, Tonelli S M, Brandolin A, and Bandoni J A 2001 Comput. Chem. Eng. 25(4) 509-515
[13] Asteasuain M, Tonelli S M, Brandolin A, and Bandoni J A 2000 Comput. Aided Chem. Eng. 8 559-564
[14] Bokis C P, Ramanathan S, Franjione J, Buchelli A, Call M L, and Brown A L 2002 Ind. Eng. Chem. Res. 41(5) 1017-1030
[15] Brandolin A, Lacunza M H, Ugrin P E, and Capiati N J 1996 Polym. React. Eng. 4(4) 193-241
[16] Agrawal N, Rangaiah G P, Ray A K, and Gupta S K 2006 Ind. Eng. Chem. Res. 45(9) 3182-3199
[17] Muhammad D, Ahmad Z, and Aziz N 2018 Materials Today: Proceedings 5(10) 21612-21619
[18] Muhammad D and Aziz N 2017 Chem. Eng. Trans. 56 757-762
[19] Bettoni A, Bravi M, and Chianese A 2000 Comput. Chem. Eng. 23(11-12) 1737-1744
[20] Seborg D E, Edgar T F, and Mellichamp D A 2004 Process Dynamics and Control: Second Edition (Hoboken NJ: John Wiley & Sons)