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Review: Control Schemes for Low Density Polyethylene Reactor

Dinie Muhammad, Norashid Aziz*

School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia,Seri Ampangan, 14300 Nibong Tebal, Seberang Perai Selatan, Penang, Malaysia.
chnaziz@usm.my

Low density polyethylene (LDPE) is one of the most common produced polymers in the world. LDPE is commonly produced using fee radical polymerisation process in high pressure environment. Polymerisation process pose significant challenges to the industrial community as the process is difficult to control with high nonlinearity behaviour and fast dynamic response. Control problems can also arise from LDPE grade switching and reactor's fouling effect. The infrequent long sampling time of laboratory measurement and unreliable online instrument measurement can make the LPDE quality monitoring become more difficult. The heart of polymerisation process is the reactor. A good control of the reactor will exhibit smooth production of LDPE. In this study, a brief review of past and recent control schemes that had been developed for LDPE process is presented. This review focused on the control schemes implemented in tubular and autoclave reactor which covers type of control scheme, process model, process estimator, and control variables used. The availability of important industrial quality parameters such as Melt flow index and Gloss index is also addressed. This review highlights the importance of nonlinear control in polymerisation process and future works related to it.

1. Introduction

Low density polyethylene (LDPE) is widely used today in a large number of applications including packaging, adhesives, coatings and films (Pladis et al., 2015). As a commodity polymer, LDPE is mass produced in continuous tubular reactor or autoclave reactor. Continuous polymerisation process is known to exhibit highly nonlinear dynamic behaviour and frequently operates in a wide operating region in order to produce polymers with properties desired by current market (Ben Amor et al., 2004). Over the years, significant efforts have been made to develop a proper understanding of polymerisation process and kinetic fundamentals. Current knowledge on polymer reaction engineering has spur the development of reliable and accurate mechanistic model and chemical aided design (CAD) software for industrial polymerisation reactors. In a way, this also prompts the development of control scheme for polymerisation reactors (Hosen et al., 2014). The knowledge of the polymerisation process can be a strong foundation to an accurate polymer process model. The profound knowledge of process operation in terms of the effect of operating variables on polymer properties can be used to design a control system in a much more straightforward strategy than would have been possible otherwise (Richards and Congalidis, 2006). The implementation of advanced process control in continuous polymerisation reactor has the potential to ensure good online control of polymer quality during the polymerisation stage which can lead to a significant improvement in polymer quality. (Jacob and Dhib, 2012). This study provides a brief review of control strategy implementations for LDPE polymerisation reactor process. Several polyethylene processes using fluidised bed reactor are also reviewed. This review will focus on the control scheme, process model, process estimator, and control variables implemented in each respective case study. The consideration for quality parameter control such as Melt flow index (MFI) and Gloss index are also addressed.

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2. LDPE Production

The basic material for polyethylene is the ethylene monomer. Ethylene is a colourless gas with a slightly sweet smell and is obtained by cracking (thermal decomposition) ethane at high temperatures in a cracker or steam furnace. Figure 1 shows the simplified industrial production of LDPE using autoclave reactor (left) and tubular reactor (right). Autoclave reactor is a stirred cylindrical reactor typically about 6.1 m long and 0.38 - 0.91 m in diameter. Tubular reactor is similar to a tube or long pipe which usually about 1.25 km long and 2.5 - 7.6 cm in diameter. In general, both production unit have similarity in term of using high temperature and pressure condition. Before entering the main unit, ethylene gas mixture had to be compressed to a pressure around 3,000 bar. In order to initiate the polymerisation reaction, either unit operation use single or multiple injections to introduce the initiator into the mixture. The temperature control on both units are critical as polymerisation of ethylene is exothermic. In autoclave reactor, proprietary baffle designs divide the unit into discrete zones enabling better molecular reaction control. For tubular reactor, molecular properties of LDPE are controlled by maintaining the reactor temperature profile. Typical ethylene conversion by using autoclave reactor is about 22 % per reactor pass while for tubular reactor is about 35 % (Butler, 2010). After the polymer exit the units, separators are used to isolate the unreacted ethylene with LDPE. The unreacted ethylene will be recycled back to the process while the molten polymer is prepared to be mixed with additives and then pelletised. Standard production rates for autoclave reactors output capacities are 75 to 225 kt/y while for tubular reactors are 100 to 250 kt/y (Butler, 2010).

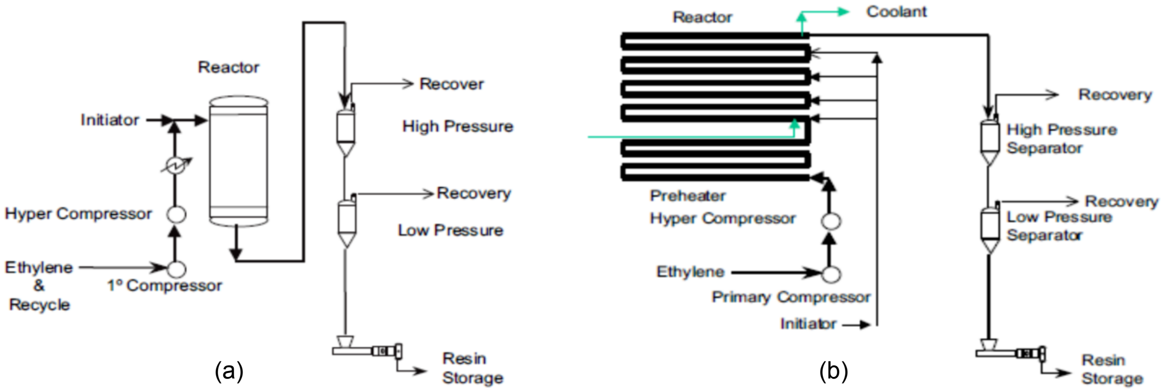

Figure 1: Simplified production of LPDE using (a) autoclave reactor and (b) tubular reactor (Butler, 2010)

3. Control in polymerisation reactor

Model predictive control is a type of model based controller that utilise explicit model to predict the process output, calculate control sequence by minimising objective function and implement receding strategy (Camacho and Alba, 2013). Based on Qin and Badgwell (2003) survey, Linear model predictive control (LMPC) has a wide acceptance in chemical process industries compared to its nonlinear counterpart, Nonlinear model predictive control (NMPC). In polymer manufacturing industries, NMPC is more preferred as LMPC would often deteriorate when they applied to process with strong nonlinearities (Seki et al., 2001). Polymerisation process also exhibit varying dead times and process gains for different polymer quality attributes with respect to reactor temperatures (Bindlish, 2015). In continuous polymerisation process, there are often polymer grade transitions to meet the market demand. Although process regulation at a single operation condition can be done by conventional linear controller, nonlinear process control is still needed to achieve good performance during grade transitions and different operating conditions. The key objective in controlling a continuous polymerisation reactor system is to maintain reactor stability in presence of any process upsets and during normal steady state operations and grade transition operations (Yoon et al., 2004). In general, commercial polymer is valued based on its final quality attributes such as melt flow index (MFI), gloss index, and impact resistances. However, in plant, these properties are hard to measure on-line and mostly have long measurement delay. In order to solve this problem, a two-tier control scheme for polymerisation reactor was proposed (Ogunnaike, 1994). The two-tier control scheme is similar to a cascade structure where a master Quality Controller (upper tier) will provide set point for the slave Composition Controller (lower tier). In the lower tier, process variables such as polymerisation temperature, reactor pressure, flow rate of monomer, initiators, chain transfer agents, and solvents are regulated to meet certain conditions based on the product recipe. Theoretically, if all these variables are tightly controlled, a consistent quality in polymer production can be achieved. The correlation between polymer properties and polymer process variables are often nonlinear. The purpose of the upper tier controller is to control the product quality and serve as a corrective control for the lower tier. The quality controller is updated with on-line or lab measurements and estimates of polymer quality properties from inferential model. In principle, any variation in product quality can be corrected if such measurement is available during the polymerisation process. In term of controller execution time, the lower tier will act faster, typically 1 min, compared to the upper tier. In absence of on-line measurement or lab data, especially during transition period, the reliability and accuracy of the quality process model is very important. Naidoo et al. (2007) had highlighted a number of practical issues and solutions that have been adopted during executing nonlinear MPC for industrial polymerisation reactor. An excellent review on traditional and advanced control techniques for batch, semi batch, and continuous polymerisation reactors are available by (Richards and Congalidis, 2006).

4. Control schemes in LDPE

In LDPE case, there are only a handful number of researchers who are involved in its control development study. Singstad et al. (1992) developed and commissioned a two-level internal nonlinear decoupling based controller for the control of an industrial multi-zone LDPE autoclave reactor. In their study, product quality control was used in the upper supervisory level while reactor stabilisation control was performed at the lower level. They showed that their control strategy accomplished superior results in closed-loop performance compared to conventional multi loop PID controllers. Ham and Rhee (1996) applied adaptive pole placement controller based on recursive least squared method for a two-compartment LDPE autoclave reactor. In their findings, the controller had shown good performance in eliminating overshoot in the reactor temperature profile and stabilising the initiator flow rate profile compared to PID controllers. The authors did not consider the direct control of polymer product quality or final properties which is very important in the industry. Berber and Coşkun (1996) tested the performance of linear Quadratic Dynamic Matrix Control (QDMC) on industrial LDPE autoclave reactor. Process nonlinearity was taken into account into the process model by integrating the autoclave reactor ODE model from current state over the prediction horizon. They demonstrated that QDMC delivered superior result compared to multi loop PI control in reactor temperature set point tracking combined with ethylene feed temperature disturbance test. Anghelea and De Keyser (2001) exploited Extended Predictive Self Adaptive Control (EPSAC) MPC approach in controlling a LDPE tubular reactor model. In their study, the controller was tested on SISO and MIMO configuration with PI controller. For MIMO case, two control approach, Solidary and Selfish control were tested. Based on the test, EPSAC controller provide satisfactory results compared to PI controller. The Solidary and Selfish control approach for MIMO case also gave similar results. Ali et al. (2003) studied two type of control schemes for fluidised bed polyethylene reactor. The first control scheme utilised a single multivariable controller to handle all the controlled variables. The second scheme used two control loops, one is a fast-dynamic loop handled by multi loop PI controllers and another is a slow dynamic loop handled by a multivariable controller. From comparison tests on both schemes, the latter one was more favourable with faster settling time and less overshoot in some cases whether LMPC or NMPC is used. In head to head comparison between LMPC and NMPC, NMPC was reported to display better superior performance in achieving offset free response and robust to model mismatch error. Ben Amor et al. (2004) applied an industrial real-time optimisation software (ROMeo) with NMPC for a simulated polymer grade transition control in a polyethylene fluidised bed reactor. The NMPC algorithm was developed using orthogonal collocation and sequential quadratic programming (SQP) was used to solve the resulting nonlinear programming problem. Luenberger observer was designed to estimate the unmeasured states. In their research, the controller and observer part were developed inside ROMeo and the mathematical process model was developed using Matlab. Both software was connected together to complete the simulation. From the test, NMPC was managed to control the four grade transitions process despite significant model uncertainty. Yao et al. (2004) studied optimal control for LDPE tubular reactor. In their study, the optimal control objective is to determine the optimal jacket temperature as a function of reactor length that would maximise the final monomer conversion of an LDPE reactor. Maximum reactor temperature and the range of reactor jacket temperature were specified as inequality process constraints. Genetic algorithm technique was used to solve the optimal control problem. Based on the comparison study, the optimal process had presented significant improvement in the final monomer conversions up to 42.33 % by using 5 initiator injections. Naidoo et al. (2007) reported on industrial implementation of NMPC in LDPE tubular reactor. The optimisation part in NMPC was handled using SQP and Kalman Filter was used to estimate the process states online. The process model was developed using Bounded Derivative Network which is an improved empirical model based on artificial neural network technique (Turner and Guiver, 2005). The NMPC control scheme was implemented using the two-tier system which is a cascaded structure where the master Quality Controller providing set-points for the slave Composition Controller. The implementation of NMPC in industry had produced positive results in reducing product offset and increasing production capacity. Zavala and Biegler

(2009) had employed several optimisation-based strategies for LDPE tubular reactor control. The reactor was modelled based on a number of Differential and algebraic equations (DAE). In their work, fouling and defouling scenario was considered as disturbance in the process. They demonstrated that Tracking NMPC was able to stabilise the reactor temperature and maintaining the melt index and production rate despite the disturbance. The addition of economic function into the tracking NMPC had provided it with better control grasp of the process without sacrificing the production rate. Moving Horizon Estimator (MHE) was also tested with NMPC as output feedback controller for the process. During the test, MHE-NMPC was able to stabilise the process despite the fouling disturbances. Jacob and Dhib (2012) discussed the application of unscented Kalman Filter (UKF) in NMPC algorithm for multi-zone multi-feed autoclave reactor. The UKF algorithm is reported to have higher degree of accuracy, wide range of application and simpler implementation than Extended Kalman filter (EKF) (Romanenko and Castro, 2004). In their work, the closed loop performance of UKF based NMPC is compared with Kalman filter based LMPC in set point tracking and disturbance rejection test under noisy process measurement and model mismatch. In both tests, UKF-NMPC performance is better than KF-LMPC. The performance UKF-NMPC was reported to be more significant compared to LMPC and PID controllers in controlling single-zone LDPE autoclave reactors (Jacob and Dhib, 2011).

Table 1: Summary of control schemes implementation in LDPE

Researcher	Reactor System	Data Source	Control Scheme	Model (Process Model)	Controller	Controlled Variable (CV) Manipulated Variable (MV)
Singstad et al., 1992	Autoclave	Industry	Two level	ODE	Multivariable based Nonlinear Decoupling	CV: Product Quality; MV: reactor pressure; temperature profile; production rate;
Ham and Rhee, 1996	Autoclave	Journal	Closed Loop	ODE	Adaptive pole placement	CV: reactor temperature; MV: initiator flow rate;
Berber and Coşkun, 1996	Autoclave	Industry	Closed Loop	ODE (Step Model)	Linear QDMC	CV: reactor temperature; MV: catalyst flow rate; zone monomer flow rate;
Anghelea and De Keyser, 2001	Tubular	Journal	Closed Loop	ODE (FPM)	EPSAC	CV: weight average degree of polymerisation; zone peak temperature; MV: solvent flow rate; initiator flow rate;
Ali et al., 2003	Fluidised Bed	Journal	Two level	ODE (FPM)	EKF-NMPC	CV: reactor partial pressure; reactor temperature; MV: feed component flow rate; bleed flow rate; coolant inlet temperature;
Ben Amor et al., 2004	Fluidised bed	Journal	Two level	ODE (FPM)	Luenberger-NMPC	CV: Melt Index; Density; Reactor pressure; Production rate; MV: Nitrogen flow rate; Hydrogen flow rate; comonomer flow rate; catalyst flow rate;
Yao et al., 2004	Tubular	Journal	Closed Loop	ODE	Optimal Control	Optimal reactor jacket temperature;
Naidoo et al., 2007	Tubular	Industry	Two level	BDN	KF-NMPC	CV: Melt Index; Gloss Index; MV: Reactor temperature; CTA concentration; Initiator flow rate;
Zavala and Biegler, 2009	Tubular	Industry	Two level	DAE (FPM)	Tracking NMPC; RTO-NMPC; MHE-NMPC;	CV: Production rate; Melt Index; Reactor temperature profile; MV: Initiator flow rate; jacket inlet temperature; jacket inlet flow; side stream temperature;
Jacob and Dhib, 2012	Autoclave	Industry	Closed Loop	ODE (FPM)	UKF-NMPC	CV: Reactor temperature profile; weight-averaged molecular weight; MV: initiator flow rate; reaction zone monomer feed flow rate;

The summary of the control schemes implementation is shown in Table 1. Based on the table, most of the researchers developed their reactor model based on mathematical model using ordinary differentials equation (ODE). The availability of much model (or also known as first principle model, FPM) will facilitate the NMPC development as such model can be used as its nonlinear process model. As for empirical modelling, only a single case was reported. The Bounded Derivative Network (BDN) is an analytical integral of neural network which has capability of incorporating process knowledge inside it. It worth to mentioned that the application of empirical modelling in polymerisation process is still viable as mentioned by Hosen et al. (2014). Empirical modelling has the advantage over FPM modelling when there is less fundamental understanding of the process. The popularity of model based controller (LMPC and NMPC) is profound in the survey. The wide application of MPC in research community and industry is due its general and intuitive design in solving the process control problem in time domain (Camacho and Alba, 2013). The survey also reveals that NMPC was given more attention than LMPC. This was expected since polymerisation reactor process typically suffers from high nonlinearity and dynamic behaviour. Such behaviours can occur due to uneven polymerisation, thermal runaway and during grade transition. In regards to polymerisation process predicament, the application of NMPC is more appropriate. It was noted that there were two control schemes that was occasionally used by the researchers. The closed loop type is more towards using a single multivariable controller to control all the parameters inside the process. Two level control scheme utilise dual layer of control where a supervisory (or upper) control loop which typically handle quality parameters and regulatory (or lower) control loop to control the basic parameters typically temperature, flow rate and pressure. Although both implementations had reported success in their respective studies, Ali et al. (2003) had reported that the latter one is more preferable in term of regulatory control performance and robustness. The application of state estimator in control scheme was reported to be essential in order to estimate unmeasurable polymer properties and improve controller robustness (Jacob and Dhib, 2012). The selection of controlled variables (CV) and manipulated variables (MV) are varies among researchers and mainly depend on the type of reactor used. Some researchers use tight operation control (typically temperature profile) in order to achieve desired final polymer properties. Others use the quality controller which can control directly the final end-use polymer properties via reliable correlation of certain polymer parameter e.g. weight average molecular weight (WAMW) (Jacob and Dhib, 2012). Based on Shenoy and Saini (1986) study, polymer WAMW had shown a good correlation with industrial final end-use polymer properties such as melt flow index (MFI). Application of soft sensors to estimate MFI had also produced good results in estimating the quality parameter real time using industrial data (Farsang et al., 2015).

5. Conclusions

A brief review on control schemes application in LDPE polymerisation reactor was conducted. The review had shown that application of advanced process control especially model predictive control was well accepted. This primarily due to the nonlinearity and dynamic behaviour of polymerisation reactor. Implementation of NMPC in industry has been reported to produce significant results in increasing plant capacity, reducing off spec product during grade transition and stabilising the process during steady state operation (Naidoo et al., 2007). Most of the reactor models involved in the LPDE polymerisation process are developed based on mechanistic model. This open for model development study using hybrid or black box modelling technique such as Adaptive Neuro-Fuzzy Inference System (ANFIS) and Artificial Neural Network (ANN). This also brings to the development study of NMPC based on empirical model rather than in first principle model (FPM) as practiced by many before in the respective area. Two tier control scheme appears to be more promising to be implemented in the polymerisation reactor compared to the single multivariable control system. The important matter is the end-use polymer properties must be properly determined using any techniques, for example, state estimator to ensure the final product quality. The incorporation of this knowledge to the controller would be greatly valuable.

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Reference

Ali E., Al-Humaizi K., Ajbar A., 2003, Multivariable Control of a Simulated Industrial Gas-Phase Polyethylene Reactor. Industrial and Engineering Chemistry Research 42 (11), 2349-2364.

Anghelea M., De Keyser R., 2001, Predictive control of a low density polyethylene plant, European Control Conference (ECC), 4-7 Sept 2001, Porto, Portugal, 2267-2272.

Ben Amor S., Doyle F.J., Mc Farlane R., 2004, Polymer grade transition control using advanced real-time optimization software, Journal of Process Control 14 (4), 349-364.

Berber R., Coşkun S., 1996, Dynamic simulation and quadratic dynamic matrix control of an industrial low density polyethylene reactor, Computers & Chemical Engineering 20, S799-S804.

Bindlish R., 2015, Nonlinear model predictive control of an industrial polymerisation process, Computers and Chemical Engineering 73, 43 - 48.

Butler T.I., 2010, Chapter 2-PE Processes, Ed. Wagner J.R., Multilayer Flexible Packaging, William Andrew Publishing, Boston, USA, 15-30.

Camacho E.F., Alba C.B., 2013, Model predictive control, Springer Science & Business Media, London, UK.

Farsang B., Balogh I., Nemeth S., Szekvolgyi Z., Abonyi J., 2015, PCA based data reconciliation in soft sensor development – application for melt flow index estimation, Chemical Engineering Transactions 43, 1555-1560.

Ham J.Y., Rhee H.K., 1996, Modelling and control of an LDPE autoclave reactor, Journal of Process Control 6 (4), 241 - 246.

Hosen M.A., Hussain M.A., Mjalli F.S., Khosravi A., Creighton D., Nahavandi S., 2014, Performance analysis of three advanced controllers for polymerisation batch reactor: An experimental investigation, Chemical Engineering Research and Design 92 (5), 903-916.

Jacob N.C., Dhib R., 2011, Unscented Kalman filter based nonlinear model predictive control of a LDPE autoclave reactor, Journal of Process Control 21 (9), 1332 - 1344.

Jacob N.C., Dhib R., 2012, Nonlinear MPC of a multi-zone multi-feed LDPE autoclave reactor, Journal of Industrial and Engineering Chemistry 18 (5), 1781- 795.

Naidoo K., Guiver J., Turner P., Keenan M., Harmse M., 2007, Experiences with nonlinear MPC in polymer manufacturing, Assessment and Future Directions of Nonlinear Model Predictive Control 358, 383 - 398.

Ogunnaike B.A., 1994, On-line modelling and predictive control of an industrial terpolymerisation reactor, International Journal of Control 59, 711-729.

Pladis P., Meimaroglou D., Kiparissides C., 2015, Prediction of the Viscoelastic Behaviour of Low-Density Polyethylene Produced in High-Pressure Tubular Reactors, Macromolecular Reaction Engineering 9 (3), 271 - 284

Qin S.J., Badgwell T.A., 2003, A survey of industrial model predictive control technology, Control engineering practice 11 (7), 733 - 764.

Richards J.R., Congalidis J.P., 2006, Measurement and control of polymerisation reactors, Computers and Chemical Engineering 30 (10-12), 1447-1463.

Romanenko A., Castro J.A.A.M., 2004, The unscented filter as an alternative to the EKF for nonlinear state estimation: a simulation case study, Computers and Chemical Engineering 28, 347 - 355.

Seki H., Ogawa M., Ooyama S., Akamatsu K., Ohshima M., Yang W., 2001, Industrial application of a nonlinear model predictive control to polymerisation reactors, Control engineering practice 9, 819-828.

Shenoy A.V., Saini D.R., 1986, Melt flow index: More than just a quality control rheological parameter - Part II, Advances in Polymer Technology 6 (2), 125-145.

Singstad P., Nordhus H., Strand K., Lien M., Lyngmo L.B., Moen O., 1992, Multivariable non-linear control of industrial LDPE autoclave reactors, American Control Conference, 24-26 June 1992, Chicago, Illinois, US, 615-619.

Turner P., Guiver J., 2005, Introducing the bounded derivative network- superseding the application of neural networks in control, Journal of Process Control 15 (4), 407 - 415.

Yao F.Z., Lohi A., Upreti S.R., Dhib R., 2004, Modelling, simulation and optimal control of ethylene polymerisation in non-isothermal, high-pressure tubular reactors, International Journal of Chemical Reactor Engineering 2 (1), DOI: 10.2202/1542-6580.1152.

Yoon W.J., Kim Y.S., Kim I.S., Choi K.Y., 2004, Recent advances in polymer reaction engineering: modelling and control of polymer properties, Korean Journal of Chemical Engineering 21 (1), 147-167.

Zavala V.M., Biegler L.T., 2009, Optimization-based strategies for the operation of low-density polyethylene tubular reactors: nonlinear model predictive control, Computers and Chemical Engineering 33 (10), 1735-1746.