

Control of Polyethylene Properties using Nonlinear Model Predictive Control

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Abstract: This paper deals with the control of the melt index and density of polymers produced. Nonlinear Model predictive control (NLMPC) is used for this purpose. A nonlinear reactor model combined with correlations for predicting polymer melt index and density are used to simulate the process. The simulations revealed the effectiveness of NLMPC to drive the polymer properties to follow a series of grade changeover in the absences and presence of modeling errors. Grade transition is achieved with zero offset but with relatively large settling time. Rapid grade changeover is limited by the large residence time and broad residence time distributions for both the gas phase and formed polymers.

1. INTRODUCTION

Polyethylene industry is forced to produce polymers with various grades to meet the growing and diverse customer requirements. Each polymer grade is defined by specific polymer properties such as density and melt index. To achieve these properties, the plant should be operated at different operating conditions. Moving from one operating condition to another requires a good regulatory control system. The control system is also necessary to maintain the process safety by regulating the reactor temperature and pressure.

The concept of grade transition control of polymerization reactors has been investigated by several researchers. McAuley and McGregor (1992) presented optimal grade transition policy for gas phase polyethylene reactors by solving offline optimization problem. McAuley and McGregor (1993) extended their work to include a controller based on input/output linearization to implement their optimal strategy. Debling et al. (1994) studied a number of grade transition operations using the simulation package POLYRED. Sato et al. (2000) tested a gain scheduling approach to switch between different grades using a linearized model of the polyethylene reactor process and its product properties. Biegler et al. (2002) determined optimal grade transition strategies for the whole polyethylene plant that produces polymer in tubular reactor. The proposed strategy solves a large open-loop optimization problem. Ohshima et al. (2000) and Wang et al. (2000) determined the grade transition trajectories by solving an open-loop optimization function that minimizes the off-specs products and the transition time required to reach the new operating condition. They also proposed a combination of feedforward and feedback controllers to make the controlled variables follow the optimal trajectories. Kiparissides et al. (2003) augmented their optimal grade changeover control with a methodology to find the control structure configuration. The integrated approach requires solving a mixed integer programming problem. Ben Amor et al. (2004) followed the

same approach proposed by Wang et al. (2000), but they used a nonlinear Model Predictive Control (NLMPC) to track the trajectories obtained by the open-loop optimization. Bonvin et al. (2005) considered the optimization of grade transition via the tracking of necessary condition of optimality. No regulatory controller is considered to enforce the optimal path. Lo and Ray (2006) carried out a comprehensive parametric analysis to show how reactor inputs can be manipulated to reach specific polymer qualities over nickel catalyst. The study neither involves determining optimal trajectories nor implementing advance control strategy. The offline optimization methods produce input trajectories with their switching times that provide optimal grade transition in the sense of minimum off-specs products. The reduction of off-specs products is achieved through in terms of minimum overshoot and/or settling time in the products property response. However, obtaining the optimal input trajectories is not enough because in the presence of modelling error and/or unmeasured disturbances, the product properties may diverge away from their nominal values. In this case, a feedback control is necessary to regulate the process.

According to the above investigations, the control of polymer grade changeover is handled via two approaches. One approach is an iterative online optimization approach, i.e. receding horizon control. The other approach is the integrated feedforward and feedback controls. Only the work of Doyle et al. (2003) falls in the first approach. Apparently, the second approach requires determining the optimal reactor input signals over the entire transition time that will be used as reference values for the controlled variables and the manipulated variables. On the other hand, the optimization-based controllers such as NLMPC can bypass this requirement, i.e. calculating the input and output reference values beforehand. NLMPC optimizes online a cost function in an open-loop mode. The first action of the derived optimal sequences is implemented on the process. The procedure is then repeated every sampling instant. The result is that the process response stays close to the optimal tracks.

2. THE PROCESS MODEL

The polyethylene reactor process is depicted in Fig. 1. The process model was developed by McAuley et al. (1995) and is given below. This model is chosen because its kinetic parameters were validated against plant data (McAuley et al., 1990). Further details of the model, and the definition of the various states and parameters of the model is given elsewhere (Ali et al., 2003)

$$V_g \frac{dC_{M1}}{dt} = F_{M1} - x_{M1} B_t - R_{M1} \quad (1)$$

$$V_g \frac{dC_{M2}}{dt} = F_{M2} - x_{M2} B_t - R_{M2} \quad (2)$$

$$V_g \frac{dC_H}{dt} = F_H - x_H B_t - R_H \quad (3)$$

$$V_g \frac{dC_N}{dt} = F_N - x_N B_t \quad (4)$$

$$\frac{dY_c}{dt} = F_c a_c - k_d Y_c - O_p Y_c / B_w \quad (5)$$

$$(M_r C p_r + B_w C p_p) \frac{dT}{dt} = HF + HG - HR - HT - HP \quad (6)$$

$$M_w C p_w \frac{dT_g}{dt} = F_g C p_g (T_{g_i} - T_g) + F_w C p_w (T_{w_i} - T_{w_o}) \quad (7)$$

The Melt index and Density can be correlated to the gas concentration as follows:

$$\ln(MI) = 3.5 \ln \left(k_0 + k_1 \frac{CM_2}{CM_1} + k_3 \frac{CH_2}{CM_1} \right) \quad (8)$$

$$\rho = p_0 + p_1 \ln(MI) - \left(p_2 \frac{CM_2}{CM_1} + p_3 \frac{CM_3}{CM_1} \right)^{p_4} \quad (9)$$

The cumulative Melt index and polymer density can be obtained from the following differential equation (Sato et al., 2000):

$$\frac{dMI_c}{dt} = \frac{3.5 O_p}{B_w} \left(MI^{3.5} MI_c^{2.5} - MI_c \right) \quad (10)$$

$$\frac{d(1/\rho_c)}{dt} = \frac{O_p}{B_w} \left(\frac{1}{\rho} - \frac{1}{\rho_c} \right) \quad (11)$$

The model equations listed above are slightly modified than those given by McAuley et al. (1995). For simplicity, only one active site for the catalyst is considered here. Moreover, the energy balance around the cooler considers the dynamic of the recycle temperature explicitly instead of the heat removal as used by McAuley et al. (1995). In due course, the cooling process is modelled as well mixed system. The thermal effect of the recycle compressor is also included in this model.

2. THE ON-LINE NLMPC ALGORITHM

In this work, the structure of the MPC version developed by Ali and Zafiriou (1993) that utilizes directly the nonlinear model for output prediction is used. A usual MPC formulation solves the following on-line optimization:

$$\min_{\Delta u(t_k), \dots, \Delta u(t_{k+M-1})} \sum_{i=1}^P \|\Gamma(y(t_{k+i}) - R(t_{k+i}))\|^2 + \sum_{i=1}^M \|\Lambda \Delta u(t_{k+i-1})\|^2 \quad (12)$$

subject to

$$A^T \Delta U(t_k) \leq b \quad (13)$$

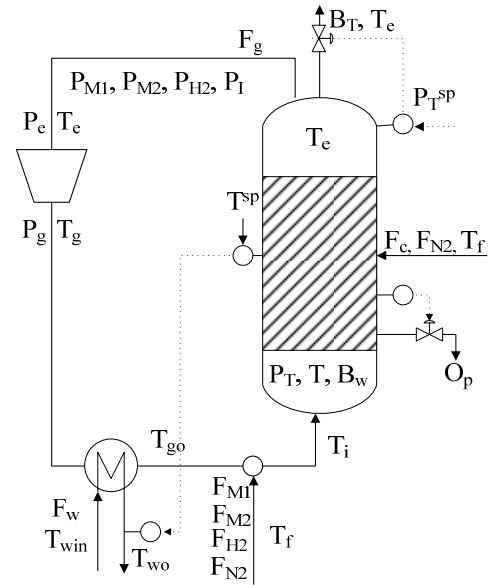


Fig.1. Schematic of the polyethylene reactor

For nonlinear MPC, the predicted output, y over the prediction horizon P is obtained by the numerical integration of:

$$\frac{dx}{dt} = f(x, u, t) \quad (14)$$

$$y = g(x) \quad (15)$$

from t_k up to t_{k+P} where x and y represent the states and the output of the model, respectively. The symbols $\| \cdot \|$ denotes the Euclidean norm, k is the sampling instant, Γ and Λ are diagonal weight matrices and $R = [r(k+1) \dots r(k+P)]^T$ is a vector of the desired output trajectory. $\Delta U(t_k) = [\Delta u(t_k) \dots \Delta u(t_{k+M-1})]^T$ is a vector of M future changes of the manipulated variable vector u that are to be determined by the on-line optimization. The control horizon (M) and the prediction horizon (P) are used to adjust the speed of the response and hence to stabilize the feedback behaviour. Γ is usually used for trade-off between different controlled outputs. The input move suppression, Λ , on the other hand, is

used to penalize different inputs and thus to stabilize the feedback response. The objective function (Equation 12) is solved on-line to determine the optimum value of $\Delta U(t_k)$. Only the current value of Δu , which is the first element of $\Delta U(t_k)$, is implemented on the plant. At the next sampling instant, the whole procedure is repeated. To compensate for modelling error and eliminate steady state offset, a regular feedback is incorporated on the output predictions, $y(t_{k+1})$ through an additive disturbance term. Therefore, the output prediction is corrected by adding to it the disturbance estimates. The latter is set equal to the difference between plant and model outputs at present time k . More details on improving the NLMPC robustness by the integration of Kalman Filter are given elsewhere (Ali and Zafiriou, 1993).

3. RESULTS

The control objective here is to move the process through different operating condition depending on the target values for the MI and density. The controller should also keep the production rate constant during transition. These objectives will be handled via NLMPC using the feed flow rate of the monomer, comonomer, hydrogen and catalyst as manipulated variables. It is also necessary to maintain process safety through regulating the reactor temperature and pressure. This second control objective is achieved via independent PI control loops that manipulate the reactant coolant water T_w , and bled flow rate BT. The design and tuning parameters for these loops is given elsewhere (Ali et al., 2003). Simulation of the process for a series of three set point changes using a sampling time of 0.1 hr gives the results shown in Figs. 2 and 3. A control horizon of $M=1$ and prediction horizon of $P=15$ is used in NLMPC. The weights on the manipulated variables are chosen $\Lambda=[1 \ 1 \ 1 \ 10]$ and the weights on the controlled outputs are chosen $\Gamma=[1 \ 10 \ 5000]$ which corresponds to MI, density and production rate (PR). It can be seen from Figure 2 that the polymer properties are well maintained at their prospective set points. The production rate is successfully kept at its desired value despite some spikes that occur at instant when the grade changeover starts which is associated with sudden changes in the manipulated variables as shown in Fig. 3. These outliers in the production rate are still acceptable as it lies within $\pm 0.5\%$ of the set point. It should be noted that settling time for the MI ranges between 15 to 26 hours depending on the set point value. For the polymer density, the settling time ranges between 16 to 18 hours. No overshoot was observed.

Fig. 3 illustrates how the manipulated variables change in order to maintain the output responses shown in Fig. 2. The figure also depicts the reaction of BT and T_w which are the manipulated variables for the external PI loops. These MV's are varied because changing the feed flow rates creates disturbance to the temperature and pressure control loops.

The sampling time used in the previous simulation ($T=0.125$ hr) is short. In practice, measurements of polymer properties are available only at sampling frequency of 2 hours. For this reason we repeat the simulation for sampling time of 1 hour assuming the polymer property remains constant for each two hours. The simulation results are illustrated in Figs. 4 and 5

for different set point sequences. The prediction horizon is changed to $P=2$ because the sampling time is long enough. Once again successful responses were obtained with almost the same settling times. The production rate demonstrated slight overshoot at the third set point change. Nevertheless, the overall performance is acceptable.

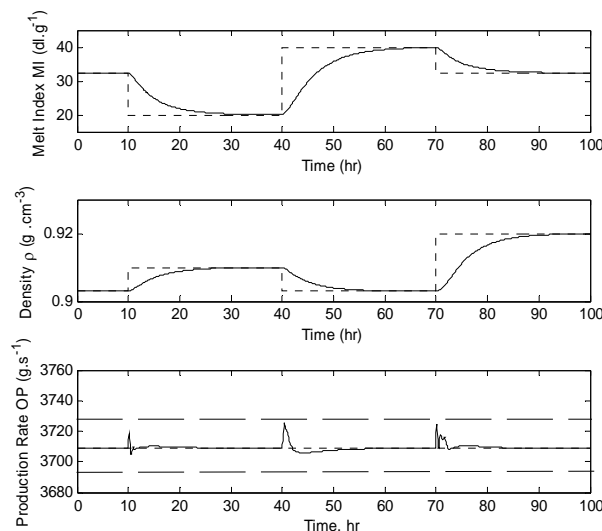


Fig.2. Controlled outputs using NLMPC with $T=0.1$ hr, dotted line: set point, solid line: output response, dashed line: tolerance limit

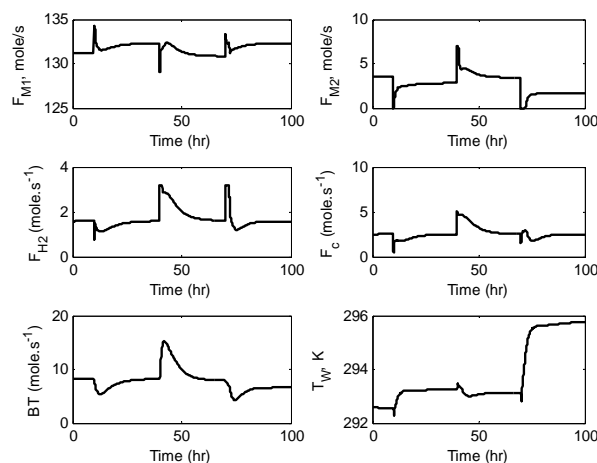


Fig.3. Manipulated variables for $T=0.1$ hr. F_{M1} : monomer feed rate; F_{M2} : comonomer feed rate; F_C : catalyst federate; F_{H2} : hydrogen feed rate; T_w : coolant temperature and BT: bled flow rate.

The previous simulations are carried out assuming perfect model. However, this is not always true in real practice. To test the robustness of NLMPC to reject the effect of modelling errors, the simulation is repeated with $+10\%$ error in the reaction rate constant and catalyst activity, and $+5\%$ in the parameters of the density correlation (9). The results are shown in Fig. 6 to 8. It is evident that NLMPC was able to

keep good control performance despite the severe modelling errors. It was found that the simple additive disturbance estimates were sufficient to help the NLMPC overcome the influence of the model uncertainty. Fig. 8 demonstrates the severity of the modelling errors as significant mismatch between the response of the model and plant states is apparent. Fortunately, the mismatch is constant with time which can be easily represented by step-like disturbance. This explains why additive disturbance estimates were enough to improve the NLMPC performance. Kalman filtering or rigorous state estimation is necessary in case of slow drift disturbances and/or internally unstable processes (Ali and Zafiriou, 1993). In our case, the process stability is maintained because the reactor temperature and pressure are well controlled (McAuley et al., 1995). Figure 8 shows that the monomer concentration is drastically affected by modelling error while the other gases were marginally affected because they are indirectly influenced by the inaccuracy in reaction rate. Evidently, Melt index and density are strongly affected by the model imperfection because they are directly related to the gases ratio. In addition, direct error in the density correlation is imposed.

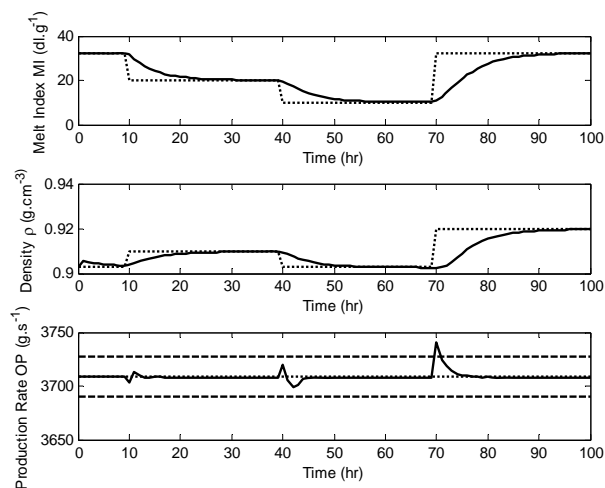


Fig.4. Controlled output response for $T=1$ hr, dotted line: set point, solid line: output response, dashed line: tolerance limit

Typical optimal grade transition involves minimizing the transition time. The settling time can not be incorporated directly in the standard MPC formulation. Instead, faster response can be achieved by setting $P=M$ and using minimum values for the input weights. Our attempts to create quicker responses via controller tuning, is found to produce aggressive and oscillatory feedback behaviour. Rapid transition may not be successfully achievable because it requires drastic changes in the operating conditions which may result in run-away situations (Ohshima and Tanigaki, 2000). Moreover, Gas phase polyethylene reactors are well known of having large gas inventory, long residence times, and broad residence time distributions (Lo and Ray, 2006).

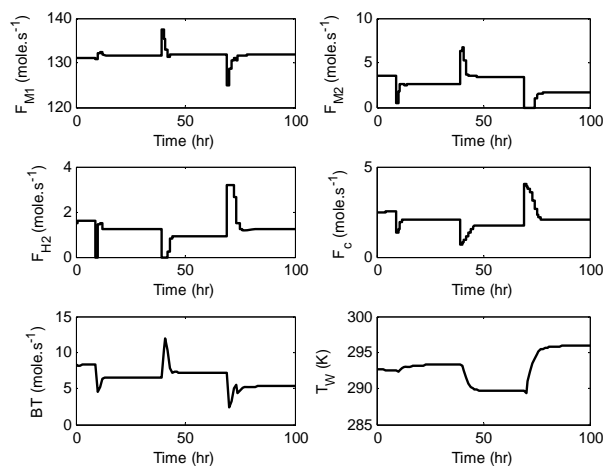


Fig.5. Manipulated response for $T=1$ hr. F_{M1} : monomer feed rate; F_{M2} : comonomer feed rate; F_c : catalyst federate; F_{H2} : hydrogen feed rate; T_w : coolant temperature and BT: bleed flow rate.

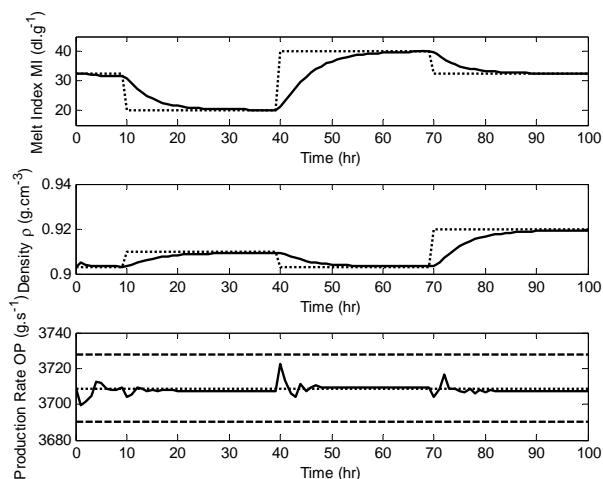


Fig.6. Controlled output response for $T=1$ hr in the presence of modelling errors, dotted line: set point, solid line: output response, dashed line: tolerance limit

4. CONCLUSIONS

The problem of desirable polymer grade transition is investigated in this paper. The required transition is handled via feedback control using nonlinear model predictive control. The NLMPC is based on nonlinear dynamic model of the gas phase polyethylene reactor and a nonlinear correlation for the polymer properties. Effectiveness of the control system to satisfy the grade transition is tested through simulation for perfect model case and for the case where severe modelling errors are imposed in the reaction kinetics, catalyst activity and density correlation parameters. The results indicate the efficiency of NLMPC to deal with the changeover requirements. Reduction of off-specs products can be partially achieved through eliminating response overshoot. Further reduction via minimizing the transition

time is not possible because of the long residence time of the process and the process safety do not serve the cause.

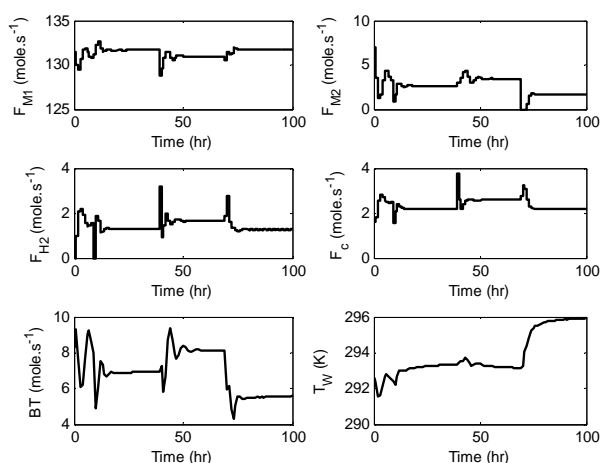


Fig. 7. Manipulated response for $T=1$ hr in the presence of modelling error. F_{M1} : monomer feed rate; F_{M2} : comonomer feed rate; F_C : catalyst feed rate; F_{H2} : hydrogen feed rate; T_w : coolant temperature and BT: bled flow rate.

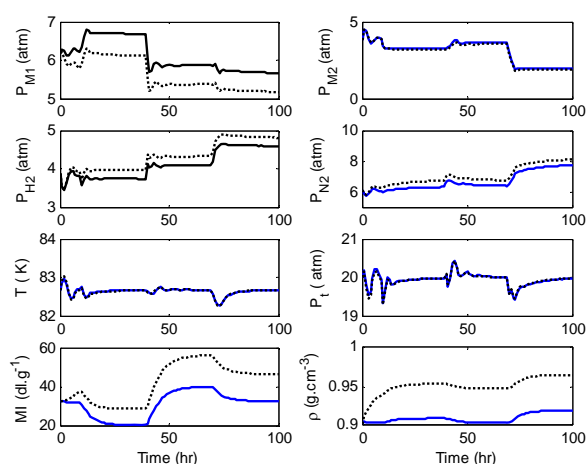


Fig. 8. Plant and model states responses corresponding to the test in Figure 6, dashed line: model, solid line: plant. P_{M1} : monomer partial pressure, P_{M2} : partial pressure of comonomer, P_{H2} : hydrogen partial pressure, P_{N2} : nitrogen partial pressure, P_t : total pressure.

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