Periodic Control of Gas-phase Polyethylene Reactors

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Abstract: Nonlinear model predictive control algorithm is used for the on-line control of polymer molecular weight distribution. The control of chain-length distribution is achieved by selecting a collection of points in the distribution and using it as set points for the control algorithm. An on-line Kalman filter is used to incorporate infrequent and delayed off-line molecular weight measurements. Through simulation; the control algorithm is evaluated, under tracking conditions as well as plant-model mismatch. The results demonstrate that the control algorithm can regulate the entire molecular weight distribution with high computational efficiency and minimum steady state error.

Keywords: Molecular weight distribution, nonlinear model predictive control, Kalman filter, polymerization reactor control, fluidized bed reactor, polyethylene

1. INTRODUCTION

Polymers today are crucial products that are used in all parts of our daily life. The range of applications includes standard applications as packaging materials and textile fibers, and special ones in the automobile and electrical industries. Molecular weight distribution (MWD) is considered as one of the fundamental properties that determines polymer properties and thus its applications. Therefore, it is important to monitor and control MWD during the industrial production of polymers. A significant amount of research has been done in the area of control, monitoring and modelling of polymerization reactors; Excellent reviews have been given by several researchers (Elicabe and Meira, 1988, Embirucu et al., 1996, Congalidis and Richards, 1998, Richards and Congalidis, 2006). A careful study of previous works, with focus on the description of polymer MWD, results in the following conclusions:

1. Most of the work that was done described polymer MWD by the weight average molecular weight (M_w), in addition to polydispersity index (PDI). Few researchers used the entire molecular weight distribution in their control studies. The use of Mw and PDI to describe polymer quality is helpful. However, sometimes, the molecular weight averages can be misleading when the molecular weight distribution shows bimodalities and/or it has high molecular weight tails. Besides, it is very useful to describe polymer quality by using the entire molecular weight distribution because in many polymer applications such as paints and paper coatings, it is required to specify such distribution properly (Sayer et al., 2001).

2. In polyolefins polymerization, the work done to control the entire MWD of the produced polymer used mixtures of different metallocenes (Chatzidoukas et al., 2007, Heiland and kaminsky, 1992) or a hybrid catalyst of Ziegler-Natta and metallocene catalysts in a one stage process (Shamshoum et al., 2003). The use of single reactor to produce the desired polymer is cost-efficient alternative. However, the mixture of different catalysts may lead to complex undesirable catalyst interactions and non-reproducible catalyst behaviour due to the high variability of the polymerization rate of each catalyst (Nele and Pinto, 2000). Additionally, the implementation of such catalyst systems requires a deep understanding of polymerization mechanisms using these catalysts; which is not a simple task. Finally, this method is still in the research phase and, it may take a long time before it can be (if it is developed successfully) widely implemented in industry. An alternative approach is to vary the polymerization conditions periodically in a single polymerization reactor. The periodic operation of continuous chemical reactors can improve the performance of the reacting system and allow better design and control of the molecular weight distribution in a single reactor (Nele and Pinto, 2000, Schiffino, 1995).

The scope of this work is to investigate the production of polyethylene, in a fluidized bed reactor, with a well-defined molecular weight distribution using nonlinear model predictive controller (NLMPC).

2. PROCESS MODEL

In fluidized-bed polyethylene reactors, the co-polymerization of ethylene and -olefin monomers is carried out using a multi-site Ziegler-Natta catalyst, which consists of three different types of active sites. Each active site produces polymer with molecular weight distribution that can be described by Schulz-Flory distribution. The polyethylene reactor process is depicted in Fig 1. The process model was

developed by (McAuley et al., 1995), modifications made in this model were described in (Ali et al., 2003).

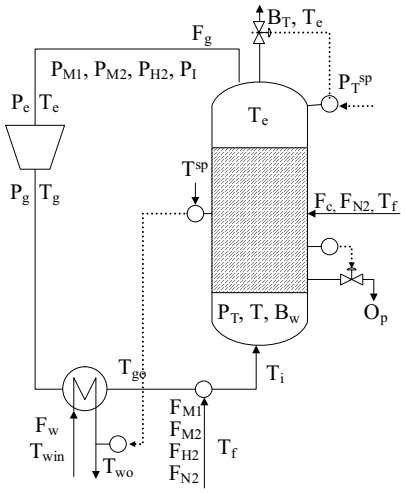

Fig. 1. Polyethylene reactor.

2.1 Molecular Weight Distribution Model

The instantaneous molecular weight distribution for each type of active sites can be described by Flory-Schulz exponential function (Kissin et al., 2005)

$$y_j^d = j \cdot q^2 \cdot \exp(-j \cdot q) \tag{1}$$

with q is the termination probability, j is the number of repeating units and y_j^d instantaneous weight distribution. As assumed above, the catalyst consists of three different active sites and the distribution of the polymers produced by each site type can be represented by Flory's most probable distribution. Thus, the overall distribution of the produced polymer can be calculated by the weighted sum of the three distributions as given below

$$y_{j,ins} = \sum_{i=1}^{3} w_i \cdot (y_j^d)_i \tag{2}$$

where $y_{j,ins}$ is the overall instantaneous molecular weight distribution, and w_i is the mass fraction of each site. The molecular weight distribution of the polymer accumulated in the reactor after a certain polymerization time can be calculated using the following equation:

$$\frac{dy_j}{dt} = \frac{O_p \cdot (y_{j,ins} - y_j)}{B_w} \tag{3}$$

here y_j is the cumulative molecular weight distribution, O_p is polymer production rate and B_w is mass of polymer in the reactor bed. Finally the GPC reading of the MWD is calculated by the following equation:

$$GPC = j \cdot y_j \cdot ln(10) \tag{4}$$

3. 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:

$$\min_{\Delta u(t_k),\ldots,\Delta u(t_{k+M-1})} \sum_{i=1}^{P} \left\| \Gamma(y(t_{k+i}) - R(t_{k+i})) \right\|^2 + \sum_{i=1}^{M} \left\| \Lambda \Delta u(t_{k+i-1}) \right\|^2 \tag{5}$$

subject to

$$A^T \Delta U(t_k) \le b \tag{6}$$

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

$$\frac{dx}{dt} = f(x,u,t) \tag{6}$$

$$y = g(x) \tag{7}$$

from t_k up to t_{k+P} where x and y represent the states and the output of the model, respectively. The symbols || . || denotes the Euclidean norm, k is the sampling instant, Γ and Λ are diagonal weight matrices and $R = [r(k+1) \ldots r(k+P)]^T$ is a vector of the desired output trajectory. $\Delta U(t_k)=[\Delta u(t_k) \ldots \Delta u(t_{k+M-1})]^T$ 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 behavior. 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 (Eq. 5) 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 modeling 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 as follows:

$$d(k) = y_p(k) - y(k) \tag{7}$$

The disturbance estimate, d, is assumed constant over the prediction horizon due to the lack of an explicit means of predicting the disturbance. However, for severe modeling errors, or open-loop unstable processes the regular feedback is not enough to improve the NLMCP response. Hence, state or parameter estimation is necessary to enhance the NLMPC performance in the face of model-plant mismatch. In this work, Kalman filtering (KF) will be incorporated to correct the model state and thus, to address the robustness issue. Utilization of the NLMPC with KF requires adjusting an additional parameter, σ. More details on the integration of KF

with the NLMCP algorithm are given elsewhere (Ali and Zafiriou, 1993). In addition to state estimation by KF, the predicted output will be also corrected by the additive disturbance estimates of Eqn.7.

The main objective of the NLMPC is to control the entire MWD. It is also necessary to maintain acceptable polymer production rate. Process stability is another important issue which is handled through regulating the total gas pressure and the bed temperature. These two controlled variables are adapted via separate PI control loops. The design and tuning parameters of these loops are given elsewhere (Ali et al., 2003).

4. RESULTS AND DISCUSSION

It is worth mentioning that determining input trajectories that provide the desired distribution is difficult as the final polymer quality is sensitive to hydrogen concentration (X) value and the mass of the produced polymer. In this sense, maintaining the desired MWD during process operation is even more challenging. In the presence of model-plant mismatch and/or when unmeasured disturbances enter the plant, the situation becomes more complex. The control objective here is to produce broad polyethylene with well-defined MWD starting from narrow distribution and maintain it there. The results of this case are shown in Figs. 2 and 3. Four manipulated variables, which are the monomer, hydrogen, nitrogen and catalyst flow rates, are used. The weighting factors for these inputs are Λ=[0 0 20 50]. Four controlled variables, which represent specific points in the target MWD, are considered as shown by the dots in Fig 3. The weighting factor for all outputs is given the same value of Γ=[1 1 1 1]×100. The lower limit for the manipulated variables is set to zero and the upper limit is set to twice their nominal values. The MWD target function contains 103 points, however only four points were selected as controlled outputs to reduce the computation effort consumed by the NLMPC calculations. The input horizon (M) and output horizon (P) are taken equal to 1 and 4, respectively. A sampling time of 1 hr is used. Usually the GPC measurements are available at low frequency. Advanced measurement sensors that can provide measurements in the order of minutes are available but at high cost.

Fig. 3 demonstrates the ability of NLMPC to maintain the new set point for the polymer distribution with minor distortion in the distribution function. More interesting is the response of the manipulated variables as shown in Fig. 2. The resulted response of the manipulated variables is in the form of periodic functions. Long prediction and moving horizon capability of NLMPC helped the controller to understand the dynamic nature of the process to an extent that it produced cyclic input sequences. Moreover, Fig. 2 shows how the bleed flow rate (B_T) and the cooling water inlet temperature (T_w) varies by separate PI controllers to maintain the total pressure at 20 atm and the reactor temperature at 82 ^oC. Note that the manipulated variables used by NLMPC are plotted in discrete form because the NLMPC works in discrete time fashion.

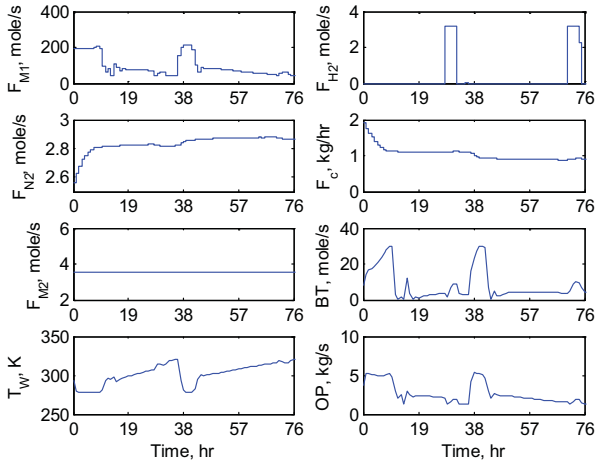

Fig. 2. Manipulated variable response using NLMPC.

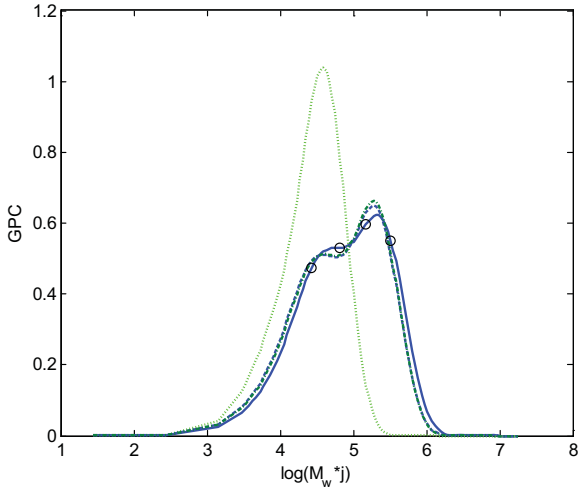

Fig. 3. MWD using NLMPC. Dotted line: initial distribution, solid: target, dashed: controlled distribution.

Next the algorithm was tested for targeting another MWD. In this case, seven points on the GPC curve is taken as the controlled variables with their weights are fixed at G=[1 100 100 200 100 50] ×102. The lower limit of F_{M1} is set to 40 mole/s to keep high monomer concentration in the reactor. The value of the rest of the parameters remains the same as before. The simulation results are shown in Figs. 4 - 5. Evidently, NLMPC generated suitable periodic input sequences that produce MWD close to the desired one as shown in Fig. 5. The MWD suffered from minor distortion; however exact match of the target function is not necessary especially when we know that the relative error in GPC measurements is around 10%. This outcome can be obtained at shorter simulation time. The small production rate is obvious from Fig. 4; in fact, the average production rate is found to be 2.42 kg/s. To improve the production rate, the latter is incorporated as a controlled variable in the NLMPC algorithm. Using γ=0.1 for the production rate, NLMPC managed to increase the polymer production to 2.86 kg/s but with notable loss of the MWD. Results are not shown here for simplicity. Increasing the weight of the designated

controlled output further will of course propagates the production rate but the MWD will depart away from the desired set point. Our investigation revealed the existence of trade-off between the production rate and broadening the MWD. Widening the distribution requires pronounced changes in hydrogen concentration inside the reactor. Increasing hydrogen concentration is achieved by feeding more hydrogen to the reactor this reduces ethylene polymerization rate and as a consequence reduces the overall production rate. Whereas, reducing hydrogen concentration is achieved by opening the vent (Lo and Ray, 2006) that allows hydrogen concentration in the reactor to escape, causing hydrogen concentration to fall quickly. Such reduction in the concentration affects positively on the production rate.

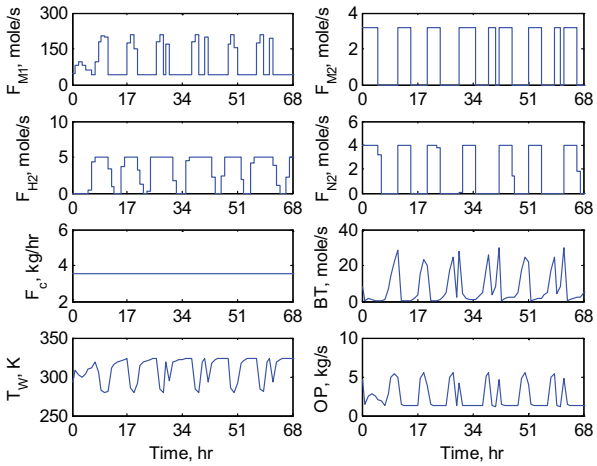

Fig. 4. Manipulated variable response using NLMPC. Decreasing polymer average molecular weight.

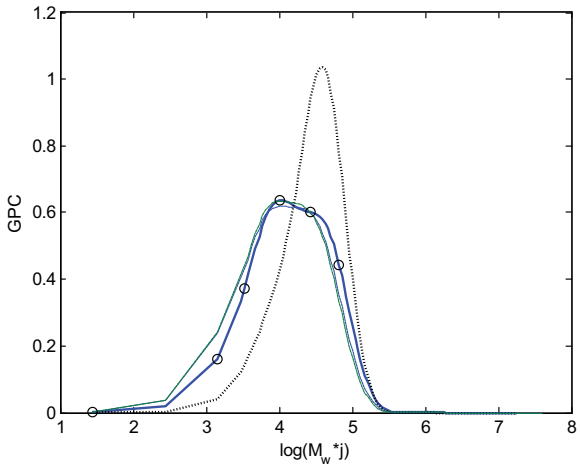

Fig. 5. MWD using NLMPC. Dotted line: initial distribution, solid: target, dashed: controlled distribution.

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 modeling errors, the simulation of targeting higher molecular weight is repeated with−20% error in the reaction rate constant and catalyst activity. The results are shown in Figs. 6 - 7. It is evident that NLMPC is able to keep good control performance despite minor loss of controller performance.

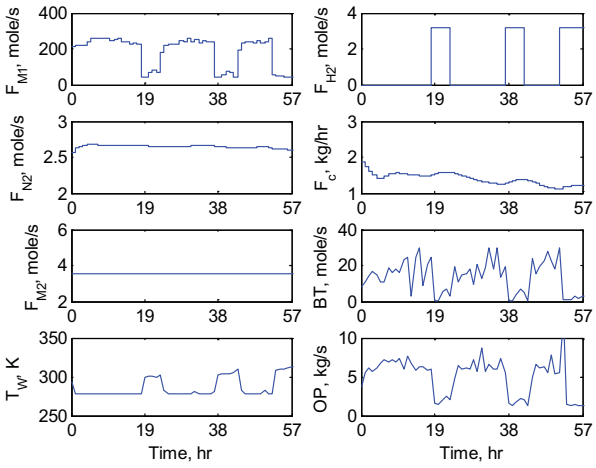

Fig. 6. Manipulated variable response using NLMPC in the presence of -20% in catalyst activation and reaction rate constant.

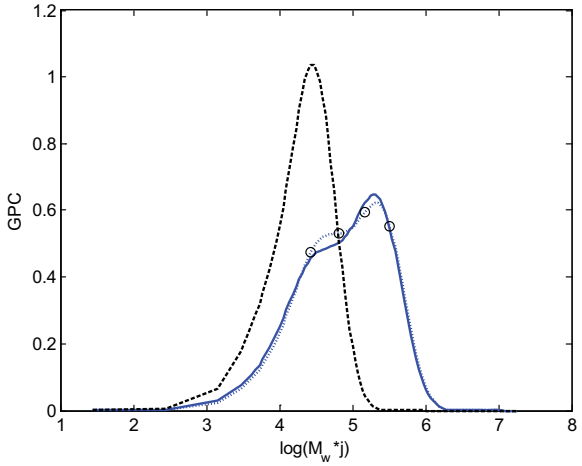

Fig. 7. MWD using NLMPC in the presence of -20% error in catalyst activation and reaction rate constant. Dotted line: initial distribution, solid: target, dashed: controlled distribution.

It is worth mentioning that controller performance could be improved more if the dynamics of hydrogen is faster. Since, hydrogen is not consumed in the reactor and large fluctuations in hydrogen concentration are required to broaden polymer distribution, improving controller performance would not be an easy task. This challenge can be solved using either a catalyst that is highly-sensitive to hydrogen as metallocenes or hydrogen consuming agent. The first approach depends on implementing a relatively new catalyst that is not widely used industrially (Galli and Vecellio, 2001). The second approach still needs more investigation to prove its applicability for the studied process. Finally, note that venting is usually used to reduce hydrogen concentration, as described above, however; venting reactor contents is not an economical choice because monomer also

escapes from the reactor. Nonetheless, no other choices are available.

5. CONCLUSIONS

In industrial applications, the molecular weight distribution of the produced polymer is usually measured using molecular weight averages and polydispersity index. In this article, we have presented an on-line MWD control technique to produce polymers with a target distribution in a fluidized-bed polymerization process. This strategy uses detailed polymerization process model, and Kalman filter to correct model states. A NLMPC controller is designed to control polymer MWD and polymerization process productivity. For the calculation of the MWD, selected points in polymer distribution curve are used as set-points for the controller that manipulates monomer, hydrogen, nitrogen and catalyst feed rates. To test the feasibility of the proposed MWD control technique, simulations have been carried out for ethylene gas-phase polymerization using conventional Zielger-Natta catalyst. The simulations suggest that the proposed control strategy can be useful new technique to control the MWD of polymer in continuous polymerization processes. The performance of the developed control algorithm can be improved more if the dynamic response of hydrogen concentration inside the polymerization reactor is less sluggish.

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