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Property Control in a Continuous MMA Polymerization Reactor using EKF based Nonlinear Model Predictive Controller

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Abstract

A mathematical model was developed for a continuous reactor in which free radical polymerization of methyl methacrylate (MMA) occurred. Elementary reactions considered in this study were initiation, propagation, termination, and chain transfers to monomer and solvent. The reactor model took into account the density change of the reactor contents and the gel effect. A control system was designed for a continuous reactor using extended Kalman filter (EKF) based nonlinear model predictive controller (NLMPC) to control the conversion and the weight average molecular weight of the polymer product. Control input variables were the jacket inlet temperature and the feed flow rate. For the purpose of validation of the control strategy, on-line digital control experiments were conducted with densitometer and viscometer for the measurement of the polymer properties. Despite the complex and nonlinear features of the polymerization reaction system, the EKF based NLMPC performed quite satisfactorily for the property control of the continuous polymerization reactor.

1. Introduction

Continuous polymerization reactors are widely used to produce the synthetic polymers. With an increasing demand for high-quality polymers, it is necessary to build a control strategy that would minimize the production of off-spec polymer during the start-up or grade change operations. However, polymerization processes are difficult to control effectively due to their severe nonlinearity. As a result, several kinds of nonlinear control strategies have been developed for polymerization processes.

Congalidis et al. [1] designed a feedforward and feedback control scheme to regulate polymer production rate, molecular weight, and reactor temperature. Adebekun and Schork [2, 3] demonstrated nonlinear estimation and control method to be suitable for the control of a continuous MMA polymerization reactor. They have obtained satisfactory results even when the desired steady state was open-loop unstable. Kurtz and Henson[4] studied the control of monomer concentration and reactor temperature using a technique which combined input-output decoupling and linear model predictive control.

Despite all these simulation studies, there have been only a few published reports on the actual implementation of such control schemes to continuous polymerization reactor systems through experiments. The globally linearizing control (GLC) method was implemented experimentally to control conversion and temperature by Soroush and Kravaris [5]. Their experimental study showed that conversion could not be controlled effectively by manipulating the flow rate of the inlet initiator stream. Mutha et al. [6] designed the control strategy to treat control nonaffine systems (nonlinear in the manipulated variables). They presented the experimental evaluation of a nonlinear model-based estimator and predictive control strategy on a continuous MMA solution polymerization reactor.

From a review of earlier works, it is apparent that what is in demand is not only a more effective control algorithm but also actual implementation of the control strategy on the continuous polymerization reactor system.

In this study, the extended Kalman filter based nonlinear model predictive controller [7] was implemented experimentally to control the conversion and the weight-average molecular weight of polymer product in a continuous MMA polymerization reactor. Manipulated variables were the jacket inlet temperature and the feed flow rate. In order to measure the properties of polymer on line, the densitometer and the viscometer were utilized.

2. Polymerization Reactor Model

The polymerization system considered in this work is a continuous stirred tank reactor for MMA polymerization. The reaction kinetics are assumed to follow the free radical polymerization mechanism including chain transfer reactions to both solvent and monomer.

From the free radical polymerization mechanism, the following mass balance equations can be derived for each of initiator, monomer and solvent:

$$\frac{d(IV)}{dt} = q_f I_f - qI - k_d IV \tag{1}$$

$$\frac{d(MV)}{dt} = q_f M_f - qM - \{2fk_d I + (k_p + k_{trm})MG_0\}V \tag{2}$$

$$\frac{d(SV)}{dt} = q_f S_f - qS - k_{trs} SG_0 V \tag{3}$$

in which V and q denote the volume of the reaction mixture and the volumetric flow rate, respectively, while I, M, S, and G_0 represent the concentrations of initiator, monomer, solvent and living polymer, respectively. Subscript f denotes the feed stream.

The method of moments was adopted to calculate the number-average molecular weight (*Mn*) and the weight-average molecular weight (*Mw*). The definitions of the moments are as follows:

$$G_k = \sum_{n=1}^{\infty} n^k R_n(t) \quad k = 0,\ 1,\ 2 \tag{4}$$

$$F_k = \sum_{n=1}^{\infty} n^k P_n(t) \quad k = 0,\ 1,\ 2 \tag{5}$$

where G_k and F_k are the kth moments of living and dead polymer concentrations, respectively. One can derive balance equations for the first three moments of the living and dead polymer concentrations as follows:

$$\frac{d(G_0V)}{dt} = -qG_0 + \{2fk_dI - k_tG_0^2\}V \tag{6}$$

$$\frac{d(G_1V)}{dt} = -qG_1 + \{2fk_dI + k_pMG_0 - k_tG_0G_1 + (k_{trm}M + k_{trs}S)(G_0 - G_1)\}V \tag{7}$$

$$\frac{d(G_2V)}{dt} = -qG_2 + \{2fK_dI + k_pM(G_0 + 2G_1) - k_tG_0G_2 + (k_{trm}M + k_{trs}S)(G_0 - G_2)\}V \tag{8}$$

$$\frac{d(F_0V)}{dt} = -qF_0 + \left\{\frac{1}{2}(k_t + k_{td})G_0^2 + (k_{trm}M + k_{trs}S)G_0\right\}V \tag{9}$$

$$\frac{d(F_1V)}{dt} = -qF_1 + \{(k_tG_0 + k_{trm}M + k_{trs}S)G_1\}V \tag{10}$$

$$\frac{d(F_2V)}{dt} = -qF_2 + \{(k_{td}G_0 + k_{trm}M + k_{trs}S)G_2 + k_{tc}(G_0G_2 + G_1^2)\}V \tag{11}$$

As the monomer is converted to the polymer, the density of the reaction mixture increases and thus the volume V of the reactor contents changes as the reaction proceeds.

It is well-known that free radical polymerization kinetics exhibit the gel effect, which results from the self-acceleration of the polymerization rate and diffusion controlled termination reaction among the large polymer radicals. At high conversion, the propagation rates may also be diffusion controlled when the polymerization temperature is below the glass transition temperature of the polymer being synthesized. In this work, we adopted the gel effect correlation proposed by Schmidt and Ray [8].

The temperature dependence of the rate constants is assumed to follow the Arrhenius law. The kinetic data used for the plant model of this study are taken from the literature [9]. Based on the mass balance equations, the conversion, the number- and weight-average molecular weights are defined by the following equations:

$$X = \frac{V_p\rho_p}{V\rho_r} \tag{12}$$

$$Mw = w_m \times \frac{(G_2 + F_2)}{(G_1 + F_1)} \tag{13}$$

$$Mm = w_m \times \frac{(G_1 + F_1)}{(G_0 + F_0)} \tag{14}$$

where subscripts p and r denote the polymer and reactant, respectively.

The energy balances for reactor and jacket can be formulated as follows:

$$\frac{d(V(\rho C_p)_{mean}T_r)}{dt} = (\rho C_p)_{mean}q_fT_f - (\rho C_p)_{mean}qT_r + (-\Delta H)k_pMG_0 - UA(T_r - T_j) + Q_{loss} \tag{15}$$

$$\frac{d(V_j(\rho C_p)_cT_j)}{dt} = (\rho C_p)_cq_fT_{jin} - (\rho C_p)_cq_cT_{jout} + UA(T_r - T_j) + U_aA_a(T_a - T_j) \tag{16}$$

where ΔH, U, A, and Q_{loss} denote the heat of reaction for propagation, the overall heat transfer coefficient, the heat exchange area and the rate of heat loss, respectively. Further, the subscript r, j, c and a represent the reaction mixture, jacket, heating-cooling water and ambient air, respectively. As the conversion increases, the heat transfer efficiency becomes poorer. In this study, UA, U_aA_a and Q_{loss} are assumed to be unmeasured disturbances.

3. Extended Kalman Filter based NLMPC

3.1 Process model

We assume that the process model is expressed through the following nonlinear differential equation:

$$\dot{x} = f(x,u,d) \tag{17}$$

$$y = g(x,d) \tag{18}$$

the state vector x, the manipulated input vector u, the unmeasured disturbance d and the output vector y are defined as

$$x = \left[\frac{I}{I_f}\ \frac{M}{M_f}\ \frac{S}{S_f}\ \frac{F_0}{F_{00}}\ \frac{F_1}{F_{10}}\ \frac{F_2}{F_{20}}\ \frac{T_r}{T_a}\ \frac{T_j}{T_a}\right]^T,\quad u = \left[\frac{T_{jin}}{T_a}\ \frac{q_f}{q_{f0}}\right]^T$$
$$d = [UA\ \ U_aA_a\ \ Q_{loss}]^T,\quad y = \left[\frac{T_r}{T_a}\ X\ Mw\right]^T \tag{19}$$

The kth moment of the dead polymer concentration is much larger than that of the living polymer concentration. Therefore, the quasi-steady-state approximation is valid for the moments of the living polymer concentration.

For digital controller design, u and d can be assumed to be constant between the sampling instants. Hence, a discrete version of the process model can be expressed as follows [7]:

$$x_k = F_{ts}(x_{k-1}, u_{k-1}, d_{k-1}) \tag{20}$$

$$y_k = g(x_k, d_k) \tag{21}$$

where $F_{ts}(x_{k-1}, u_{k-1}, d_{k-1})$ denotes the terminal state vector obtained by integrating the ordinary differential equation (17) for one sampling interval with the initial condition of x_{k-1} and constant inputs of $u=u_{k-1}$ and $d=d_{k-1}$. In general, F_{ts} cannot be written in closed form.

For the purpose of state estimation, it is common to express the unmeasured disturbance signal d as an integrated white noise. It is also possible that the measurements of y_k are corrupted by measurement noise v_k. Combining (20) and (21) with unmeasured disturbance model, we arrive at the following augmented model:

$$\begin{bmatrix} x_k \\ x_k^w \end{bmatrix} = \begin{bmatrix} F_{ts}\left(x_{k-1}, u_{k-1}, C^w x_{k-1}^w\right) \\ A^w x_{k-1}^w \end{bmatrix} + \begin{bmatrix} 0 \\ B^w \end{bmatrix} w_{k-1} \tag{22}$$

$$\hat{y}_k = g(x_k, C^w x_k^w) + v_k \tag{23}$$

where w_k is discrete-time white noise with covariance R^w and v_k is white noise with covariance of R^v.

3.2 State estimation: extended Kalman filter (EKF)

The basic idea of EKF is to perform linearization at each time step to approximate the nonlinear system as a time-varying system affine in the variables to be estimated, and apply the linear filter theory to it. In the EKF, the discrete process model equation is linearized as follows:

$$\tilde{A}_{k-1} = \frac{\partial f(x,u,d)}{\partial x} \Big| (x = x_{k-1|k-1}, u = u_{k-1}, d = C^w x_{k-1|k-1}^w) \tag{24}$$

$$A_{k-1} = \exp(\tilde{A}_{k-1} t_s) \tag{25}$$

$$\tilde{B}_{k-1}^d = \frac{\partial f(x,u,d)}{\partial d} \Big| (x = x_{k-1|k-1}, u = u_{k-1}, d = C^w x_{k-1|k-1}^w) \tag{26}$$

$$B_{k-1}^d = \int_0^{t_s} \exp(\tilde{A}_{k-1}\tau) d\tau \cdot \tilde{B}_{k-1}^d \tag{27}$$

$$C_k = \frac{\partial g(x,d)}{\partial x} \Big| (x = x_{k|k-1}, d = C^w x_{k|k-1}^w) \tag{28}$$

$$C_k^d = \frac{\partial g(x,d)}{\partial d} \Big| (x = x_{k|k-1}, d = C^w x_{k|k-1}^w) \tag{29}$$

If the Jacobian matrices of f and g with respect to x and d are used, the augmented state and the measured output vector are linearly approximated as follows:

$$\begin{bmatrix} x_k \\ x_k^w \end{bmatrix} \approx \begin{bmatrix} F_{ts}(x_{k-1|k-1}, u_{k-1}, C^w x_{k-1|k-1}^w) \\ A^w x_{k-1|k-1}^w \end{bmatrix} + \Phi_{k-1} \begin{bmatrix} x_{k-1} - x_{k-1|k-1} \\ x_{k-1}^w - x_{k-1|k-1}^w \end{bmatrix} + \Gamma^w w_{k-1} \tag{30}$$

$$\hat{y}_k \approx g(x_{k|k-1}, C^w x_{k|k-1}^w) + \Xi_k \begin{bmatrix} x_k - x_{k|k-1} \\ x_k^w - x_{k|k-1}^w \end{bmatrix} + v_k \tag{31}$$

$$\Phi_{k-1} = \begin{bmatrix} A_{k-1} & B_{k-1}^d C^w \\ 0 & A^w \end{bmatrix}, \Gamma^w = \begin{bmatrix} 0 \\ B^w \end{bmatrix}, \Xi_k = \begin{bmatrix} C_k & C_k^d \cdot C^w \end{bmatrix} \tag{32}$$

Under the assumption that the nonlinear system (17) and (18) are well approximated by the affine system (30) and (31) obtained via local linearization, the Kalman filter provides the optimal estimator. The extended Kalman filter algorithm is summarized by the occurrence formulas:

Model prediction:

$$\begin{bmatrix} x_{k|k-1} \\ x_{k|k-1}^w \end{bmatrix} = \begin{bmatrix} F_{ts}(x_{k-1|k-1}, u_{k-1}, C^w x_{k-1|k-1}^w) \\ A^w x_{k-1|k-1}^w \end{bmatrix} \tag{33}$$

Measurement correction:

$$\begin{bmatrix} x_{k|k} \\ x_{k|k}^w \end{bmatrix} = \begin{bmatrix} x_{k|k-1} \\ x_{k|k-1}^w \end{bmatrix} + L_k \left(\tilde{y}_k - g(x_{k|k-1}, C^w x_{k|k-1}^w)\right) \tag{34}$$

where

$$L_k = \Sigma_{k|k-1} \Xi_k^T \left(\Xi_k \Sigma_{k|k-1} \Xi_k^T + R^v\right)^{-1} \tag{35}$$

$$\Sigma_{k|k-1} = \Phi_{k-1} \Sigma_{k-1|k-1} \Phi_{k-1}^T + \Gamma^w R^w \left(\Gamma^w\right)^T \tag{36}$$

$$\Sigma_{k|k} = (I - L_k \Xi_k) \Sigma_{k|k-1} \tag{37}$$

The model update equation (33) requires nonlinear integration of ODE (17) with known initial condition and constant inputs, so that this is usually the most time-consuming step.

3.3 Multistep prediction equation

Model predictive control algorithms use a model to predict the effect of past control inputs on the process output and then calculate the current and future control actions required to move the predictive process outputs along their desired setpoint trajectories. We assume that the controlled variable y_c is expressed as

$$y_k^c = h(x_k, d) \tag{38}$$

In order to develop a prediction equation for y_c that is linear with respect to the undecided input moves, we again linearize the above expression with respect to $x_{k|k}$:

$$y_k^c \approx h(x_{k|k}, C^w x_{k|k}^w) + \begin{bmatrix} H_k & H_k^d \cdot C^w \end{bmatrix} \begin{bmatrix} x_k - x_{k|k} \\ x_k^w - x_{k|k}^w \end{bmatrix} \tag{39}$$

where the Jacobian matrices are defined as

$$H_k = \frac{\partial h(x,d)}{\partial x} \Big| (x = x_{k|k}, d = C^w x_{k|k}^w) \tag{40}$$

$$H_k^d = \frac{\partial h(x,d)}{\partial d} \Big| (x = x_{k|k}, d = C^w x_{k|k}^w) \tag{41}$$

The prediction equation for p sampling intervals into the future can be written as

$$\begin{bmatrix} y_{k+1|k}^c \\ y_{k+2|k}^c \\ \vdots \\ y_{k+p|k}^c \end{bmatrix} = \begin{bmatrix} I \\ I \\ \vdots \\ I \end{bmatrix} \left(h\left(x_{k|k}, C^w x_{k|k}^w\right) - H_k x_{k|k} - H_k^d C^w x_{k|k}^w\right) + \begin{bmatrix} H_k F_{ts}\left(x_{k|k}, u_{k-1}, C^w x_{k|k}^w\right) \\ H_k F_{2ts}\left(x_{k|k}, u_{k-1}, C^w \left(A^w\right)^i x_{k|k}^w \Big|_{0 \le i \le 1}\right) \\ \vdots \\ H_k F_{pts}\left(x_{k|k}, u_{k-1}, C^w \left(A^w\right)^i x_{k|k}^w \Big|_{0 \le i \le p-1}\right) \end{bmatrix} + \begin{bmatrix} H_k^d C^w A^w \\ H_k^d C^w \left(A^w\right)^2 \\ \vdots \\ H_k^d C^w \left(A^w\right)^p \end{bmatrix} x_{k|k}^w + \begin{bmatrix} H_k B_k'' & 0 & \cdots & 0 \\ H_k \left(A_k B_k'' + B_k''\right) & H_k B_k'' & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=0}^{p-1} H_k A_k^i B_k'' & \cdots & \cdots & H_k B_k'' \end{bmatrix} \begin{bmatrix} \Delta u_k \\ \Delta u_{k+1} \\ \vdots \\ \Delta u_{k+m-1} \end{bmatrix} \tag{42}$$

In order to keep the notation simple, we will express the above prediction equation as

$$\begin{aligned} Y_{k+1|k} &= \Im\left(h\left(x_{k|k}, C^w x_{k|k}^w\right) - H_k x_{k|k} - H_k^d C^w x_{k|k}^w\right) \\ &\quad + S_k^x \left(x_{k|k}, u_{k-1}, x_{k|k}^w\right) + S_k^{x^*} x_{k|k} + S_k'' \Delta U_k = Y_{k+1|k}^0 + S_k'' \Delta U_k \end{aligned} \tag{43}$$

where the term $Y_{k+1|k}^0$ can be calculated from the state estimates by performing integration of the nonlinear ODE and calculating the Jacobian matrices. S_k'' is a matrix that must be recomputed at each time step based on the updated Jacobian matrices.

3.4 Computation of control moves

On the basis of the multistep prediction equation (43), a sequence of optimal control moves can be computed, which minimizes a chosen norm of the expected future error. The objective function and constraints for the EKF based NLMPC are as follows:

$$\min_{\Delta u_k} \left\| \Lambda^y \left[Y_{k+1|k} - R_{k+1|k} \right] \right\|_2^2 + \left\| \Lambda^u \Delta U_k \right\|_2^2 \tag{44}$$

$$u_{k+l}^{low} \le u_{k+l} \le u_{k+l}^{high}, \quad 0 \le l \le m-1 \tag{45}$$

$$-\Delta u_{k+l}^{\max} \le \Delta u_{k+l} \le \Delta u_{k+l}^{\max}, \quad 0 \le l \le m-1 \tag{46}$$

$$y_{k+l}^{low} \le y_{k+l}^{c} \le y_{k+l}^{high}, \quad 0 \le l \le p \tag{47}$$

where $R_{k+l|k}$ is the future reference vector for y_c available at time k. Λ^y and Λ^u are weighting matrices that are chosen as diagonal matrices in most cases.

In the presence of constraints, the optimization can be solved via quadratic programming. A detailed solution procedure was studied by Ricker [10]. The control moves are implemented in receding horizon fashion; that is, only the first move is implemented and the optimization procedure is repeated at the next sampling time.

4. Experimental

Figure 1 shows the schematic diagram of the continuous MMA polymerization reactor system used in this study. The jacketed glass overflow reactor has a capacity of 1L and is equipped with a stirrer for the mixing of the reactants. An inverter is adopted to maintain the stirring speed at 300 rpm. Heating and cooling of the reaction mixture are carried out by heating-cooling water through the jacket. The valve stem positions of the hot and cold water lines were adjusted, in a cascade control configuration, in such a way that the jacket inlet temperature was kept equal to the desired value specified by the master controller.

A variable-speed, remote setpoint pump is used for pumping monomer, solvent and initiator solution into the reactor. This pump is piston-operated metering pump from FMI LAB (Model QVG50). The speed of pump motor is controlled by stroke rate controller (Model V200). The reaction product flows out of the reactor via an overflow line. In order to measure the density and viscosity of the reaction mixture, the circulation line is attached to the reactor. The product is circulated by the diaphragm metering pump through the circulation line, in which the on-line densitometer and viscometer are installed. The measured values of density are used to calculate the conversion and the viscosity measurements along with conversion data were used to determine the weight-average molecular weight. The on-line measurement techniques are well described in the literature [11].

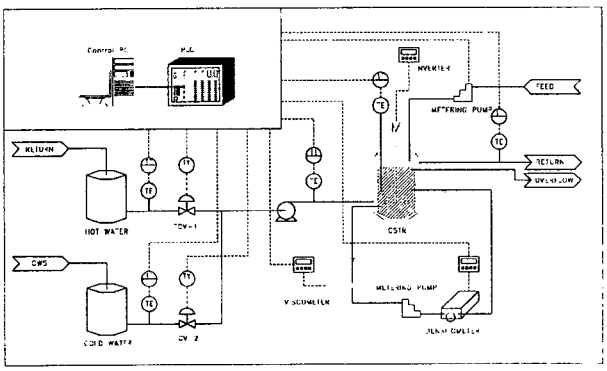

Figure 1. Schematic diagram of the continuous MMA polymerization reactor system.

Table 1. Reference conditions for the continuous MMA polymerization

Item	Value
Initial charge	
Monomer	450 ml
Solvent	450 ml
Initiator	4.5g
Feed concentration	
Monomer	4.65 mol/L
Solvent	5.04 mol/L
Initiator	0.02 mol/L
Operating conditions	
Reactor temperature	70-80 °C
Feed flow rate	5-15 ml/min

Ethylacetate (EA), benzoylperoxide (BPO), and methylmetacrylate (MMA) are used as solvent, initiator, and monomer, respectively. The inhibitor contained in the monomer is eliminated by using a 0.1M NaOH solution. Nitrogen is bubbled through the reaction mixture for about 30 minutes to purge the monomer and solvent of oxygen. The reactor temperature is raised to the desired starting temperature and then the purified initiator dissolved in solvent is fed to start the

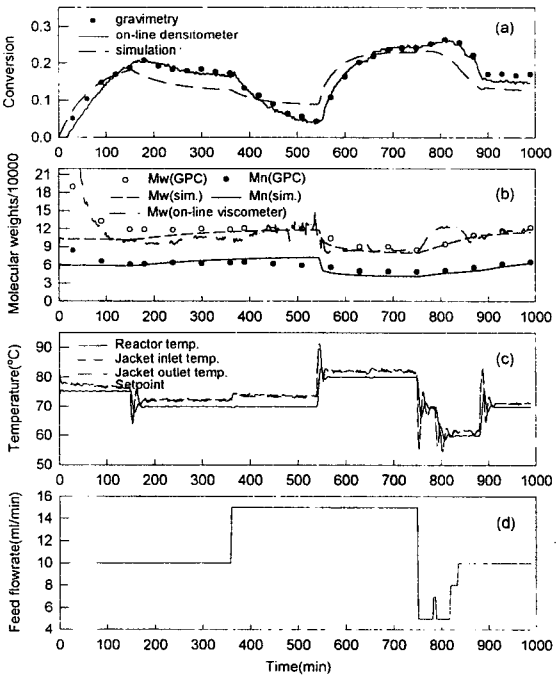

Figure 2. Histories of conversion and molecular weights when the setpoints of the reactor temperature and the feed flow rate undergo a series of step changes, respectively.

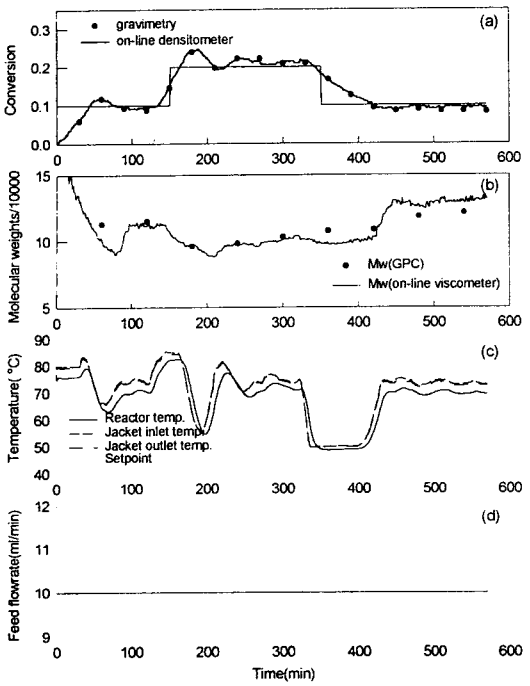

Figure 3. Servo and regulatory responses of EKF based NLMPC for step changes in the setpoint for conversion.

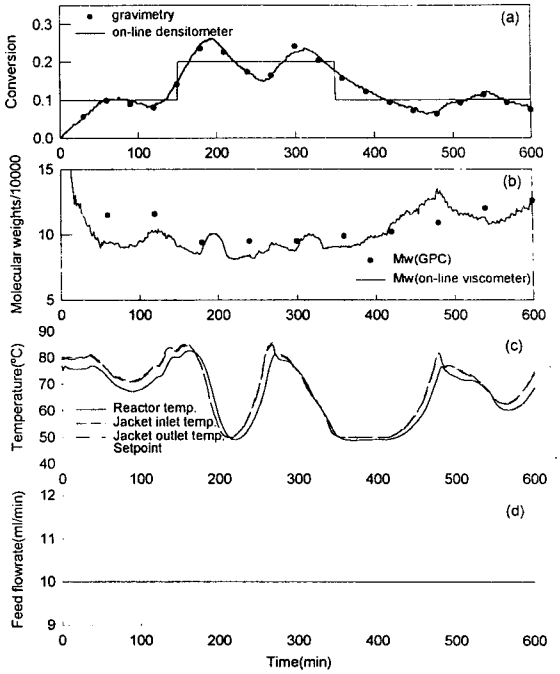

Figure 4. Servo and regulatory responses of linear MPC for step changes in the setpoint for conversion.

polymerization. Also the switch of the feeding pump is turned on to feed the monomer, solvent, and initiator solution into the reactor. The set of reference conditions for the experiment is given in Table 1. The reaction mixture is sampled at successive times and the conversion is measured by the gravimetric method, while the average molecular weights are measured by the gel permeation chromatography.

5. Results and Discussion

5.1 Model validation and on-line measurement

The polymerization reaction experiment was conducted and the polymer properties were measured both on-line and off-line in such a way that the proposed model and measurement technique could be validated. Figure 2 shows the comparison between the experimental (filled keys) and simulation (curves) results when the setpoints of reactor temperature and the feed flow rate undergo a series of step changes, respectively. The two are in fairly good agreement not only in terms of the conversion but also in view of the molecular weights. Therefore, it may be concluded that the model developed in this study is adequate to be used for model predictive controller.

The on-line measurement values of conversion and weight-average molecular weight are presented in Figure 3 (Part (a) and (b)). Clearly, the values are found to agree well with the off-line measurement values. Hence, it is justified to use the measured values for on-line state estimation.

5.2 Controller performance : SISO case

In this case, the manipulated variable is the jacket inlet temperature and the controlled variable is the conversion. The design parameters are chosen as follows:

$$\Sigma_{0|0} = diag(10^{-10}\ 10^{-10}\ 10^{-10}\ 10^{-4}\ 10^{-4}\ 10^{-10}\ 10^{-10}\ 10^{-2}) \quad (48)$$

$$R^{y} = diag(10^{-6}\ 10^{-8}\ 10^{-2}) \quad (49)$$

$$p = 30,\ m = 5,\ \Lambda^{y} = 1,\ \Lambda^{u} = 2.5 \quad (50)$$

The maximum and minimum constraints of the jacket inlet temperature are 85 and 50°C, respectively.

Figure 3 shows the servo and regulatory responses of EKF based NLMPC for step changes in the setpoint for conversion. In less than 100 minutes, the controller drives the conversion to its setpoint. When there is a step change in the conversion setpoint from 0.1 to 0.2, the controller output (the setpoint of the jacket inlet temperature) increases to its maximum limit, 85°C, and finally it varies around its steady-state value (Figure 3(c)). Part(b) shows variations of the weight-average molecular weight. The curves and the filled keys represent the on-line and off-line data, respectively.

The performance of the linear MPC (LMPC) is presented in Figure 4. This MPC is designed using a linear model derived at the nominal steady state. The servo response is indeed worse than that of EKF based NLMPC. The setpoint change causes larger, poorly-damped oscillation in conversion (Part (a)). Also, the reactor temperature does not reach its steady-state value as shown in part (c).

5.3 Controller performance : MIMO case

In this case, the manipulated values are the jacket inlet temperature and the feed flow rate whereas the controlled variables are the conversion and the weight-average molecu-

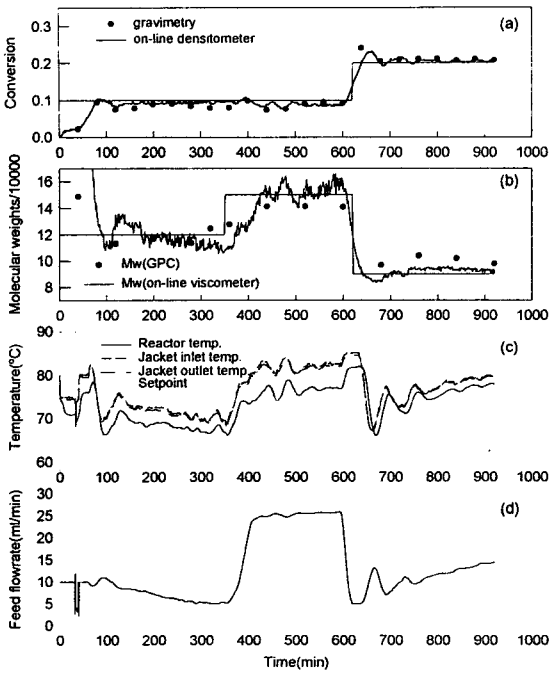

Figure 5. Servo and regulatory responses of EKF based NLMPC for step changes in the setpoints of conversion and molecular weight.

lar weight.

The maximum and minimum constraints of feed flow rate are 30 and 5 ml/min, respectively. The weighting matrices are *diag*(10, 0.05) for the output and *diag*(30,2) for the input. The other parameters are the same as for the case of SISO.

In Fig. 5, part(a) and (b) present the profiles of the controlled outputs when there are step changes in the setpoints of conversion and molecular weight. The corresponding profiles of the jacket inlet temperature and the feed flow rate are shown in parts (c) and (d). The setpoint of molecular weight is changed from 120,000 g/mol to 150,000 g/mol at 350 min., while the setpoint of conversion remains unchanged. Since the reactor has interactive dynamics, the controller increases the feed flow rate (to increase the weight-average molecular weight) and also increases the jacket inlet temperature (to maintain the conversion at 0.1) simultaneously to compensate for the interaction. However, the controller cannot fully compensate for the effect of molecular weight setpoint change and thus the conversion slightly oscillates. Finally, the conversion returns to its setpoint at about 500 min.

6. Conclusions

An EKF based nonlinear model predictive controller was implemented experimentally to control the conversion and the weight-average molecular weight in a continuous MMA polymerization reactor. For this a mathematical model was developed for a continuous reactor in which free radical polymerization of methyl methacrylate (MMA) occurred. In order to measure the properties of polymer on line, the densitometer and the viscometer were utilized.

Based on the experimental results, it is concluded that the EKF based NLMPC performs better than the LMPC in the sense of better regulation and less oscillation.

Despite the complex and nonlinear features of the polymerization reaction system, the EKF based NLMPC performed quite satisfactorily for the property control of the continuous polymerization reactor. It seems evident that the proposed control strategy may be applied to other continuous polymerization processes to minimize the production of off-spec polymer.

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