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TEMPERATURE CONTROL OF A BATCH PMMA POLYMERIZATION REACTOR USING ADAPTIVE PREDICTIVE CONTROL ALGORITHM

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Abstracts An adaptive unified predictive control (UPC) algorithm is applied to a batch polymerization reactor for poly(methyl methacrylate) (PMMA) and the effects of controller parameters are investigated. Computational studies are performed for a batch polymerization system model developed in this study. A transfer function in parametric form is estimated by recursive least squares (RLS) method, and the UPC algorithm is implemented to control the reactor temperature on the basis of this transfer function. The adaptive unified predictive controller shows a better performance than the PID controller for tracking set point changes, especially in the latter part of reaction course when gel effect becomes significant. Various performance can be acquired by selecting adequate values for parameters of the adaptive unified predictive controller; in other words, the optimal set of parameters exists for a given set of reaction conditions and control objective.

Keywords Adaptive control, UPC, RLS method, PMMA, Batch polymerization

1. INTRODUCTION

Predictive control is a control scheme in which the controller determines a control output profile that optimizes a given objective function on a time interval extending from the current time to the current time plus prediction horizon. Since the concept of predictive control was introduced by Richalet, many different predictive controllers have been proposed in the literature, and Soeterboek (1990) proposed the unified predictive controller encompassing the features of several well-known predictive controllers.

Because of complex reaction mechanism, strong inherent nonlinearities, and the absence of steady state, the control of a batch polymerization process has many problems. Further, like most other chemical processes, model uncertainties are unavoidable and this characteristics make the application of model-based controllers difficult. Adaptive control scheme is a possible solution and some studies have been performed in the domain of polymerization. Houston and Schork (1987) applied adaptive predictive control algorithm to semibatch polymerization reactor on a linear approximation and Kiparissides *et al.* (1990) used long-range predictive control method for the control of molecular weight in a batch polymerization reactor.

In this work, a control system for the temperature control of a batch PMMA polymerization reactor was designed using adaptive unified predictive control algorithm, and then the performance of the controller and the effects of the controller parameters were investigated by simulation.

2. REACTOR MODEL

The system considered in this study is batch,solution polymerization of methyl methacrylate (MMA) using benzoyl peroxide (BPO) as an initiator. The physical system consists of jacketed reactor, the reaction mixture, and the heating-cooling water.

2.1 Kinetic Mechanism

The kinetic mechanism for the free radical solution polymerization of PMMA is given in Table 1. In this table, R_j and P_j denote living and dead polymer with chain length j, respectively.

Table 1. Kinetic mechanism for the free radical solution polymerization

Initiation	$I \xrightarrow{k_d} 2\varphi\cdot$ $\varphi\cdot + M \xrightarrow{k_i} R_1\cdot$
Propagation	$R_j\cdot + M \xrightarrow{k_p} R_{j+1}\cdot$
Termination by combination	$R_i\cdot + R_j\cdot \xrightarrow{k_{tc}} P_{i+j}$
Termination by disproportionation	$R_i\cdot + R_j\cdot \xrightarrow{k_{td}} P_i + P_j$
Chain transfer to monomer	$R_i\cdot + M \xrightarrow{k_{trm}} P_i + R_1\cdot$
Chain transfer to solvent	$R_i\cdot + S \xrightarrow{k_{trs}} P_i + S\cdot$

2.2 Mass Balance Equations

From the kinetic mechanism, the following differential equations may be derived to represent dynamics of the different species in the polymerization reactor.

Initiator

$$\frac{1}{V}\frac{d(IV)}{dt} = -k_d I \tag{1}$$

Monomer

$$\frac{1}{V}\frac{d(MV)}{dt} = -2fk_d I - k_p M G_0 - k_{trm} M G_0 \tag{2}$$

Solvent

$$\frac{1}{V}\frac{d(SV)}{dt} = -k_{trs} S G_0 \tag{3}$$

Moment of living polymer concentration

$$\begin{aligned} \frac{1}{V}\frac{d(G_0V)}{dt} &= 2fk_d I - k_t G_0^2 \\ \frac{1}{V}\frac{d(G_1V)}{dt} &= 2fk_d I + k_p M G_0 - k_t G_0 G_1 \\ &\quad + k_{trm} M (G_0 - G_1) + k_{trs} S (G_0 - G_1) \\ \frac{1}{V}\frac{d(G_2V)}{dt} &= 2fk_d I + k_p M (G_0 + 2G_1) - k_t G_0 G_2 \\ &\quad + k_{trm} M (G_0 - G_2) + k_{trs} S (G_0 - G_2) \end{aligned} \tag{4}$$

Moment of dead polymer concentration

$$\begin{aligned} \frac{1}{V}\frac{d(F_0V)}{dt} &= \frac{1}{2}k_t G_0^2 + \frac{1}{2}k_{td} G_0^2 + k_{trm} M G_0 \\ &\quad + k_{trs} S G_0 \\ \frac{1}{V}\frac{d(F_1V)}{dt} &= k_t G_0 G_1 + k_{trm} M G_1 + k_{trs} S G_1 \\ \frac{1}{V}\frac{d(F_2V)}{dt} &= k_{tc}(G_0 G_2 + G_1^2) + k_{td} G_0 G_2 \\ &\quad + k_{trm} M G_2 + k_{trs} S G_2 \end{aligned} \tag{5}$$

where I, M, and S are the concentrations of initiator, monomer, and solvent, respectively. G_k and F_k are the kth moments of living and dead polymer concentrations, respectively, which are defined by

$$\begin{aligned} G_k &= \sum_{j=1}^{\infty} j^k R_j \\ F_k &= \sum_{j=1}^{\infty} j^k P_j \qquad (k = 0, 1, 2) \end{aligned} \tag{6}$$

Gel effect is an important phenomenon in free radical polymerization which occurs at high monomer conversion and in this work, it is considered by introducing the correlations for the gel and glass effects proposed by Schmidt and Ray (1981).

2.3 Energy Balance Equations

The cold and hot water at constant temperatures are mixed by means of a three-way valve and the heating-cooling water flowrate through the jacket is maintained constant. The dynamics of the mixer is not considered, thus the temperature of the jacket inlet water is given by

$$T_{j,in} = (1-\beta)T_{cold} + \beta T_{hot} \tag{7}$$

where $T_{j,in}$ is the jacket inlet water temperature, T_{cold} is the cold water temperature, T_{hot} is the hot water temperature and β is the position of the three-way valve.

Provided that the jacket temperature is arithmetic mean of jacket inlet temperature and jacket outlet temperature, the dynamics of reactor and jacket are described by

$$\begin{aligned} \frac{d(\rho C_p V_r T_r)}{dt} &= (-\Delta H_p) k_p M G_0 V_r - UA(T_r - T_j) \\ \frac{d(\rho_c C_{pc} V_j T_j)}{dt} &= 2\rho_c C_{pc} q_c (T_{j,in} - T_j) + UA(T_r - T_j) \\ &\quad - U_\infty A_\infty (T_j - T_\infty) \end{aligned} \tag{8}$$

where ΔH_p is the reaction enthalpy of propagation, U is overall heat transfer coefficient, and A is heat transfer area. Further, the subscript r, j, and ∞ indicate reactor, jacket, and ambient air, respectively. The heat exchange between reactor and ambient air is neglected.

3. CONTROLLER DESIGN

For time-varying processes such as batch systems, the parameters of the model are not constant. They change because of internal or external influences and must be updated with time for model-based control systems. In this work the recursive least squares (RLS) method is used for real-time system identification with a parametric process model. Based on the estimated model, a UPC controller manipulates the position of three-way valve for the control of reactor temperature. Fig. 1 shows the control system structure.

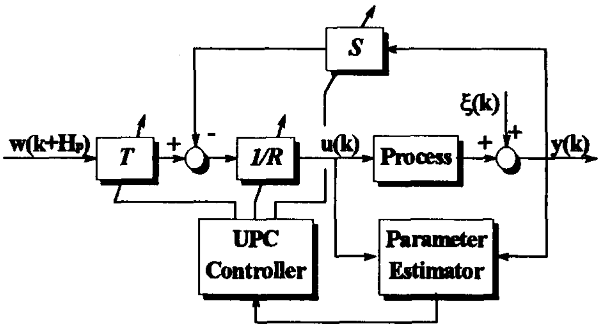


Fig. 1. Structure of the constructed control system.

3.1 Process Model

The parametric process model used in this study is represented by

$$y(k) = \frac{q^{-d}B(q^{-1})}{A(q^{-1})}u(k-1) + \frac{C}{D}e(k) \tag{9}$$

where q^{-1} is the shift operator, d is the time-delay of the process and the polynomials A and B are given by

$$\begin{aligned} A(q^{-1}) &= 1 + a_1 q^{-1} + \cdots + a_{n_A} q^{-n_A} \\ B(q^{-1}) &= b_1 + b_2 q^{-1} + \cdots + b_{n_B} q^{-n_B+1} \end{aligned} \tag{10}$$

in which n_A and n_B are the degrees of polynomials A and B, respectively. The second term of Eq.(9) represents disturbance appearing on the output of the process and $e(k)$ denotes a discrete white noise sequence.

3.2 System Identification

The RLS parameter estimation algorithm with forgetting factor λ is realized by the following equations:

$$\hat{\theta}(k)=\hat{\theta}(k-1)+\left\{\frac{P(k-1)\phi(k)\,[y(k)-\phi^T(k)\hat{\theta}(k-1)]}{\lambda+\phi^T(k)P(k-1)\phi(k)}\right\}/\lambda$$

$$P(k)=\left\{P(k-1)-\frac{P(k-1)\phi(t)\phi(k)^T P(k-1)}{\lambda+\phi(k)^T P(k-1)\phi(t)}\right\}/\lambda \tag{11}$$

with

$$\phi(k) = [\,-y^T(k-1)\ \cdots\ -y^T(k-n_A)\quad u^T(k-d-1)\ \cdots\ u^T(k-d-n_B)\,]^T \tag{12}$$

$$\hat{\theta} = [\ \hat{a}_1\ \cdots\ \hat{a}_{n_A}\ \ \hat{b}_1\ \cdots\ \hat{b}_{n_B}\ ]^T$$

3.3 Unified Predictive Controller Design

The i-step-ahead predictor used in UPC is

$$P\hat{y}(k+i) = G_i u(k+i-\hat{d}-1) + \frac{H_i}{\hat{A}}u(k-1) + \frac{F_i}{T}[y(k)-\hat{y}(k)] \tag{13}$$

where P is a polynomial which is introduced to improve the servo behavior of the control system and G_i, H_i, and F_i are solved from the following diophantine equations:

$$\frac{\hat{C}P}{\hat{D}} = E_i + q^{-i}\frac{F_i}{\hat{D}}$$
$$\frac{\hat{B}P}{\hat{A}} = G_i + q^{-i+\hat{d}}\frac{H_i}{\hat{A}} \tag{14}$$

The unified criterion function including weighting and structuring for the controller output is given by

$$J = \sum_{i=H_m}^{H_p}[P\hat{y}(k+i) - P(1)w(k+i)]^2 + \rho\sum_{i=1}^{H_p-\hat{d}}\left[\frac{Q_n}{Q_d}u(k+i-1)\right]^2 \tag{15}$$

and it is minimized under the following constraint:

$$\phi P u(k+i-1) = 0 \qquad 1 \le H_c < i \le H_p - \hat{d} \tag{16}$$

where ρ is a weighting factor, H_m is the minimum-cost horizon, H_c is the control horizon, and H_p is the prediction horizon.

When the process model is linear, the criterion function is quadratic and there are no constraints on the controller output, the criterion function can be minimized analytically. If the criterion function J is minimized with respect to the vector $\boldsymbol{u}$, then the optimum $\boldsymbol{u}$ can be calculated by applying the condition

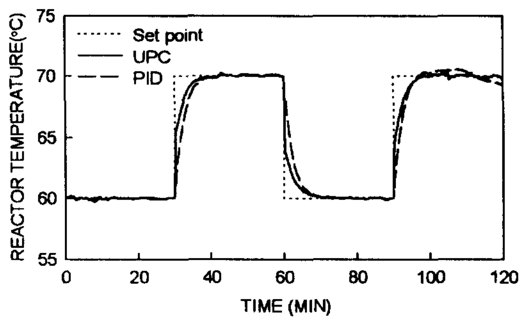
$$\frac{\partial J}{\partial \boldsymbol{u}} = 0 \tag{17}$$

and it is realized by setting the polynomials of the controller, R, S, and T (Fig. 1). The detailed calculation procedure is not repeated here and can be found in Soeterboek(1990).

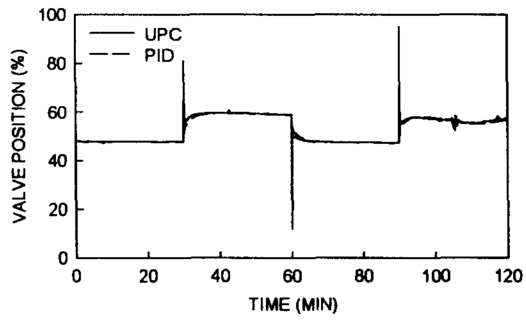
4. SIMULATION RESULTS

All simulations were carried out based on the following assumptions:

- Only level constraint exists in the manipulation of the valve position. In other words, rate constraint does not exist in actuation of the valve.
- Time delay does not exist in measurement and actuation.
- Measurement noise is white noise.



(a)



(b)

Fig. 2. Performances of UPC and PID for tracking the set point changes: (a) reactor temperature, (b) valve position.

The parameters of the UPC controller were selected by rule of thumb method, then fine tuning was performed by trial and error method. For convenience, a standard set of parameters were selected as T_s=5sec, H_p=7, H_m=1, H_c=3, P=1, $\varphi=\Delta$, ρ=0.01, $Q_n=\Delta$, Q_d=1, and λ=0.97. From now on, the value of the parameter which is not mentioned is same as that of the standard set of parameters.

4.1 Tracking of Set Point Changes

Fig.2 shows the performance of the UPC controller and the conventional PID controller in tracking the set point changes. The parameters of the PID controller were tuned by trial and error method as K_c=0.6, τ_I=5sec, and τ_d=0.03sec.

In the earlier part of the reaction course, both controllers show similarly good performances. However, in the latter part when the conversion of monomer is high and heat transfer efficiency becomes low, the UPC controller is superior to the PID controller. It can be seen that the output of the UPC controller is more active than that of the PID controller at the instant of set point change. Furthermore, the PID controller shows a little delay in action, which causes the deviation from the set point, especially in the latter part.

4.2 Rejection of Disturbance

In practical situations, robustness to unexpected disturbance is of great importance. The ability of UPC controller to reject the influence of disturbance was examined by introducing the case of abrupt shortage of the heating-cooling water. The flowrate of heating-

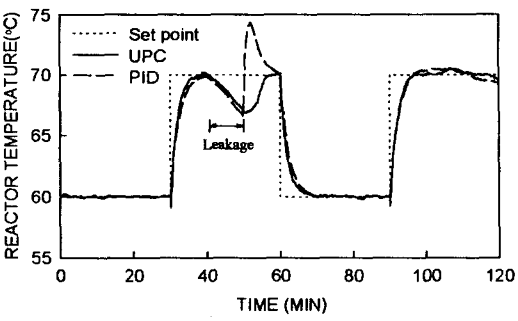


Fig. 3. Rejection of the disturbance caused by heating-cooling water shortage. (λ =0.95)

cooling water was reduced from 11 l/min to 1l/min after 40 minutes from the initiation and lasted for 10 minutes.

As can be seen in Fig. 3, the UPC controller showed a satisfactory performance in eliminating the influence of disturbance and regulating the reactor temperature.

4.3 Tracking of the Optimal Trajectory

In general, the ultimate goal of the reactor temperature control is getting desired properties of the product. Therefore, batch operation is often carried out for tracking a given trajectory. In tracking the optimal trajectory proposed by Ahn *et al.* (1994), the PID controller showed a little fluctuation and delay while the UPC controller did not. The closed-loop responses are illustrated in Fig. 4(a). Proper parameter estimation is essential for desirable performance of an adaptive controller. Fig. 4(b) shows the estimated values of transfer function parameters and the estimated reactor temperature by RLS parameter estimator. The parameters keep changing during the operation and the estimated reactor temperature seems to be nearly identical with the actual one. Fig. 4(c) shows the profiles of number average and weight average molecular weights of polymer and the conversion of monomer during the reaction.

4.4 Effects of the Controller Parameters

The adaptive UPC controller has many design parameters and this means that various performances can be acquired by selecting an appropriate set of parameters.

Fig. 5 shows the effect of the prediction horizon H_p on the performance of the controller. As the prediction horizon decreases the response becomes somewhat faster, but excessively small H_p may cause undesirable response as can be seen in the figure. This phenomenon can be explained by the fact that both the delay margin and the gain margin increase as H_p becomes large.

The effect of the forgetting factor λ on the response is given in Fig. 6. As λ increases, the reflection of the process change to the transfer function becomes slower and hence, the response becomes less sensitive. As is expected, however, measurement noise may affect the response of controller seriously when λ is too small. Thus, the choice of the forgetting factor λ must be based on the compromise between greater elimination of the noise and better tracking of time-varying process parameters.

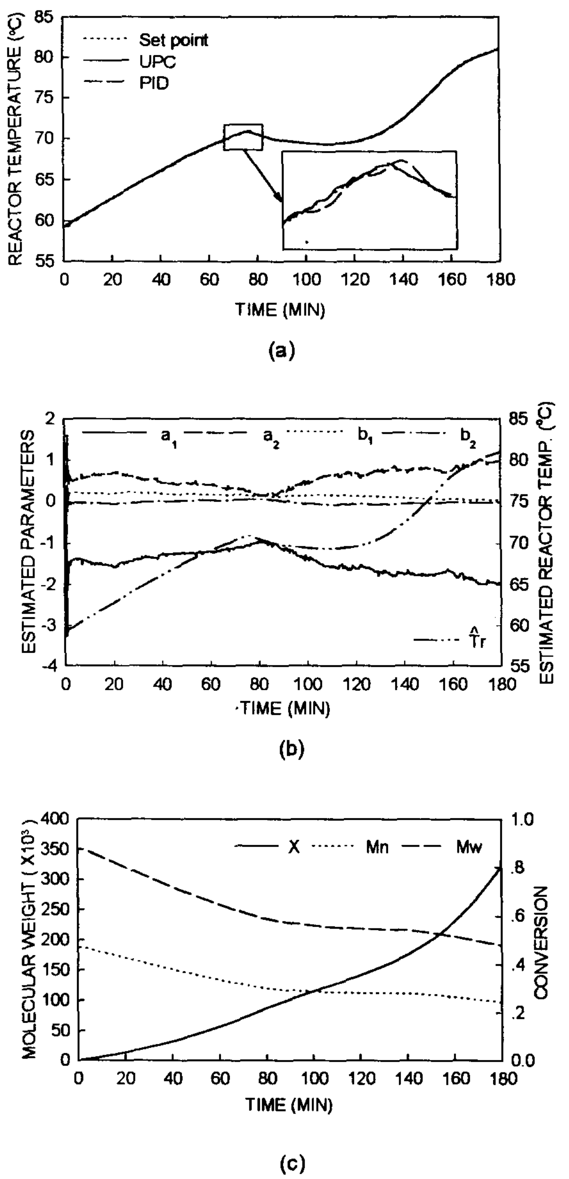


Fig. 4. Performances of UPC and PID for tracking the optimal trajectory: (a) reactor temperature, (b) estimated parameters and estimated reactor temperature, (c) number and weight average molecular weights and monomer conversion.

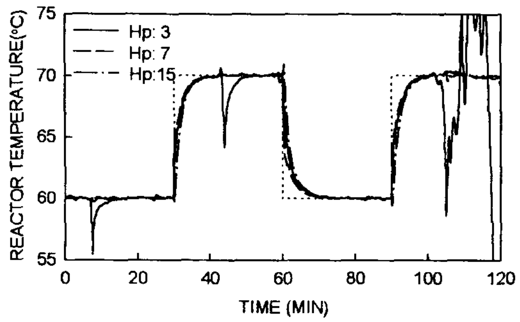


Fig. 5. Performances of UPC for various values of the prediction horizon.

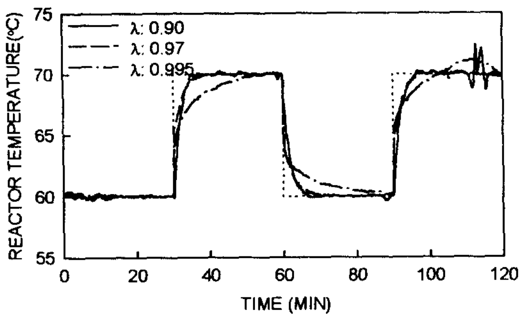


Fig. 6. Performances of UPC for various values of the forgetting factor.

5. CONCLUSIONS

An adaptive UPC controller which is applied to the batch polymerization process showed better performance than the conventional PID controller in both set point tracking and disturbance rejection. Also, the reactor temperature estimated by RLS parameter estimator was nearly identical to the actual one.

It turned out that sufficiently large H_p is necessary for acceptable performance, and as λ increases the controller becomes robuster to the measurement noise though the response becomes slower. Therefore, proper set of parameters should be selected considering given set of reaction conditions and control objective.

It seems evident that the adaptive UPC controller developed using a parametric model can be applied to other polymerization processes without additional efforts.

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