Optimal Temperature Tracking Control of a Polymerization Batch Reactor by Adaptive Input-Output Linearization

Kap Kyun Noh, Dongil Shin, En Sup Yoon, and Hyun Ku Rhee

Abstract: The tracking of a reference temperature trajectory in a polymerization batch reactor is a common problem and has critical importance because the quality control of a batch reactor is usually achieved by implementing the trajectory precisely. In this study, only energy balances around a reactor are considered as a design model for control synthesis, and material balances describing concentration variations of involved components are treated as unknown disturbances, of which the effects appear as time-varying parameters in the design model. For the synthesis of a tracking controller, a method combining the input-output linearization of a time-variant system with the parameter estimation is proposed. The parameter estimation method provides parameter estimates such that the estimated outputs asymptotically follow the measured outputs in a specified way. Since other unknown external disturbances or uncertainties can be lumped into existing parameters or considered as another separate parameters, the method is useful in practices exposed to diverse uncertainties and disturbances, and the designed controller becomes robust. And the design procedure and setting of tuning parameters are simple and clear due to the resulted linear design equations. The performances and the effectiveness of the proposed method are demonstrated via simulation studies.

Keywords: nonlinear systems control, polymerization reaction, time-variant input-output linearization, parameter estimation, reference trajectory tracking control

I. Introduction

The transition from the bulk to the small-volume specialties of versatile properties designed to specific purposes has been a trend in the industry[1]. Batch processes have much more flexibility than continuous processes and so they will be preferred to be a candidate to cope with the changes. But, batch processes, particularly batch reactor in which polymerization reactions proceed with time, have several challenging problems in the control point of view such as i) due to dynamic characters in its nature, how to operate over the entire batch cycle should be designed a priori, ii) they are exhibiting severe nonlinear features and those in CSTR are well known[2][3], iii) it is difficult to have a proper model describing the effects of high viscosities on both the heat transfer through a cooling system and complex reaction kinetics, and iv) real time sensors for the quality of polymer products are lacking. Only simple temperatures are usually available. Therefore, the polymerization batch reactor can be posed as a nonlinear time-varying system with uncertainties induced from the inaccurate model and lacked sensor availability.

Meanwhile, for the last two decades, considerable developments have been made in the nonlinear systems theory evolved from the differential geometry[4] and a few applications to a polymerization batch reactor have been reported. The GLC(Globally Linearizing Control) method proposed by Kravaris and Chung[5] was applied to a polymerization reactor via simulation[6] and experimentally [7] and with interpreted as a feedforward-feedback method for the system with a relative order of one, applied to a copolymerization reactor[8]. The external PID controller in the GLC was required to compensate for model errors and unknown disturbances. The adaptive control method for input-output linearizable systems with constant parametric uncertainty of Sastry and Isidori[9] was applied to track the monomer conversion trajectory along with an EKF(Extended Kalman Filter)[27] for unavailable states[10]. Adaptive control based on a linear approximate model was also implemented by researchers[11][12][13].

In this study, the control problem of tracking an optimal reference temperature trajectory in a polymerization batch reactor will be considered. The control synthesis will be carried out based on the reduced design model, derived from the energy balances, with parametric time varying uncertainties describing the effects of the excluded material balances, constitutive relationships and additional process uncertainties on the design model. Due to the introduction of time varying parameters and their nonlinear characteristics, the proposed method is a combination of the nonlinear time varying input-output linearization with on-line parameter estimation. In the following sections, MMA(MethylMetha Acrylate) polymerization reaction in a batch reactor as an application system, and a time variant input-output linearization and a parameter estimation for an adaptive linearization will be described. Finally, simulation results for illustrating the effectiveness of the method will be discussed.

II. Polymerization reaction in a batch reactor

The kinetics of a free radical solution polymerization reaction is relatively well known[14] and shown in Table 1. The reaction system consists of MMA(MethylMethaAcrylate) as a monomer, Benzene as a solvent, and AIBN as an initiator, respectively.

The mathematical model for the polymerization reaction in a batch reactor consists of i) the material balances based on the reaction kinetics, ii) the energy balances around the reactor configuration, and iii) constitutive equations describing the gel

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Table 1. Reaction kinetics of the MMA free radical polymerization

$I \xrightarrow{k_d}$		$2\dot{R}$	Initiation
$\dot{R}+M \xrightarrow{k_i}$		$\dot{P}_1$	
$\dot{P}_n+M \xrightarrow{k_p}$		$\dot{P}_{n+1}$	Propagation
$\dot{P}_n+M \xrightarrow{k_m}$		$D_n+\dot{P}_1$	Chain Transfer to Monomer
$\dot{P}_n+S \xrightarrow{k_s}$		$D_n+\dot{P}_1$	Chain Transfer to Solvent
$\dot{P}_n+\dot{P}_m \xrightarrow{k_{td}}$		D_n+D_m	Termination by Dispropotionation
$\dot{P}_n+\dot{P}_m \xrightarrow{k_{tc}}$		D_{n+m}	Termination by Combination

where I :Inintiator, $\dot{R}$:Primary Radical, M :Monomer, S :Solvent, $\dot{P}_j$:Polymer Radical of Chain Length j, D_j :Dead Polymer of Chain Length j, k :Rate Constant of Elementary Reaction

and glass effects, an overall heat transfer coefficient, the rate constants, physical properties, etc. Under some standard assumptions, the resulted model is in Table 2 and the constitutive equations regarding the rate constants and physical properties can be found in the literature[14]. Note that the quasi-steady-state assumption(QSSA) is applied to only primary radicals from the initiator decomposition, not to polymer radicals. Extension of QSSA to the polymer radicals breaks down at a high conversion[15]. The MWD(Molecular Weight Distribution) of the produced polymers is approximated by a few moments as is often the case.

The model can be divided into two parts: the one consists of the mass balances and constitutive equations, of which the states are not usually available and it forms a basis of determining the reference trajectory of section III, and the other is the energy balances, which are described in temperatures as states, and it forms a design basis for implementing the reference trajectory. The former will be referred to as a disturbance model and the latter as a design model. The controller for a tracking is designed on the design model, while the disturbance model is treated as unknown with respect to the design model. The couplings between two submodels are displayed through a polymerization reaction heat and an overall heat transfer coefficient, both of which are treated as unknown parameters in the design model. They are time-varying and severely nonlinear, which make it difficult to implement the trajectory and so requires a nonlinear control method capable of dealing with time-varying uncertainties. If the accurate disturbance model is available, the knowledge should be fully utilized in the synthesis of the controller. But, especially in the industrial reactor, this is not feasible.

A major nonlinear characteristic in a free radical polymerization is the presence of autoacceleration, called the gel effect, in the course of polymerization reaction[16]. The gel effect represents the effect of decreasing diffusivity of the live polymer radicals due to increasing viscosity of the reaction mass on the termination rate constant, k_t and is exhibited as a sharp increase in the monomer conversion and total polymer radicals concentration as well as the weight- averaged molecular weight with time. At the time which the gel effect starts, a peak in the heat of reaction begin to appear and the peak of the bell-shaped reference trajectory are also required to lower the molecular weight of polymers. At higher monomer conversions, the propagation reaction also becomes diffusion-controlled(glass effect). To incorporate the gel and glass effects into the model, the gel and glass effect models developed by Chiu et al.[15] are used and shown in Table 3.

Table 2. Model for the polymerization reaction in a batch reactor[14]

Material Balances

$$\dot{x}_1 = -\frac{k_p}{V}x_1x_4$$

$$\dot{x}_2 = -k_d x_2$$

$$\dot{x}_3 = -\frac{k_s}{V}x_3x_4$$

$$\dot{x}_4 = 2fk_d x_2 - \frac{k_t}{V}x_4^2$$

$$\dot{x}_5 = 2fk_d x_2 - \frac{k_t}{V}x_4x_5 + \left(\frac{k_m}{V}x_1 + \frac{k_s}{V}x_3\right)(x_4 - x_5) + \frac{k_p}{V}x_1x_4$$

$$\dot{x}_6 = 2fk_d x_2 - \frac{k_t}{V}x_4x_6 + \left(\frac{k_m}{V}x_1 + \frac{k_s}{V}x_3\right)(x_4 - x_6) + \frac{k_p}{V}x_1(x_4 + 2x_5)$$

$$\dot{x}_7 = \left(\frac{k_{td}}{V} + \frac{1}{2}\frac{k_{tc}}{V}\right)x_4^2 + \left(\frac{k_m}{V}x_1 + \frac{k_s}{V}x_3\right)x_4$$

$$\dot{x}_8 = \frac{k_t}{V}x_4x_5 + \left(\frac{k_m}{V}x_1 + \frac{k_s}{V}x_3\right)x_5$$

$$\dot{x}_9 = \frac{k_t}{V}x_4x_6 + \frac{k_{tc}}{V}x_5^2 + \left(\frac{k_m}{V}x_1 + \frac{k_s}{V}x_3\right)x_6$$

$$\dot{x}_{10} = -\frac{V_0}{1+\beta[M]_0V_0}\frac{(-\dot{x}_1)}{} = -\frac{\varepsilon}{(1+\beta)[M]_0}\frac{k_p}{V}x_1x_4$$

Energy Balances

$$\dot{x}_{11} = \frac{(-\Delta H_p)}{\rho C_p V^2}k_p x_1x_4 - \frac{UA}{\rho C_p V}(x_{11} - x_{12})$$

$$\dot{x}_{12} = \frac{UA}{\rho_w C_{pw} V_J}(x_{11} - x_{12}) - \frac{F_{cw}}{V_J}(x_{12} - T_{cw}) + q_{ex}$$

where $x_1 = [M]V$, $x_2 = [I]V$, $x_3 = [S]V$, $x_4 = [\lambda_0]V$, $x_5 = [\lambda_1]V$, $x_6 = [\lambda_2]V$, $x_7 = [\mu_0]V$, $x_8 = [\mu_1]V$, $x_8 = [\mu_2]V$, $x_{10} = V$, $x_{11} = T_R$, $x_{12} = T_J$, $[\lambda_k] = \sum_{n=1}^{\infty} n^k[P_n]$ $k = 0,1,2$:kth moments of live polymer radicals, $[\mu_k] = \sum_{n=1}^{\infty} n^k[D_n]$ $k = 0,1,2$:kth moments of dead polymer, ρ :density of reaction mass, C_p :heat capacity of reaction mass, A :jacket-side area for heat exchange, V_J :jacket-side volume, F_{cw} :coolant flowrate, T_{cw} :coolant temperature, q_{ex} :external heat input, ρ_w :density of coolant, C_w :heat capacity of coolant

The heat of reaction generated during the polymerization is

$$\Delta H_R = \left(\frac{-\Delta H_p}{\rho C_p V_R^2}\right)k_p x_1x_4 \tag{1}$$

where ΔH_p is the heat of propagation reaction and x_1 , x_4 are concentrations of the monomer and total live polymer radicals, respectively. To estimate the reaction heat, two states are needed. The states can be estimated by a state estimator such as EKF(Extended Kalman Filter)[17] or by an open-loop model as a feedforward disturbance estimator[8][10].

As the polymerization reactions proceed and the concentrations of produced polymer chains increase, the viscosity of the reacting medium increases significantly and sharply at the

onset of the gel effect, which results in a sharp decrease of the overall heat-transfer coefficient, U . This poses a difficult controlling problem along with the low thermal conductivity of the formed polymer. To account for this, the empirical correlation by Soroush and Kravaris[7] is adopted for simulation. The heat transfer coefficient is assumed to be a function of the monomer conversion only as follows.

Table 3. Model for the Gel and Glass Effects in a MMA Polymerization[15]

$$k_p = \frac{k_{p_o}}{1+\frac{k_{p_o}\theta_p\lambda_o}{C}} \qquad k_t = \frac{k_{t_o}}{1+\frac{k_{t_o}\theta_t\lambda_o}{C}}$$

$$\theta_p = \theta_p^0 \exp\left(\frac{E_{\theta_p}}{RT_k}\right) = 5.5445\times10^{-16}\exp\left(\frac{27.786 kcal/gmol}{RT_k}\right) \text{ (min)}$$

$$\theta_t = \frac{\theta_{p_o}^0}{[I]_o}\exp\left(\frac{E_{\theta_t}}{RT_k}\right) = 1.1548\times10^{-22}\exp\left(\frac{34.730 kcal/gmol}{RT_k}\right) \text{(mol/l min)}$$

$$A = 0.168 - 8.21\times10^{-6}(T_c - T_{gp})^2 \qquad B = 0.03$$

$$C = \exp\left(\frac{2.303(1-\Phi_p)}{A+B(1-\Phi_p)}\right)$$

In the dimensionless form

$$\frac{k_p}{k_{p_o}^o} = \frac{K_{p_o}(\bar{T})}{1+\frac{\phi_{\theta_p}K_{\theta_p}(\bar{T})K_{p_o}(\bar{T})\bar{x}_4}{C\bar{x}_{10}}} = K_p(\bar{T},\bar{x}_4,\bar{x}_{10})$$

$$\frac{k_t}{k_{t_o}^o} = \frac{K_{t_o}(\bar{T})}{1+\frac{\phi_{\theta_t}K_{\theta_t}(\bar{T})K_{t_o}(\bar{T})\bar{x}_4}{C\bar{x}_{10}}} = K_t(\bar{T},\bar{x}_4,\bar{x}_{10})$$

$$A = 0.168 - 8.21\times10^{-6}T_o^2(\bar{T}_c - \bar{T}_{gp})^2 \qquad B = 0.03$$

$$C = \exp\left(\frac{2.303(1-\Phi_p)}{A+B(1-\Phi_p)}\right)$$

where λ_o :Total Conc. of the Live Polymer Radicals, $[I]_o$:Initial Conc. of the Initiator, Φ_p :Volume Fraction of the Polymer, k_{p_o}, k_{t_o} :Rate Constants of the Propagation and Termination Reaction at no Conversion, $k_{p_o}^o, k_{t_o}^o$:Frequency Factors of the Rate Constants, k_{p_o}, k_{t_o} , T_0 :basis temperature, T_{gp} :glass transition temperature of the polymer

$$U(x) = U_o\left[a + (1-a)\exp(-bx^c)\right] \tag{2}$$

where correlation parameters are set as a=0.2 ,b=7.0 and c=3.0 and U_o is an overall heat transfer coefficient at no conversion, $x = 0$. This correlation can be utilized if measurements on the conversion of monomer are available, but which is not practical due to the viscose character of the reacting medium at a high conversion. It also depends on design details of the cooling systems around a given reactor.

The entire model covering major behaviors of a polymerization reactor will be used as a simulated process, while the control synthesis and parameter estimation proceeds around the design model.

III. Design of an optimal reference trajectory

The severe conditions caused mainly by the high viscosity of the reacting mixture make it difficult to measure the physical properties, related to the qualities of the produced polymer, such as monomer conversion and MWD(Molecular Weight Distribution), and subsequently make it difficult to control the quality by the closed-loop feedback. Thus, the common approach for a quality control of the batch reactor is to determine the reference operation trajectory leading to a polymer product of the specified quality and then to design a controller for implementing the trajectory precisely. Since at the terminal time $t = t_f$, the product qualities are sensitive to the history of the operation, i.e., deviations from the designed reference trajectory during the whole reaction, the trajectory should be tracked as tightly as possible.

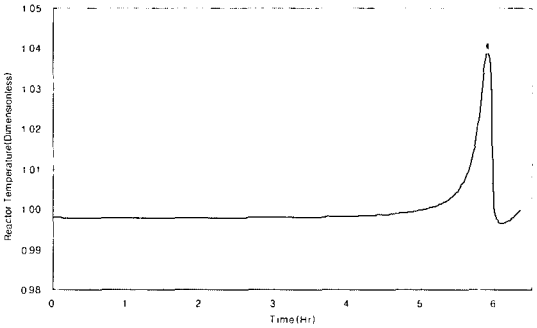


Fig. 1. An optimal reference temperature trajectory for MMA polymerization in a batch reactor.

The trajectory can be determined by minimizing the deviations from the specified targets at a final time through searching for the optimal temperature trajectory over the whole batch time. The problem takes a mathematical formulation below;

$$J = \underset{T}{Min}\left\{w_1\left(1-\frac{PDI}{PDI_d}\right)^2 + w_2\left(1-\frac{\overline{MW}_n}{\overline{MW}_{nd}}\right)^2 + w_3\left(1-\frac{x}{x_d}\right)^2\right\}_{t=t_f} \tag{3}$$

subject to

$$\dot{x} = f(x,T,\vartheta,t) \quad x(t_0) = x_0 \tag{4}$$

where the objective function is expressed in the weighted-deviation form of the number-averaged molecular weight ($\overline{MW}_n$), PDI(Polydispersity Index) defined as the ratio of the weight-averaged MW to the number-averaged MW, and monomer conversion from the respective desired value. Dynamic model as constraints consists of the material balances.

By the classical variational approach(Pontryagin Minimum Principle), above optimization problem is reduced to the two-point boundary value problem. That is, the process model equations with initial conditions are integrated in forwards and then the co-state equations with final conditions are integrated in backwards, while the Hamiltonian is minimized by using the steepest gradient method with a fixed searching size, α_1 [18]. Fig.1 shows the calculated optimal reference temperature trajectory for the MMA polymerization. The bell-typed shape is similar to the results in the literature[18][19].

In this work, the specified target values are $x_d = 1.0$, $PDI_d = 2.5$ and $\overline{MW}_{nd} = 360{,}000.$ (g/mol) and the weights in the objective are set to $w_1 = 1.$, $w_2 = 10.$ and $w_3 = 20.$ The parameter, α_1 for updating the suboptimal trajectory at each iteration is fixed to $1.0\times\ 10^{-6}$.

IV. Input-output linearization of time-varying nonlinear systems

The input-output linearization as a controller synthesis

method has been well established for nonlinear time-invariant systems[4][5] and recently extended to nonlinear time-varying systems[20], both of which result in an equivalent linear time-invariant system. The brief review will be given.

Consider a nonlinear time-varying system

$$\begin{aligned} \dot{x} &= f(x,t) + g(x,t)u \\ y &= h(x,t) \end{aligned} \tag{5}$$

where $x \in \Gamma \subset R^n$, $u \in R$ and $y \in R$ denote the state vector, the input and the output, respectively. f and g are smooth vector fields and h is a smooth scalar field, both in $\Gamma \times R$.

The standard Lie derivatives for a time-invariant system are inadequate for a time-varying system and need to be modified to account for the explicit time dependence of the model. The modified Lie derivatives are defined as follows;

$$\begin{aligned} L_f^0 h(x,t) &= h(x,t) \\ L_f^k h(x,t) &= < dL_f^{k-1} h, f > (x,t) + \frac{\partial L_f^{k-1} h}{\partial t}(x,t) \qquad k = 1,2,.. \end{aligned} \tag{6}$$

where $dL_f^{k-1}h$ means the gradient of a scalar function, $L_f^{k-1}h$ and <,> stands for the scalar product of two vectors.

Definition: For the system of eq.(5), the relative order of the output y with respect to the input u is defined as the smallest integer r such that

$$L_{g(x,t)} L_{f(x,t)}^{r-1} h(x,t) \neq 0 \qquad \forall x \times t \in \Gamma \times [t_0, \infty) \tag{7}$$

,i.e., bounded away from zero.

As in the time-invariant case, the relative order is the smallest time derivative of the output which depends explicitly on the input. The existence of a finite relative order ensures that the locally invertible state transformation and state feedback law linearizing the input-output response exist[20].

Through a suitable state transformation and state feedback, the system can be transformed into the normal form[4], in which structural characteristics of the system are clearly exposed. Since we are interested in an output tracking problem, the normal form in the error coordinates will be convenient for controller design. The transformed normal form is

$$\begin{aligned} \dot{\sigma} &= e_1 \\ \dot{\bar{e}}_r &= A\bar{e}_r + B\left(-y_{sp}^{(r)} + L_f^r h + L_g L_f^{r-1} hu\right) \\ \dot{\eta} &= \bar{\eta}_{n-r}\left(e_1 + y_{sp}, e_2 + y_{sp}^{(1)}, ..., e_r + y_{sp}^{(r-1)}, \eta, t\right) \end{aligned} \tag{8}$$

where $\bar{e}_r = [e_1, .., e_r]^T$ with $e_i = L_f^{i-1} h - y_{sp}^{(i-1)}$, i=1,..r is an error coordinate vector and the pair(A,B) is in a controllable canonical form. $\eta = [\eta_1, .., \eta_{n-r}]$ is a new states vector and $\bar{\eta}_{n-r} \in R^{n-r}$ is nonlinear maps. $y_{sp}^{(i-1)}$ is the (i-1)th derivative of a reference output and so it will be assumed that the reference output is continuously differentiable as times as necessary. The normal form above is augmented with an integral of the output error and the linearizing state feedback is not yet applied.

The state feedback law linearizing the input-output relation is clear from eq.(8);

$$u = \frac{y_{sp}^{(r)} - L_f^r h(x,t) + v}{L_g L_f^{r-1} h(x,t)} \tag{9}$$

where a new control input, v is introduced to meet additional control requirements around the linearized system and can be taken as

$$\begin{aligned} v &= \sum_{i=1}^{r} \alpha_i (L_f^{i-1} h(x,t) - y_{sp}^{(i-1)}) + \alpha_0 \int_0 (h(x,t) - y_{sp}) dt' \\ &= \sum_{i=1}^{r} \alpha_i e_i + \alpha_0 \int_0 e_1 dt' \end{aligned} \tag{10}$$

The coefficients, $[\alpha_0, .., \alpha_r]^T$ can be appropriately set for stability, performance and robustness due to the controllability of a linear part in the error coordinates.

The nonlinear dynamics in the eq.(8) is unobservable from the output and forms internal dynamics. It is called as zero dynamics when the output is constrained identically to zero by the suitable control input along with zero reference. The state feedback closed-loop system with the control law of eq.(9) and (10) is in a cascaded form, in which the linear system is stable such that an arbitrary pole placement is possible and the nonlinear system is driven by arbitrarily fast decaying errors and bounded reference trajectory. Thus, the stability of above closed-loop system is guaranteed only if the unobservable system is bounded-input-to-state stable. This feature results from the fact that the input-output linearization is a nonlinear analog of the pole-zero cancellation in a linear system. Therefore, for an internal stability, the cancelled dynamics are required to be stable. That is, the given system must be a minimum-phase system[4].

Feedback linearizing controllers are based on the exact cancellations of the nonlinearities. Therefore, uncertainty in the model would result in the control law that no longer linearizes the input-output relationship. Imperfect linearization will cause control performances to be affected or deteriorated. In case of linearly parametric uncertainty, the estimates of f and g can be obtained by using the estimated parameters and then Lie derivatives can be calculated from these estimates of the vector fields. For $r \geq 2$, the estimates of Lie derivatives are not linear in the unknown parameters. This difficulty can be avoided by redefining the multi-linear product as another unknown parameter. Note that the derivatives of the estimated parameters are also included as another parameters in the control law.

The approximate state feedback law using the estimated Lie derivatives is

$$u_a = \frac{y_{sp}^{(r)} - \overline{L_f^r h(x,t)} + \sum_{i=1}^{r} \alpha_i (\overline{L_f^{i-1} h(x,t)} - y_{sp}^{(i-1)}) + \alpha_0 \int_0 (\overline{h(x,t)} - y_{sp}) dt'}{\overline{L_g L_f^{r-1} h(x,t)}} \tag{11}$$

where the bar represents the estimates of the corresponding Lie derivatives. When u_a is applied to the system, the linear error system of eq.(8) is no longer linear and becomes

$$\dot{\bar{e}}_{r+1} = A_c \bar{e}_{r+1} + W(\bar{e}_r, \eta, t)\Theta \tag{12}$$

Here, A_c is a (r+1)× (r+1) Hurwitz matrix with the polynomial coefficients, α_i, i=0,1,..,r and $\bar{e}_{r+1} = [\sigma, \bar{e}_r]^T$. Θ is the parameter error vector of all multilinear products among the parameters and their derivatives such $\hat{\theta}_i^2, \hat{\theta}_i\hat{\theta}_j, \hat{\theta}_i\dot{\hat{\theta}}_j, \cdots$. So, the second term in the right-hand side is induced from uncertain pa-

rameters and it is perturbing or destabilizing the stable linear system. As each parameter estimate is reaching its true value, the vector Θ goes to zero and the error system is asymptotically linearized.

During the transient of the estimated parameters, the stability of the perturbed linear system of eq.(12) is ensured when the perturbation term, $W(\bar{e}_r, \eta, t)\Theta$ are bounded and the poles of the Hurwitz linear system are placed sufficiently deep into the left half of s-plane and the internal dynamics are stable.

V. Parameter estimation

The design model of section II is described in only output variables as states. The effects from the disturbance model are treated as lumped time-varying parameters which should be identified through some procedure. In this section, an estimation method of the parameters in the design model will be proposed.

Consider the nonlinear system linearly parameterized by the time-varying parameters, $\theta(t) \in R^p$

$$\begin{aligned} \dot{y} &= \left[\left(\sum_{i=1}^{p} f_i^y(y)\right) + \left(\sum_{i=1}^{p} g_i^y(y)\right)u\right]\theta(t) + \left[f_0^y(y) + g_0^y(y)u\right] \\ &= \Psi(y,u)\theta(t) + \left[f_0^y(y) + g_0^y(y)u\right] \\ y &= [y_c, y_m]^T \end{aligned} \tag{13}$$

where $\Psi(y,u)$ is a known coefficient matrix of the unknown parameters and $y_i^y \in R^p$, $g_i^y \in R^p$, i=0,1,..,p are vector fields on $y \in R^q$. In addition to the controlled output, y_c, the output vector as the state vector, y is augmented with measurable secondary outputs, $y_m \in R^{q-1}$ which are useful for parameter estimations. The above equation can be considered as linear parameterization of a general time-varying system of eq.(5) with the help of independent secondary outputs.

The estimated outputs can be obtained from the same model with the parameters replaced by their estimates as follows;

$$\begin{aligned} \dot{\hat{y}} &= \left[\left(\sum_{i=1}^{p} f_i^y(\hat{y})\right) + \left(\sum_{i=1}^{p} g_i^y(\hat{y})\right)u\right]\hat{\theta}(t) + \left[f_0^y(\hat{y}) + g_0^y(\hat{y})u\right] \\ &= \Psi(\hat{y},u)\hat{\theta}(t) + \left[f_0^y(\hat{y}) + g_0^y(\hat{y})u\right] \end{aligned} \tag{14}$$

For parameters estimation, it will be assumed that a) parameters to be identified appear explicitly in the design model and that b) the coefficient matrix of parameters has a full column rank. The nonlinear system of eq.(5) can be suitably arranged in a parametric form such that unknown parameters appear in the first derivative of the output vector as in eq.(14) and so assumption a) is satisfied. After the rearrangements, the resulted parameters often have their physical meanings in the given process. As the relative order of the output, y_c for the input, u is defined, the relative order, $r_i^{\theta_j}$ of the output, y_i for a parameter, θ_j can be defined similarily as[21]

$$r_i^{\theta_j} = \min\left[k : \left(\frac{\partial y_i^{(k)}}{\partial \theta_j}\right) \neq 0\right] \quad \exists i \in [1,..,p] \tag{15}$$

In the terminology of the parameter relative order, the assumption a) means that all the parameters appearing in the design model have the relative order of one. Similar to the input relative order of the controlled output, the parameter relative order characterizes how directly the parameter affects the output. The lower the relative order, the more direct is the effect of the parameter on the output. In short, the proposed method can estimate the parameters directly affecting one of the measurable outputs. Assumption b) is equivalent to the condition

$$rank\left\{\Psi^T \Psi(y,u)\right\} = p \tag{16}$$

As shown below, the assumption b) enables the unknown parameters to be computed directly from the parameterized system model and it can be thought of as a sort of the regularity condition for parameters observance from the first outputs derivative.

The GMC(Generic Model Control)[22] as a nonlinear control design method is to find the control law that forces the output response of the nonlinear system to follow the response of a predetermined linear system, which is given as a PI control trajectory;

$$\dot{y} = K_1(y_{sp} - y) + K_2 \int_0^t (y_{sp} - y)dt' \tag{17}$$

If the system has the input relative order of one, the control law by the GMC is directly obtained from the process model as explicitly revealed in eq.(17). The method is directly extended to the square MIMO(Multi-Input Multi-Output) system if each output has the relative order of one with respect to the input vector.

When the GMC is adapted to the parameter estimation, it is desired that the predicted outputs from the model of eq.(14) converge the measured outputs along the specified PI control trajectory as a target trajectory;

$$\dot{\hat{y}} = K_1(y - \hat{y}) + K_2 \int_0^t (y - \hat{y})dt' \tag{18}$$

where $\hat{y}$ is the predicted outputs. K_1 and K_2 are diagonal matrices whose elements are chosen to achieve a proper parameter estimation performance as tuning parameters. Due to the nonsingularity of the coefficient matrix, the parameter estimation can be done by combining eq.(14) with (18) and the resulted equation in a state space form is

$$\begin{aligned} \dot{\hat{y}} &= K_1(y - \hat{y}) + K_2 \int_0^t (y - \hat{y})dt' \\ \dot{\hat{\theta}}(t) &= \left\{\Psi^T\Psi\right\}^{-1}\Psi^T\left\{K_1(y-\hat{y}) + K_2\int_0^t (y-\hat{y})dt' - \left[f_0^y(\hat{y}) + g_0^y(\hat{y})u\right]\right\} \end{aligned} \tag{19}$$

In this equation, the driving inputs are the measured outputs The estimated parameters make the responses of the estimated outputs and the outputs error to the measured outputs be a second order linear dynamics as

$$e = \left(Is^2 + K_1 s + K_2\right)^{-2} Is^2 y \tag{20}$$

$$\hat{y} = \left(Is^2 + K_1 s + K_2\right)^{-2} (K_1 s + K_2) y \tag{21}$$

where $e = y - \hat{y}$ is the estimation output error. By choosing suitable K_1 and K_2, the predicted outputs approach the measured outputs and the output errors decay to zero, both in the prespecified 2nd order way. The design of the tuning parameters follows the procedure suggested by Lee and Sullivan[22].

When the predicted outputs approach the measured outputs, it is desirable to suppress an overshoot and an oscillation of the predicted outputs. Therefore, ξ in the formula of Lee and Sullivan[22] is advised to be greater than 3.0.

Table 4. Reaction Conditions for Simulation

V_S^o	Solvent Volume	0.3(l)
V_M^o	Monomer Volume	1.0(l)
V_R^o	Reaction Volume	1.3(l)
V_J	Jacket Volume	$0.5*V_R^o$
T_{cw}	Coolant Temp.	10(℃)
A_o	Area for Heat Transfer	500(cm^2)
C_I^o	Initiator Concentration	0.0258(gmol/l)
C_M^o	Monomer Concentration	6.9675(gmol/l)
C_S^o	Solvent Concentration	2.1019(gmol/l)
U_o	Overall Heat Transfer Coeff.	0.75(cal/min.cm^2.K)
t_f	Batch Cycle Time	380(min)

where superscript ° means the value at initial condition or at no conversion.

An integral term in the PI target trajectory makes the parameter estimates approach their true values without any offsets if unknown external disturbances are not intervened. And, in case of the existence of external disturbances, the estimates incorporate the effects of the external disturbances on the outputs and so they deviate from their true values, but it improves the robustness of the controller using the estimates.

The parameter estimation method by Tatiraju and Soroush[23] is based on the model reference system of the first order and so the responses of the estimated outputs to the measured outputs are a first order. Their form does not contain an integral term. The link between the parameter estimation in this section and the GMC is through the fact that the relative order of each parameter is one and the coefficient matrix is nonsingular.

VI. Application to a polymerization batch reactor and discussions

The input-output linearization method combined with parameter estimation is applied to a tracking problem of off-line determined temperature trajectory of a polymerization batch reactor. Application results via simulation will be discussed. Simulation conditions are summarized in Table 4. In order to prevent numerical conditioning problems, all the equations in Table 2 are appropriately nondimensionalized. The bar over the variables and parameters stands for the dimensionless of the corresponding variables and parameters. The dimensionless groups are omitted for brevity.

1. Design of the linearizing control law with an integral

In this application, the design model of the energy balances from the equations set in Table 2 can be restated in the following general form

$$\begin{aligned}\dot{\bar{x}}_{11} &= \bar{\theta}_1(\bar{x}_1,\bar{x}_4,\bar{x}_{10},\bar{x}_{11},\Xi) - \bar{\theta}_2(\bar{x}_1,\Xi)(\bar{x}_{11}-\bar{x}_{12}) \\ \dot{\bar{x}}_{12} &= \gamma\bar{\theta}_2(\bar{x}_1,\Xi) - \bar{F}_{cw}(\bar{x}_{12}-\bar{T}_{cw}) + \bar{q}_{ex}\end{aligned} \tag{22}$$

where $\bar{\theta}_1(t)$ and $\bar{\theta}_2(t)$ represent the heat of polymerization reaction and an overall heat transfer coefficient, respectively. γ is relatively constant and $\bar{q}_{ex}$ is the heat input from an external heater. Each parameter shows the dependence of the states in the disturbance model and another parameters set, Ξ. It is assumed that each is completely unknown. They can be treated as lumped parameters and have specific physical meanings. For the design of the control, the design model will be described in the state-space form of eq.(5)

$$\begin{aligned}\dot{\bar{x}} &= \begin{bmatrix}\dot{\bar{x}}_{11}\\ \dot{\bar{x}}_{12}\end{bmatrix} = f(\bar{x}_{11},\bar{x}_{12},\bar{\theta}(t)) + g(\bar{x}_{11},\bar{x}_{12},\bar{\theta}(t))\bar{u}_c \\ \bar{y} &= h(\bar{x}_{11},\bar{x}_{12}) = \bar{x}_{11}\end{aligned} \tag{23}$$

where

$$\begin{aligned}f(\bar{x},t) &= \begin{bmatrix}\bar{\theta}_1(\bar{x}_1,\bar{x}_4,\bar{x}_{10},\bar{x}_{11},\Xi) - \bar{\theta}_2(\bar{x}_1,\Xi)(\bar{x}_{11}-\bar{x}_{12})\\ \gamma\bar{\theta}_2(\bar{x}_1,\Xi)\end{bmatrix} \\ g(\bar{x},t) &= \begin{bmatrix}0\\1\end{bmatrix} \\ \bar{u}_c &= -\bar{F}_{cw}(\bar{x}_{12}-\bar{T}_{cw}) + \bar{q}_{ex}\end{aligned} \tag{24}$$

Based on the above model, the relative order, r of the output is 2 since $L_g L_f h = \bar{\theta}_2(\bar{x}_1,\Xi) \neq 0$ and it is well defined over the physical domain. Thus, the linearizing control law can be easily formulated according to the formula eq.(9)(10) and the derivations of the necessary Lie derivatives are evident. Note that the formula requires the first order derivatives of the unknown parameters since $r \geq 2$. But, as the magnitude of the derivatives are relatively small for those of the original estimates, actually applied control law may not necessarily include the derivatives of the estimates.

In the eq.(23), a combined input of eq.(24) as a control input is used. But, either the coolant flowrate or the external heat input has to be used for physical implementations. This problem is solved with ease through the coordination rules as follows[7][24];

$$\text{if } \bar{u}_c \leq 0, \quad \text{then } \bar{F}_{cw} = -\frac{\bar{u}_c}{\bar{x}_{12}-\bar{T}_{cw}}, \quad \bar{q}_{ex} = 0. \tag{25}$$

$$\text{if } \bar{u}_c \geq 0, \quad \text{then } \bar{F}_{cw} = 0., \quad \bar{q}_{ex} = \bar{u}_c \tag{26}$$

The $\bar{u}_c$ is the output calculated from the controller. Of course, each physical input may have upper and lower hard constraints as in this work; $0 \leq \bar{F}_{cw} \leq 1000.$ and $0 \leq \bar{q}_{ex} \leq 5.$ External heat input is required to heat up the initial reactor contents up to the reaction temperature during the start-up and/or to recover the reaction temperature after an excessive heat removal to the desired temperature during the normal operation. Here, the purpose of heat input is for the 2nd reason.

The polynomial coefficients of the controllable linear system in the error coordinates of eq.(8) should be selected such that the control requirements imposed on the given process be satisfied. The control law of eq.(10) does not show explicitly the existence of an external controller such as PI in the GLC[5][6][7], but due to an integral term in the control law, the coefficients can be chosen so that the resulted control law be equivalent to that of the GLC control law with an external PI controller. Therefore, the polynomial coefficients as the tuning parameters will be set in the same way as the GLC

suggests, which consists of two steps[7]. The tuning procedure is systematic and easy to understand the effects and the roles of tuning parameter on the performances at each step. At the first step, the control law linearizing the nonlinear process into an equivalent linear system of the order, r(relative order) are designed. The determination of the dynamics of the linearized linear system is usually referenced to the open-loop dynamics of the nonlinear system generated by a step test. In this application, when the reactor contains only monomer and solvent and the reaction does not occur, the responses of the reactor temperature to a stepwise coolant flowrate are used with a suitable constant heat input applied. The characteristic equation of the linear system is made to be $(\varepsilon s+1)^r$ where ε is about a time constant of the open-loop responses. The tuning parameter, ε is not used to speed up or retard the resulted linear dynamics. At the next step, an external PI controller is designed based on the linear system according to the standard tuning procedure of a linear system[25]. In this example, ε is set to 0.01 and τ_I of an external PI controller is set to 2ε and K_c is found to be 1.0×10^5 by a trial and error. After this procedure is done, the coefficients of the control law of eq.(10) are obtained by expanding the GLC control formula and equating the respective coefficient of the same s-order.

For comparisons, a classical PI controller is also applied to the tracking of the reference temperature trajectory and the controller parameters of $\tau_I = 2\varepsilon$ and $K_c = 1.1\times 10^3$ are used. As the controller parameters imply, τ_I is set from the open-loop response and K_c is found by a trial and error.
The tuning parameter found like this are used for all the simulations without retuning for specific cases. The sampling time for control and as well parameter estimation stated below is 5 sec and equivalently 2.2×10^{-4} in the dimensionless time.

2. Design of GMC-like parameter estimation

The jacket temperature is not a controlled output, but useful for the parameter estimation. The design model augmented with the jacket-side temperature, $\bar{x}_{12}$ as a secondary output can be expressed in the linearly parameterized form of eq.(13) in terms of the time-varying parameters, $\bar{\theta}_1(\cdot)$ and $\bar{\theta}_2(\cdot)$

$$\dot{\bar{x}} = \begin{bmatrix} \dot{\bar{x}}_{11} \\ \dot{\bar{x}}_{12} \end{bmatrix} = \begin{bmatrix} 1 & -(\bar{x}_{11}-\bar{x}_{12}) \\ 0 & \gamma(\bar{x}_{11}-\bar{x}_{12}) \end{bmatrix} \begin{bmatrix} \bar{\theta}_1 \\ \bar{\theta}_2 \end{bmatrix} - \begin{bmatrix} 0 \\ \bar{x}_{12}-\bar{T}_{cw} \end{bmatrix} \bar{F}_{cw} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \bar{q}_{ex} \qquad (27)$$
$$\bar{y} = [\bar{y}_c, \bar{y}_m] = [\bar{x}_{11}, \bar{x}_{12}]^T$$

and individual functions in the eq.(13) are defined as

$$f_1^y(\bar{y}) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad f_2^y(\bar{y}) = \begin{bmatrix} -(\bar{x}_{11}-\bar{x}_{12}) \\ \gamma(\bar{x}_{11}-\bar{x}_{12}) \end{bmatrix} \quad g_0^y(\bar{y}) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
$$\Psi(\bar{y},u) = \begin{bmatrix} 1 & -(\bar{x}_{11}-\bar{x}_{12}) \\ 0 & \gamma(\bar{x}_{11}-\bar{x}_{12}) \end{bmatrix} \qquad (28)$$
$$\bar{u}_c = -\bar{F}_{cw}(\bar{x}_{12}-\bar{T}_{cw}) + \bar{q}_{ex}$$

For an application of the proposed parameter estimation, the above equation obviously satisfies the assumption a) and the nonsingularity of the parameters coefficient matrix, $\Psi(\bar{y},u)$ is also met unless the cooling jacket temperature is equalizing to the temperature of the reactor. This situation may happen at the period that after a sharp decrease of the temperature in the trajectory is required, the heat input is applied to raise the reactor temperature fast up to the desired point or in case of noisy outputs when two temperatures are approaching closely. To avoid the singularity and an abrupt peak of the estimates when the matrix is close to the singular condition, the eigenvalues of the coefficient matrix as a distance measure to the singularity are used for simplicity because one eigenvalue is constant one and the other is $\gamma(\bar{x}_{11}-\bar{x}_{12})$, so allowing to use the absolute value of the difference between two temperatures as a distance measure to the singularity. The critical value for the singularity is set to 1.0×10^{-4} and noise levels carried with outputs are taken into account. When the absolute difference between two temperatures is within the critical value, previously calculated estimates are used in the control law because of the continuity of physical parameters.

The parameters estimates are computed such that the estimated outputs follow the actual outputs in the 2nd order way of eq.(21) and the output errors decay to zero in the same way of eq.(20). But, because the linear relationship of the 2nd order has a lead term, they are different from the usual 2nd order linear model. If the tuning parameters matrices, K_1 and K_2 are to be set as follows;

$$K_1 = diag\{2\xi/\varepsilon_{p_1}, 2\xi/\varepsilon_{p_2}\} \qquad (29)$$

$$K_2 = diag\{1/\varepsilon_{p_1}^2, 1/\varepsilon_{p_2}^2\} \qquad (30)$$

then, each transfer function of eq.(20)/(21) on the diagonal becomes

$$\frac{\varepsilon_p^2 s^2}{\varepsilon_p^2 s^2 + 2\varepsilon_p \xi s + 1} \qquad (31)$$

$$\frac{2\varepsilon_p \xi s + 1}{\varepsilon_p^2 s^2 + 2\varepsilon_p \xi s + 1} \qquad (32)$$

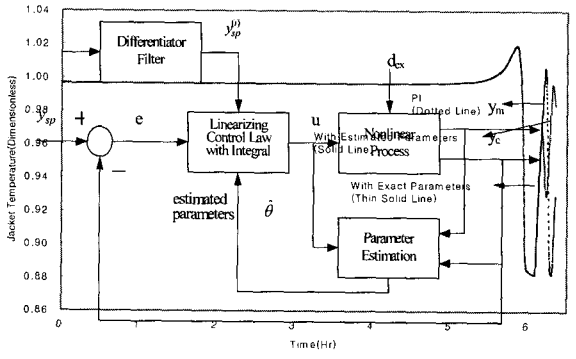
To avoid an overshoot and an oscillation, ξ is selected to be 5.0 as indicated by Lee and Sullivan[22]. In the GMC, ε_p is chosen to give an appropriate timing of the response in relation to the known output response by the control input. Parameter ε_p is set to 0.01 for both outputs.

When the parameters estimation of the state space form of eq.(19) is implemented, the first derivatives of the measured outputs caused by the lead term in the numerator are required. To obtain the approximate i-th derivatives, a standard differentiator filter(lead-lag filter)

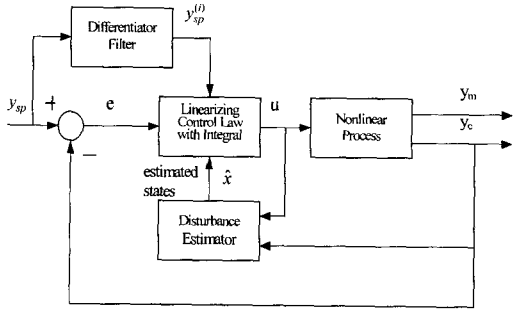
$$\frac{s^i}{(\varepsilon_d s+1)^i} \qquad (33)$$

where ε_d is a filter parameter($0<\varepsilon_d<<1$), is used. As $\varepsilon_d \to 0$, the output of the filter is more noisy and is a more accurate representation of the derivatives. ε_d for both outputs is set to 1.0×10^{-4} in the dimensionless time. The size of ε_d around the order of magnitude of the sampling time or less than one order of magnitude seems to be reasonable from the simulation results for both noiseless and noisy outputs. The approximation through the differentiator filter is also used for getting the derivatives of the reference trajectory needed in the control law.

In a tracking problem, a reference trajectory is fully available and the controller is often trying to take priori actions to follow the given trajectory. Because the parameter estimation uses control inputs by the controller, priori control inputs to catch up an anticipated and sharply changing trajectory may make a big discrepancy in the estimates. To alleviate this, the first-order dynamics of a filter type, accounting for dynamic lags between the coolant flowrate and the jacket temperature are introduced. Parameter estimation uses the filtered control input through the filter. Filter parameter in the discrete form is set to 0.2.



(a)



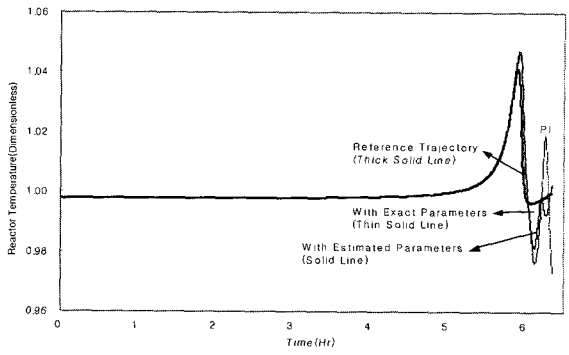
(b)

Fig. 2. Block diagram of (a) an input-output linearization with parameter estimation and (b) an input-output linearization with a disturbance estimator.

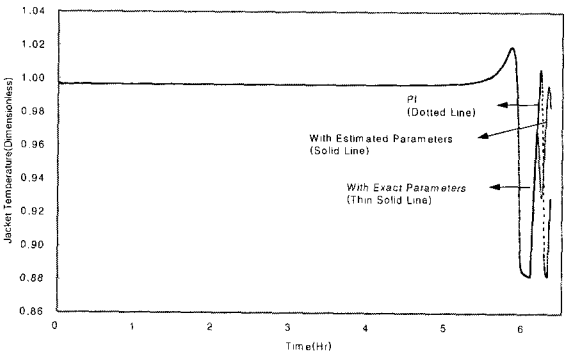
Parameters are calculated by using approximated first derivatives of the measured outputs and control inputs by the controller. These features need a filter for the raw parameter estimates and their filtered values through the filter are used in the control law. The same filters with constants of 0.05 are used for both parameter estimates.

3. An open-loop disturbance estimator and its use for control

The disturbance model excluded in the control design can be utilized as a feedforward disturbance estimator in an open-loop mode, which is already stated at the previous section and has been a common practice in the control of chemical processes[26]. Although a closed-loop disturbance estimator, called as the state observer, such as EKF(Extended Kalman Filter)[27] and other nonlinear observers[28][29] developed lately, but not up to a desirable level, can be adopted to estimate the states involved in the parameters, its design is an another challenging problem, especially for a polymerization batch reactor, mainly caused by the coexistence of frequent and infrequent measurements, convergence speed to true states within a batch cycle time, dynamically varying characteristics over a whole operation and so on[30]. Therefore, linearization with the open-loop model as a simple estimator will be considered for comparisons with the adaptive input-output linearization. An open-loop observer like this is well accepted for unavailable states in the control law such as GLC[5][6][7][8] and NIMC(Nonlinear Internal Model Control)[31]. The con-



(a)



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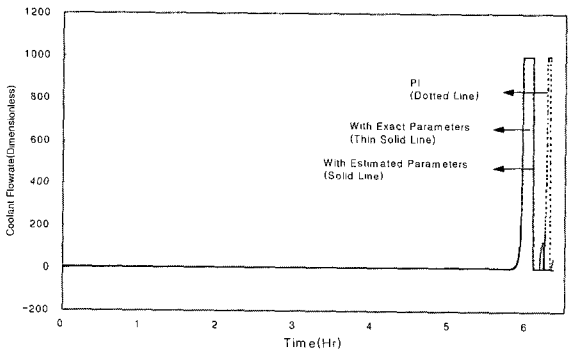


(c)

Fig. 3. Comparisons of the control performances of an input-output linearizations with exact parameters available, an input-output linearization with estimated parameters and PI control; (a) the tracking performances of the reference trajectory; (b) the jacket temperatures accompanied by each control; (c) the coolant flowrates manipulated by each control.

trol scheme of an input-output linearization with a disturbance estimator, which is equivalent to the GLC, is shown in Fig.2(b) along with that of the input-output linearization with a parameter estimator of Fig.2(a).

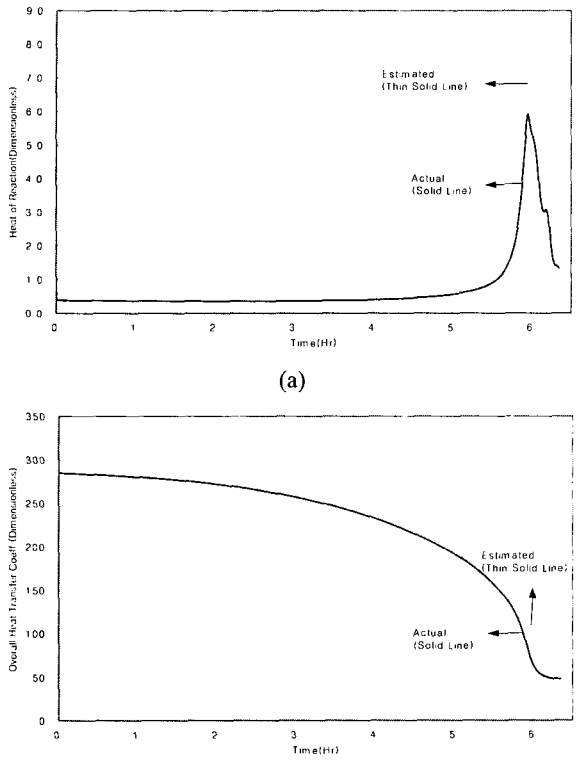


Fig. 4 Comparisons of the estimated parameters from the parameter estimator with their actual values; (a) the heat of polymerization reaction; (b) the overall heat transfer coefficient.

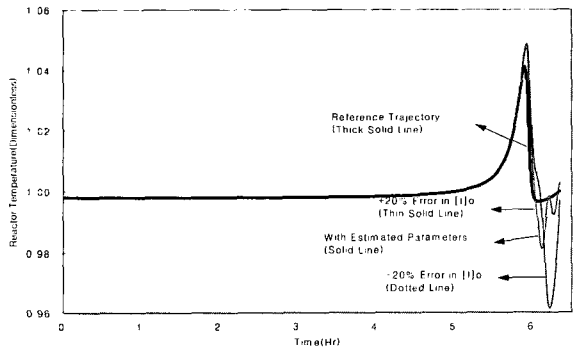


Fig. 5. Comparisons of the control performances of an adaptive input-output linearization and an input-output linearization with a disturbance estimator(case a).

Although many diverse realistic cases for a disturbance estimator can be postulated, the following cases are considered to be typical enough for illustrations.

Case a: initial loading(conditions) errors, particularly of the initiator.

Case b: modeling errors such as the ignorance of the glass effects at the high conversion and a simple linear dependence of an overall heat transfer coefficient on the estimated monomer conversion.

Case c: errors in kinetic parameters such as frequency factors of the rate constants of the propagation reaction and the decomposition reaction of the initiator.

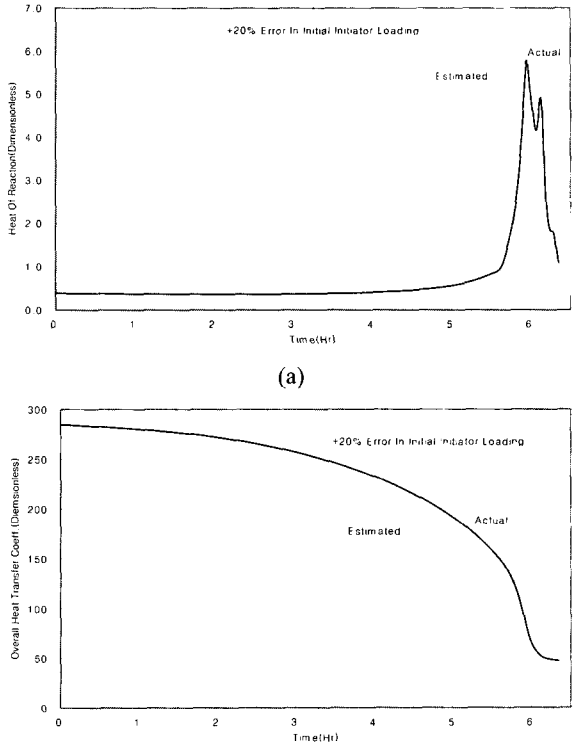


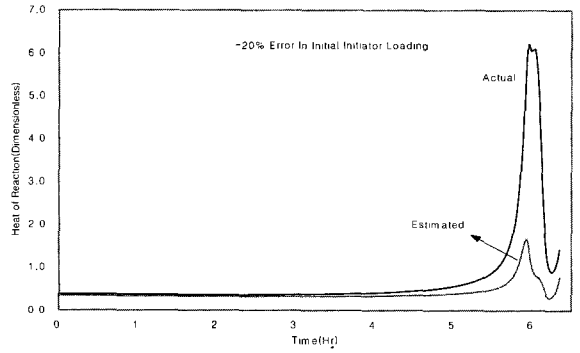
Fig. 6. Comparisons of the predicted parameters from the disturbance estimator with actual parameters; (a) the heat of polymerization reaction; (b) the overall heat transfer coefficient (case a: +20% loading errors of initiator).

Performances of the input-output linearization with a simple model-based disturbances estimator can be varied significantly case-by-case, depending on the extent of magnitude and speed of its deviations from the actual process, but in contrast, a PI controller and an input-output linearization with the parameter estimation gives the unchanged performance except for changes in the actual process.

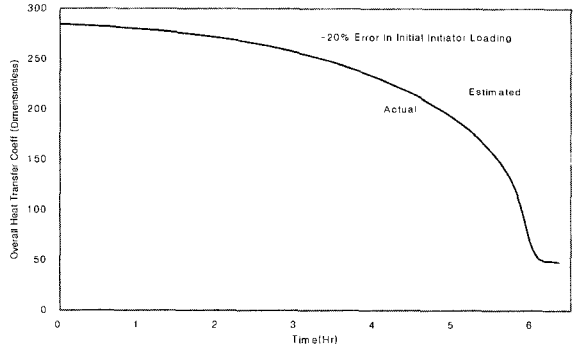
4. Discussions on simulation results

Fig.3(a) shows the control performances of the exact input-output linearization, the adaptive input-output lineraization and a conventional PI controller. Fig.3(b) and (c) shows the accompanying jacket temperatures and control input movements of each control. When exact parameters are available, an exact linearization in the input-output response is possible and it can be played as a basis for comparisons. The control performance of the exact linearization seems to be reasonable because a good tracking of the reference trajectory resulted and compared with the other two controls, the least control movements are consumed.

The performance of the input-output linearization with estimated parameters will depend on the extent of the agreements of the estimated parameters with true parameters. The estimates by the proposed parameter estimation are shown in Fig.4 along with their true values. As shown in Fig.4, true parameters are slowly varying before the gel effects, but when the gel effects start to be prevailing, the changes of parameters become significant in the speed and magnitude. The overall heat transfer coefficient changes exponentially according to the monomer conversion and faster at the on-set of the gel effect because a sharp increase of monomer conversion takes place. The heat of reaction also changes fast from the beginning of the gel effects and shows even a peaking at the culmination of the gel effect. The peaking is partly caused by the shape of the reference temperature trajectory. The increase of the reaction temperature promotes the decomposition of the initiator and subsequently the reaction rate of polymerization. Increasing the temperature is to adjust and lower the averaged molecular weight of the produced polymers to a specified value. The estimates excellently agree with the true values for both parameters during the gel effect in spite of the presence of a peaking in the reaction heat. Therefore, as shown in Fig.3, the control performances and input actions are comparable to those of the exact linearization. Note that while big and steep input changes are required to track the trajectory, the estimates show smooth behaviors.



(a)



(b)

Fig. 7. Comparisons of the predicted parameters from the disturbance estimator with actual parameters; (a) the heat of polymerization reaction; (b) the overall heat transfer coefficient (case a: -20% loading errors of initiator).

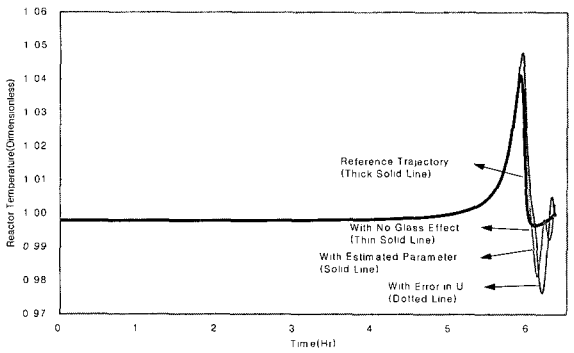
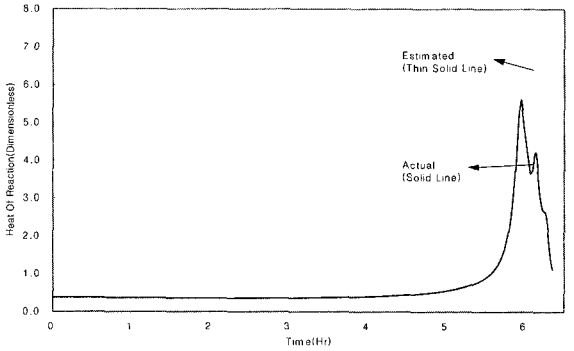
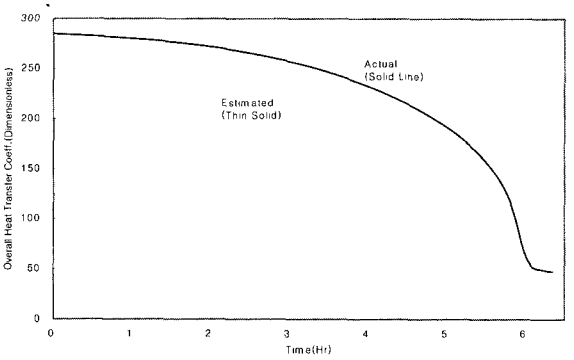


Fig. 8. Comparisons of the control performances of an adaptive input-output linearization and an input-output linearization with a disturbance estimator (case b).



(a)



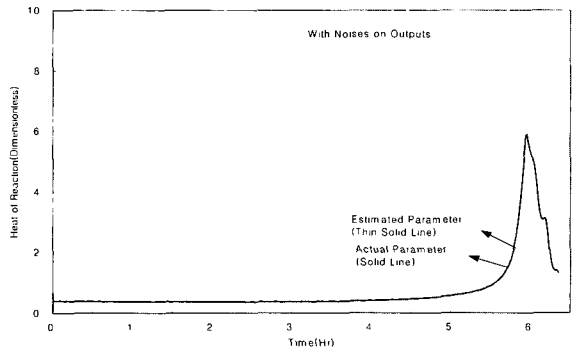
(b)

Fig. 9. Comparisons of the predicted parameters from the disturbance estimator with actual parameters; (a) the heat of polymerization reaction without glass effect; (b) the overall heat transfer coefficient with linear conversion dependence (case b).

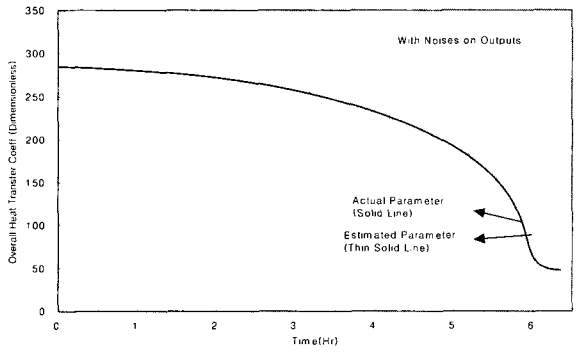
As expected, a PI control gives the poorest performance and the largest control input(Fig.3). At the end of batch time, big fluctuations appear to be continuing.

Fig.5 shows the control performances of the linearization with a disturbance model for case (a) of the subsection 3 and for comparison, the control result of the adaptive linearization is also plotted together. Usually, initial loadings of an initiator are uncertain. The linearization with a disturbance estimator incorrectly initialized gives worse control performances because inappropriate knowledges are utilized in the control and

so the right control actions on time cannot be applied. This fact can be confirmed from the predicted parameters via the disturbance model in relation to the actual values.(Fig.6/7) In case of +20% initiator loading error, the changes of the predicted values of the heat of reaction and an overall heat transfer coefficient precede those of their respective actual values far in advance as shown in Fig.6. So, early deviations occur at the head of the rising reference temperature because a priori control action of increasing the coolant flowrate is applied. In case of -20% loading error, since the predicted parameters do not reflect the magnitude of actual parameters (Fig.7), insufficient and out-of-time control inputs, solely depending on the feedback of the reaction temperature, are applied and as a result, very low reaction temperature is induced like the case of the PI control.



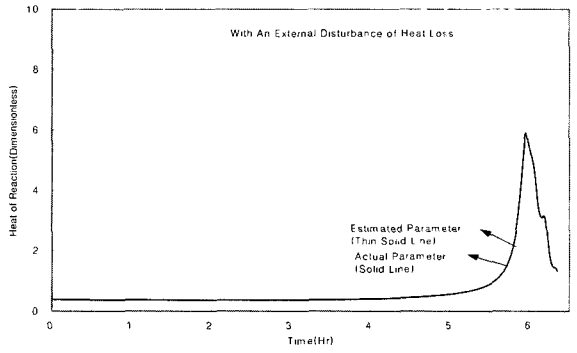
(a)



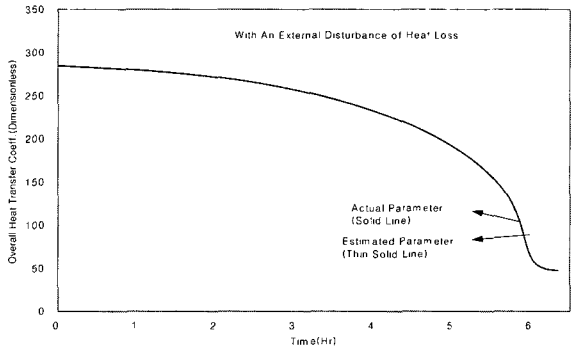
(b)

Fig. 10. Estimated parameters from the parameter estimator with noisy output; (a) the heat of polymerization reaction; (b) the overall heat transfer coefficient.

The results for case (b) are shown in Fig.8/9. The glass effects is exhibited at the higher monomer conversion than the gel effects, of which the absence leads to the completeness of the polymerization reaction and of which the effects on the heat of reaction is shown in Fig.9(a). Due to the glass effects, a complete monomer conversion is not possible in practice. Effects on the heat transfer coefficient are very slight and not shown. The result of a linear approximation to an actual overall heat transfer coefficient using the monomer conversion from a disturbance model is shown in Fig.9(b). As in Fig.9(b), the approximation is rough, but reasonable for the control use only if no other errors in the model exist. The control performances for case b are displayed in Fig.8 and the performances are a little poorer than those of an adaptive linearization. In case there exist errors in kinetic parameters, particularly such as the rate constants of the propagation reaction and initiator decomposition reaction, which are affecting directly the monomer conversion and the heat of polymerization reaction, the predicted behaviors of both parameters are similar to those of the initial loadings error cases and so the control performances between two cases(a/c) are alike. Therefore, detailed results for this case are not given.



(a)



(b)

Fig. 11. Estimated parameters from the parameter estimator with an external disturbance; (a) the heat of polymerization reaction; (b) the overall heat transfer coefficient.

Next, two issues, related with the performances of the adaptive linearization method, such as the effects of measurement noise and the existence of unknown external disturbances on the estimates, will be considered. Small noises are imposed on two measured outputs; random noise with a standard deviation of $0.01\,^{\circ}K$ for reaction temperature and random noise with a standard deviation of $0.015\,^{\circ}K$ for jacket temperature, respectively. Any filtering is not done for noisy outputs and all design parameters related with the parameter estimation are not changed. The estimated parameters for noisy outputs are shown in Fig.10. For the heat of reaction, although small fluctuations exist until the gel effects start, the results are the same as the noiseless case.(Fig.10(a)) But, for the heat transfer coefficient, relatively large fluctuations appear before the gel effects.(Fig.10(b)) The fluctuations largely come from the fluctuating control inputs because the control input is used in the

parameter estimation and the control law is tightly tuned for tracking the reference temperature of the bell-shaped, particularly sharp downward part of the shape. In spite of relatively large fluctuations, the control performances of the adaptive linearization do not show noticeable deteriorations. (Not shown)

When external disturbances affecting the outputs are introduced, the estimated parameters based on the measured outputs will inevitably reflect the effects of these disturbances into the estimates and so the estimates deviate from their actual values with a nonvanishing offset if the disturbances do not vanish. The heat losses to the surrounding from the reactor jacket are taken into account in the jacket-side energy balance of eq.(27) as follows;

$$\bar{x}_{12} = \gamma\bar{\theta}_2(\bar{x}_1, \Xi) - \bar{F}_{cw}(\bar{x}_{12} - \bar{T}_{cw}) + \bar{q}_{ex} - \bar{\theta}_{\infty}(\bar{x}_{12} - \bar{T}_a) \qquad (34)$$

where $\bar{\theta}_{\infty}$ is an overall heat transfer coefficient between the reactor and the surroundings and $\bar{T}_a$ is the ambient constant temperature. The heat loss is always negative. The estimated parameters are shown in Fig.11. There is a noticeable deviation in the overall heat transfer coefficient and a very slight deviation in the heat of reaction. Because the estimates include the existence of external disturbances and are directly used in the control law, the performances of the adaptive linearization do not change against the external disturbances.

VII. Conclusions

An input-output linearization method linked with parameter estimation was proposed to control the system with time-varying parametric uncertainties and applied to the tracking problem of the optimal temperature trajectory of a polymerization reaction in a batch reactor. The good performance of the proposed method resulted from the good capability of the parameter estimation method which showed good agreement with fast varying parameters. Because uncertain time-varying parameters can include the unknowns from several sources such as disturbances, uncertain constant parameters and inaccurate nonlinearities, in spite of the complexity of a polymerization reaction, the design model for controller synthesis is in a simple form. And, since the estimates reflect theses uncertainties, the robustness of the controller using the estimated parameters can be improved. Simulation results showed that the proposed method was effective and easy to implement. And, the necessity of unavailable states in the control law and the parameter estimation is eliminated, which is caused by the form of the design model in only output variables.

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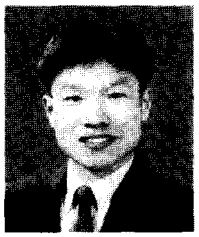

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