Nonlinear Control of a Batch Ester-Interchange Reactor

Seung Young Park and Sunwon Park*†

LG Chemical Research Park, Yusong-Gu, Munji-Dong, 104-1, Taejon 305-380, Korea
*Department of Chemical Engineering, Korea Advanced Institute of Science and Technology,
373-1, Kusong-Dong, Yusong-Gu, Taejon 305-701, Korea

Abstract–Nonlinear control algorithms using feedback input-output linearization and sliding mode control are applied to a lab-scale batch ester-interchange reaction system. Batch ester-interchange reaction requires no overshoot of reaction temperature in earlier stage of reaction and tight temperature control throughout the reaction to keep uniform quality of the final product and to prevent variation of the amount of the byproduct such as diethylene glycol at each batch. Through experimentation we find that the nonlinear controller of input-output linearization algorithm shows better control performance both at setpoint tracking and disturbance rejection than the conventional PID controller. Further, sliding mode control algorithm is supplemented and simulated to show that it improves robustness against plant-model mismatch.

INTRODUCTION

One of the most typical methods for dealing with the nonlinear characteristics of chemical processes has been to linearly approximate the process around the operating condition and to apply linear control theory. The approximation is, however, valid only on the local region and requires a great deal of computation to recursively approximate the process as the operating condition changes. Besides, the growing competition of product quality between chemical companies imposes more severe constraints to be satisfied on the operating conditions. Many advanced control algorithms have been developed to solve these problems, and the nonlinear control algorithm is one of them. Its basic concept is to set up a nonlinear model representing the system dynamics and to transform a nonlinear system into a linear system exactly or partially from the input-state or input-output point of view using differential geometric method. This algorithm, socalled feedback linearization, is experimentally verified in this study. A batch ester-interchange reaction system, which is the first stage of manufacturing Poly(ethylene terephthalate) (PET), is chosen for the study.

PET is one of the widely used polyesters for films, plastics, fibers, etc. Generally, the PET process is divided into two stages. In the first stage, called trans-esterification stage, bis-hydroxyethylterephthalate (BHET) is made from dimethyl terephthalate (DMT) and ethylene glycol (EG) under the so-called ester-interchange reaction. In the second polycondensation stage, PET polymer is made from BHET monomers via condensation reaction.

The mechanism of the PET reaction process is known to be complex and many researchers have made efforts to model the process and analyze the kinetics. Ravindranath and Mashelkar

[1981] constructed a mathematical model of the batch ester-interchange reaction and studied the effects of some key factors, e.g. EG/DMT ratio, temperature variation, and catalyst concentration which can seriously affect product quality. Datye and Raje [1985] studied the kinetics and also Choi and Khan [1988] studied state estimation of the ester-interchange reaction in a continuous stirred tank reactor.

The ester-interchange reaction is endothermic and does not bring about any unstable or catastrophic results by failure of control as in conventional exothermic reaction. In earlier region of the reaction, however, the process is nearly a zero load. That is, it is easy to put heat on the system but difficult to take out. Thus, in case overshoot of reaction temperature is induced by whatsoever, it is hard to cool it down to the desired temperature trajectory. By this reason, the reaction temperature is controlled quite below the desired temperature trajectory with the conventional PID control algorithm. In the industry, they say about 5 degrees below the reference temperature trajectory is maintained to prevent overshoot. This approach is definitely not desirable because the reaction temperature does not lie on the trajectory we really want. Moreover, it is hard to produce products with consistent quality because operators will concentrate more on keeping the reaction temperature below the specified limit, not on controlling the temperature to make consistent trajectories batch after batch. In PET process, side products such as diethylene glycol (DEG) can degrade the quality of final products seriously even with a small amount of it; this means consistent temperature trajectory at every batch is required to maintain uniform product quality.

The aim of the research is to propose a feedback linearization algorithm for tight and consistent temperature control of the batch ester-interchange reactor. The control performance is verified through experimentation under the given setpoint temperature trajectory. The supplementary aim of the research is to modify the feedback linearization algorithm to improve robust-
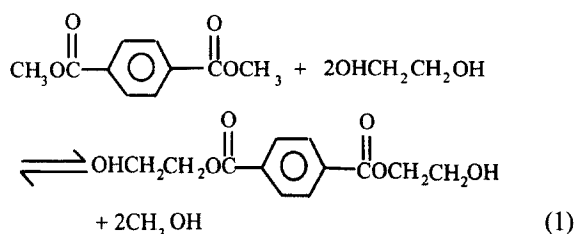
†To whom correspondence should be addressed.
E-mail: swpark@hanbit.kaist.ac.kr

ness. Feedback linearization is model-based and it does not guarantee any acceptable control performance when plant-model mismatch occurs. The sliding mode control (SMC) algorithm is proposed and combined with the feedback linearization algorithm. The performance is verified through numerical simulation.

EXPERIMENTAL

The monomer for the manufacture of PET is bis-hydroxyethyl terephthalate (BHET) and BHET is manufactured through the following two routes: (a) trans-esterification of dimethyl terephthalate (DMT); (b) direct esterification of terephthalic acid. In this study only route (a) is dealt with. In the ester-interchange reaction, DMT is esterified with ethylene glycol (EG) to give BHET and methanol as follows:

$$\text{CH}_3\text{OC}\langle\text{O}\rangle\text{COCH}_3 + 2\text{OHCH}_2\text{CH}_2\text{OH}$$

$$\rightleftharpoons \text{OHCH}_2\text{CH}_2\text{OC}\langle\text{O}\rangle\text{COCH}_2\text{CH}_2\text{OH}$$

$$+ 2\text{CH}_3\text{OH} \tag{1}$$

This reaction is known as the trans-esterification or ester-interchange reaction, and the product is never BHET alone but consists of several oligomers of BHET. DMT and EG are prepared by mole ratio of 1 : 2. In this experiment 400 g of DMT and 255.4 g of EG are used. Catalysts used in the ester-interchange reaction vary according to the specific quality of final products, and the mixture of zinc acetate and calcium acetate catalysts is used in this experiment.

The experimental apparatus of the batch reactor is shown in Fig. 1. The reactor is a 1.0 liter flask with four mouths and the reacting mixture is mixed by a two-paddle agitator which is connected to a variable RPM motor. Stirring is executed throughout the batch operation with constant RPM. The heating system of the reactor is an electrical heater and no cooling system exists. There are four temperature sensors: three 0-400 °C resist-

Fig. 1. Lab-scale batch reactor system.

ance temperature detectors (RTD) with accuracy of ±0.1 °C and one 0-400 °C thermocouple with accuracy of ±0.2 °C. The thermocouple is used to measure the jacket temperature and three RTDs are for reaction temperature, top and bottom temperatures of the distillation column, respectively.

The distillation column is a packed type and used to trap volatile EG and feeding it back into the reaction mixture. The reflux is used also to prevent EG from escaping the reaction mixture. If the top temperature of the distillation column exceeds the boiling point of methanol (64.7 °C), EG is supposed to escape and the condensate reflux is required. Distilled methanol is weighed automatically at every sampling time, which gives information on the extent of reaction. The computer is an IBM PC 386DX and is connected to analog/digital and digital/analog I/O boards. The converters used in these boards are 12-bit converters. The data acquisition software is programmed using C language.

MATHEMATICAL MODELING

Applying the nonlinear control algorithm requires mathematical modeling of the process in the state space form. Though there have been many studies in the modeling of the ester-interchange reaction, they are very complex and lack the heat balance which is the key factor in synthesizing the control system. So they are not quite suitable to be used practically for con-trol purposes. A simpler dynamic model is provided in this study.

1. Reaction Kinetics

In this study the reaction rate of DMT is simplified to give

$$-\frac{d[\text{DMT}]}{dt} = k[\text{DMT}]^n \tag{2}$$

where [DMT] is the concentration of DMT, k is the reaction rate constant, and n is the reaction order. The effect of EG concentration can be eliminated in the above equation because EG and DMT are prepared in their stoichiometric ratios. The effect of catalyst concentration is also excluded under the assumption that the concentration of catalysts does not change during a batch cycle. For convenience, instead of using a concentration based equation, a mass based reaction equation is preferred because during the reaction methanol is continuously extracted, resulting in the change of the overall mass of the reaction mixture. The number of moles of methyl groups of DMT on a unit mass (kilogram base) of the reaction mixture is provided as a new unit of the reaction. Let X be the extent of reaction, then X can be expressed as follows:

$$X = \frac{N_0 - N}{N_0} \tag{3}$$

where N_0 and N are the number of moles of methyl groups at time 0 and t, respectively. Let m_0 and m be the weight of the reaction mixture at time 0 and t, respectively, and m_{MeOH} the weight of methanol released at time t. If we define

$$C = \frac{\text{number of moles of methyl groups at time t}}{\text{mass of mixture at time t}} \tag{4}$$

then
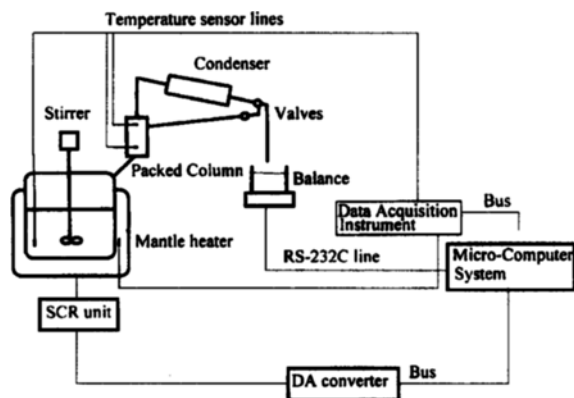
$$C = \frac{N}{m} = \frac{N_0(1-X)}{m_0 - m_{MeOH}} = \frac{N_0(1-X)}{m_0 - 0.032N_0X} = \frac{C_0(1-X)}{1-0.032C_0X} \quad (5)$$

We rewrite the reaction kinetics of Eq. (2) as follows:

$$-\frac{dC}{dt} = kC^n \quad (6)$$

and using X rather than C gives

$$\frac{dX}{dt} = \frac{kC_0^{n-1}(1-X)^n}{(1-0.032C_0)(1-0.032C_0X)^{n-2}} \quad (7)$$

2. Reaction Order Calculation

Let Eq. (7) be expressed as an integral form:

$$\int_{X_i}^{X} \frac{(1-0.032C_0X)^{n-2}}{(1-X)^n} dX = \frac{kC_0^{n-1}}{1-0.032C_0}(t-t_i) \quad (8)$$

Under the isothermal condition (195 °C) integration is calculated numerically by using Simpson's rule and plotted versus time. The value of X can be obtained from the mass of methanol accumulated under the assumption that there is little holdup in the distillation column at high temperature. The reaction order n which gives a straight line is calculated through regression to be 2.5.

3. Rate Constant Calculation

The rate constant k is conventionally assumed to have an Arrhenius type expression:

$$k = k_0 \exp\left(-\frac{E}{RT}\right) \quad (9)$$

From Eq. (7)

$$\frac{dX}{dt} = k_0 \exp\left(-\frac{E}{RT}\right) \frac{C_0^{1.5}(1-X)^{2.5}}{(1-0.032C_0X)(1-0.032C_0)^{0.5}} \quad (10)$$

Under the nonisothermal region (140-195 °C), where temperature increases in a ramp function, plotting

$$\ln\left[\frac{(1-0.032C_0X)^{0.5}(1-0.032C_0)}{C_0^{1.5}(1-X)^{2.5}}\frac{dX}{dt}\right] \text{ versus } \frac{1}{T} \text{ gives a linear line}$$

by regression with a slope of $-\frac{E}{R}$ and a y axis intercept of ln k_0. Table 1 shows the data of the activation energy and the frequency factor.

4. Dynamic Modeling

With all the information on the reaction kinetics and the heat balance we can set up the overall dynamic model of the batch ester-interchange reaction system as follows:

$$\frac{dC}{dt} = -k_0 \exp\left(-\frac{E}{RT}\right)C^{2.5} \quad (11)$$

Table 1. The values of the activation energy and the frequency factor

Activation energy	0.1641×10^5 J/mol·K
Frequency factor	8.2636×10^8 kg$^{1.5}$/mol$^{1.5}$·s

$$\frac{dT}{dt} = -\frac{UA}{mC_p} + (T-T_j) - \frac{1}{mC_p}[\Delta H_{-rxn}]k_0\exp\left(-\frac{E}{RT}\right)C^{2.5} \quad (12)$$

$$\frac{dT_j}{dt} = -\frac{UA}{M_jC_{pj}}(T_j-T) - \frac{U_\infty A_\infty}{M_jC_{pj}}(T_j-T_\infty) + \frac{Q}{M_jC_{pj}} \quad (13)$$

where ΔH_{-rxn} represent the heat of reaction, whose value is obtained from Choi and Khan [1988] and used with no modification. Above equations can be expressed as a general form of Eqs. (14) and (15):

$$\dot{x} = f(x) + g(x)u \quad (14)$$

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

$$x \in R^3, \, f, \, g \in R^3, \, u, \, y \in R$$

where

$$x = [X, \, T, \, T_j]^T \quad (16)$$

$$f(x) = [f_1(x), \, f_2(x), \, f_3(x)]^T \quad (17)$$

$$f_1(x) = \alpha_1 \frac{(1-x_1)^{2.5}}{(1-\alpha_2 x_1)^{0.5}}\exp\left(-\frac{E}{Rx_2}\right) \quad (18)$$

$$f_2(x) = -\alpha_3(x_2-x_3) - \alpha_4[\Delta H_{-rxn}]\frac{(1-x_1)^{2.5}}{(1-\alpha_2 x_1)^{1.5}}\exp\left(-\frac{E}{Rx_2}\right) \quad (19)$$

$$f_3(x) = -\alpha_5(x_3-x_2) - \alpha_6(x_3-T_\infty) \quad (20)$$

$$g(x) = \begin{bmatrix} 0 \\ 0 \\ \alpha_7 \end{bmatrix} \quad (21)$$

$$y = h(x) = x_2 \quad (22)$$

$$u = Q \quad (23)$$

Parameters α_i used for brevity of expressions are shown as Eqs. (24), (25), and (26).

$$\alpha_1 = \frac{k_0C_0^{1.5}}{1-0.032C_0}, \, \alpha_2 = 0.032C_0, \, \alpha_3 = UA/MC_p, \quad (24)$$

$$\alpha_4 = k_0m_0C_0^{2.5}/MC_p, \, \alpha_5 = UA/M_jC_{pj}, \quad (25)$$

$$\alpha_6 = U_\infty A_\infty/M_jC_{pj}, \, \alpha_7 = 1/M_jC_{pj} \quad (26)$$

5. Parameters Estimation

The values of α_i can be determined from the physical data or estimated through estimation techniques. All the linear slopes for the estimation are obtained by linear regression and no data filtering is used. The estimation procedure for these values is as follows:

• Estimation of $U_\infty A_\infty$: At the steady state (T and T_j constant) with EG in the reactor, a plot of the heater power (Q) versus the difference between the jacket temperature and room temperature (T_j-T_∞) is linear with a slope of 0.33 ($U_\infty A_\infty = 0.33$ J/Ks).

• Estimation of α_6: When there is a step change in the heater power (Q) with only stagnant air in the reactor, while there is little temperature change in air, a plot of $\ln[(T_j-Q/U_\infty A_\infty-T_\infty)/(T_{j0}-Q/U_\infty A_\infty-T_\infty)]$ versus time is linear with a slope of -0.0035 ($\alpha_6 = 0.0035$ s^{-1}).

• Estimation of α_3 and α_5: With EG in the reactor, for any given heater power a plot of dT/dt versus T$-$T$_j$ is linear with a

Table 2. The values of system parameters

α_1	0.63×10^{10} s^{-1}
α_2	0.2013
α_3	0.0009 s^{-1}
α_4	8.99×10^7 mol·K/J·s
α_5	0.0057 s^{-1}
α_6	0.0035 s^{-1}
α_7	0.0106 s^{-1}

slope of -0.0009 ($\alpha_3 = 0.0009$ s^{-1}) and with known α_6 and no heat input, a plot of $dT_j/dt + \alpha_6(T_j - T_\infty)$ versus $T_j - T$ is linear with a slope of -0.0057 ($\alpha_5 = 0.0057$ s^{-1}).
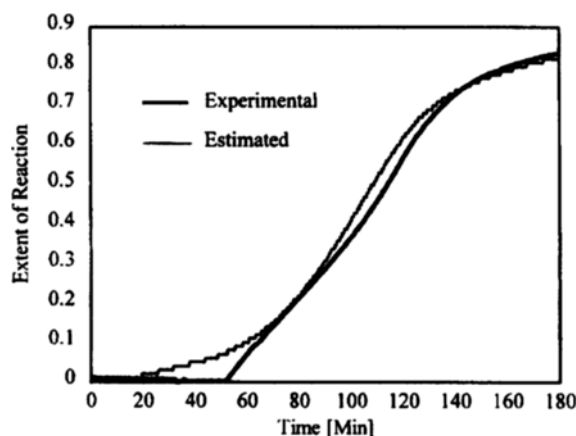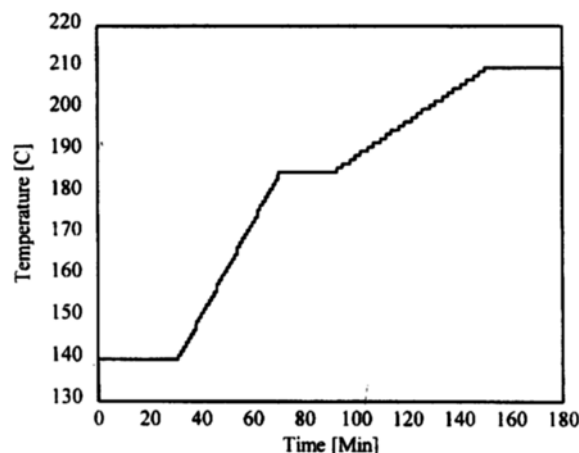
With the above estimated values, all the values of α_i are determined and shown in Table 2.

6. Validation of the Kinetic Model

Before using the developed dynamic model to synthesize the nonlinear controller, we need to validate if the model represents the real system dynamics appropriately. We compared the extent of reaction data gathered from the dynamic model with those from the experiment. Under no reflux condition the extent of reaction of the model and that of the experiment are shown in Fig. 2. The discrepancy in the earlier stage is due to the distillation column holdup before the top temperature of the distillation column exceeds the boiling point of methanol. It shows that the experimental data agrees well with those calculated by the model.

7. Operating Condition

There have been studies on the optimal reaction temperature trajectory under the various specifications of final products [Kumar et al., 1984; Ravindranath and Mashelkar, 1981]. According to a simulation study on the optimization of the ester-interchange reaction system [Kumar et al., 1984], it is desirable to increase the temperature in the earlier stage of the reaction for fast reaction and to decrease the temperature in the final stage of the reaction to reduce side reactions. In industry, a linear increase of the reaction temperature, which begins at around 140 °C and ends at around 220 °C, is conventionally used. Thus, with the knowledge from industrial practice and the simulation

Fig. 2. Experimental and estimated trajectories of the extent of reaction.

Fig. 3. Temperature setpoint trajectory.

study, we choose the setpoint temperature trajectory as in Fig. 3.

SYNTHESIS OF NONLINEAR CONTROL ALGORITHMS

1. Relative Order

Before the nonlinear controller is synthesized, the relative order of the system needs to be known. By definition [Isidori, 1989], relative order of the system is calculated as in Eqs. (27) and (28) with the general form of Eqs. (14) and (15).

$$L_g h(x) = 0 \tag{27}$$

$$L_g L_f h(x) = L_g f_2(x) = \alpha_3 \neq 0 \tag{28}$$

where L is a Lie derivative and

$$L_g h(x) = \sum_{i=1}^{n} g_i(x) \frac{\partial h}{\partial x_i}(x) \tag{29}$$

$$L_g L_f h(x) = \sum_{i=1}^{n} g_i(x) \frac{\partial (L_f h)}{\partial x_j}(x) \tag{30}$$

From Eqs. (27) and (28) we know that the relative order of the system is 2.

2. Stability of Internal Dynamics

Since the dimension of the system is 3 from Eq. (16) and the relative order is 2, one-dimensional internal (hidden) dynamics exists. Stability of this one dimensional dynamics should be validated before nonlinear controller is implemented into the system. Stability of the internal dynamics is easily studied through transformation into the normal form [Isidori, 1989]. In order to find the normal form let us take

$$\zeta_1 = h(x) = x_2 \tag{31}$$

$$\zeta_2 = L_f h(x) = f_2 \tag{32}$$

The third function $\eta(x)$ required to complete the transformation should satisfy Eq. (33).

$$L_g \eta = \frac{\partial \eta}{\partial x_3} \alpha_7 = 0 \tag{33}$$

One solution of this equation may be

$$\eta = x_1 \tag{34}$$

Considering the state transformation $z=(\zeta_1, \zeta_2, \eta)^T$, its Jacobian matrix is

$$\frac{\partial z}{\partial x} = \begin{bmatrix} 0 & 1 & 0 \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \alpha_3 \\ 1 & 0 & 0 \end{bmatrix} \tag{35}$$

which is nonsingular for any physically reliable values of x. The inverse transformation is given by

$$x_1 = \eta$$

$$x_2 = \zeta_1$$

$$x_3 = \zeta_1 + \frac{1}{\alpha_3}\left[\zeta_2 + \alpha_4 \frac{[\Delta H_{rxn}]}{(1-\alpha_2\eta)^{1.5}}(1-\eta)^{2.5}\exp\left(-\frac{E}{R\zeta_1}\right)\right] \tag{36}$$

Thus, the state transformation is deffeomorphism and is valid globally [Isidori, 1989]. With the above set of new coordinates, the system dynamics is put into the normal form:

$$\frac{d}{dt}\begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} = \begin{bmatrix} \zeta_2 \\ a(\zeta,\eta)+b(\zeta,\eta)u \end{bmatrix} \tag{37}$$

$$\frac{d\eta}{dt} = -\alpha_1 \frac{(1-\eta)^{2.5}}{(1-\alpha_2\eta)^{0.5}}\exp\left(-\frac{E}{R\zeta_1}\right) \tag{38}$$

The stability of the internal dynamics is determined by the stability of the zero dynamics and letting $\zeta_1=\zeta_2=0$ results in the stable zero dynamics.

$$\frac{d\eta}{dt} = 0 \tag{39}$$

The control input u* required to maintain ζ_1 and ζ_2 at zero is

$$u^* = -\frac{a(0,\eta)}{b(0,\eta)} = -\frac{a(0,\eta)}{\alpha_3} \tag{40}$$

Since the control input u* is finite and the zero dynamics is stable, it is concluded that the one-dimensional internal dynamics is stable.

3. Input/Output Linearization

The idea of input/output linearization is to find out linear relations between control input u and system output y. This is achieved by differentiating the system output y repeatedly until it is explicitly related by the control input u. In the case of a single input single output (SISO) nonlinear process which is described by a general form of Eqs. (14) and (15), when the relative order of the system is r, differentiating r times the system output y repeatedly results in Eq. (41) [Isidori, 1989]

$$\frac{d^r y}{dt^r} = L_f^r h(x) + L_g L_f^{r-1} h(x)u \tag{41}$$

then a linear relation between $y^{(r)}$ and v is set up as

$$\frac{d^r y}{dt^r} = v \tag{42}$$

This procedure corresponds to partially linearizing the original n dimensional nonlinear system to a r dimensional linear system. Dimension r is linearized according to the above proce-

dure and the other n-r dimension constitutes the hidden or internal dynamics. From Eqs. (41) and (42) nonlinear controller is synthesized to be:

$$u = \frac{v - L_f^r h(x)}{L_g L_f^{r-1} h(x)} \tag{43}$$

For tracking problems, i.e., the system output should follow the desired output trajectory $y_d(t)$, if we let

$$v = y_d^{(r)} + \alpha_{r-1}e_{(r-1)} + \alpha_{r-2}e_{(r-2)} + \cdots + \alpha_0 e_0 \tag{44}$$

where α_i is from a Hurwitz polynomial [Isidori, 1989]

$$d(p) = p^r + \alpha_{r-1}p^{r-1} + \cdots + \alpha_1 p + \alpha_0 \tag{45}$$

and the error e(t) is defined as

$$e_i(t) = y_d^{(i)}(t) - y^{(i)}(t) \tag{46}$$

then the state feedback law of Eq. (43) is of the form

$$u = \frac{1}{L_g L_f^{r-1} h(x)}[-L_f^r h(x) + y_d^{(r)} + \alpha_{r-1}e_{(r-1)} + \cdots + \alpha_0 e_0] \tag{47}$$

and the closed loop error dynamics is of the form

$$e_{(r)} + \alpha_{r-1}e_{(r-1)} + \cdots + \alpha_0 e_0 = 0 \tag{48}$$

which makes the error dynamics be exponentially convergent to zero.

Following the above procedure with the system model, we calculate the control input u as Eq. (49)

$$u = \frac{1}{\alpha_3\alpha_7}\left\{-\sum_{i=1}^{3}\frac{\partial f_2(x)}{\partial x_i}f_i + \frac{d^2 y_d}{dt^2} + \beta_1\left(\frac{dy_d}{dt} - \frac{dy}{dt}\right) + \beta_2(y_d - y)\right\} \tag{49}$$

By this control input u the error dynamics of the system is of the form of Eq. (50) and for any positive values of β_1 and β_2 the error dynamics is stable. In this study β_1 and β_2 are chosen to be 0.1 and 0.001 respectively.

$$\frac{d^2 e}{dt^2} + \beta_1\frac{de}{dt} + \beta_2 e = 0 \tag{50}$$

where $e = y_d - y$ \hfill (51)

4. Sliding Mode Control Combined with Input/Output Linearization

Since the relative order of the system is 2, a companion form [Slotine and Li, 1991] of the system from the general form of Eqs. (14) and (15) is expressed as follows:

$$\dot{z}_1 = z_2 \tag{52}$$

$$\dot{z}_2 = p(x) + q(x)u \tag{53}$$

$$y = z_1 \tag{54}$$

where $p(x) = L_f^2 h(x)$, $q(x) = L_g L_f h(x)$ \hfill (55)

thus the sliding mode control input based on input/output linearization can be formulated [Slotine and Li, 1991] as Eq. (56).

$$u = \frac{1}{q(x)}\left[p(x) - \hat{y}_d^{(2)} - \lambda\dot{e} + K sat\left(\frac{S}{\Phi}\right)\right] \tag{56}$$

where

$$e(t) = y_d(t) - y(t) \tag{57}$$

$$S = \dot{e} + \lambda e \tag{58}$$

$$K = \gamma\delta + (\gamma-1)|{-}p(x)+\dot{e}+\ddot{e}+y_d^2| \tag{59}$$

There are three parameters K, λ and Φ in Eq. (56). Since the value of K is calculated from γ and δ, the values of four parameters γ, δ, λ and Φ should be determined appropriately for good control performance. Among these parameters γ is explicitly related to the model uncertainty. Thus, the plant-model mismatch may need to be considered to properly choose the values of this parameter. Here we assume that the uncertainty is only in the heat transfer coefficient, and if the value of the heat transfer coefficient in the current batch is assumed to vary 30% below from the previous batch,

$$\frac{\hat{q}}{q} = \frac{1}{0.7} = 1.43 \tag{60}$$

where $\hat{q}$ represents the nominal value (the value of the previous batch in this case). Thus, if we choose

$$\gamma \geq 1.43 \tag{61}$$

we can set up the sliding mode controller for the model uncertainty of the heat transfer coefficient. The width of the boundary layer Φ is nomally chosen as 1 and δ and λ are chosen as 0.01 and 0.05, respectively.

RESULTS AND DISCUSSION

1. PID Control

The PID control algorithm is applied to the batch ester-interchange reaction system, and the performance of the PID controller is compared to that of the nonlinear controllers.

Tuning: Under the assumption of no reaction the overall dynamics reduces to the form

$$\frac{dT}{dt} = -\alpha_3(T-T_j) \tag{62}$$

$$\frac{dT_j}{dt} = -\alpha_5 + (T_j-T)-\alpha_6(T_j-T_\infty)+\alpha_7 u \tag{63}$$

where α_3, α_5, α_6, α_7 are from Table 2.
Defining deviation variables

$$\partial T = T-T_s \tag{64}$$

$$\partial T_j = T_j-T_{js} \tag{65}$$

and applying Laplace Transform gives

$$\frac{\partial T(s)}{U(s)} = \frac{3.0286}{317460s^2+3205.71s+1} \tag{66}$$

Now from the IMC-based PID tuning technique the values of Kc, τ_I and τ_D are obtained as 20, 3206, and 99, respectively.

Experimental Test : The performance of the PID control law with the parameters given by the above procedure is tested with only EG in the reactor. Fig. 4 shows that the tuning is satisfactory.

2. Setpoint Tracking Performance

The nonlinear controller based on Input/Output Linearization (IOLIN) is applied to the batch ester-interchange reaction system. The performance of the IOLIN controller and that of the PID controller are compared and shown in Fig. 5. We can see
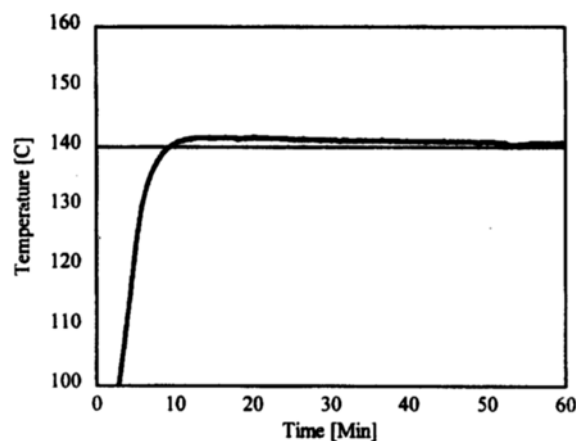
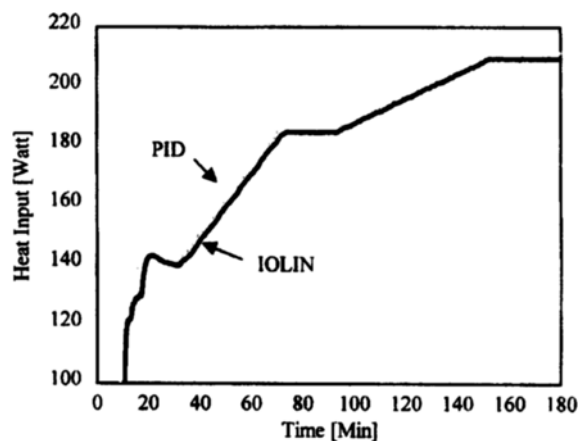Fig. 4. PID controller parameter tuning test with EG.

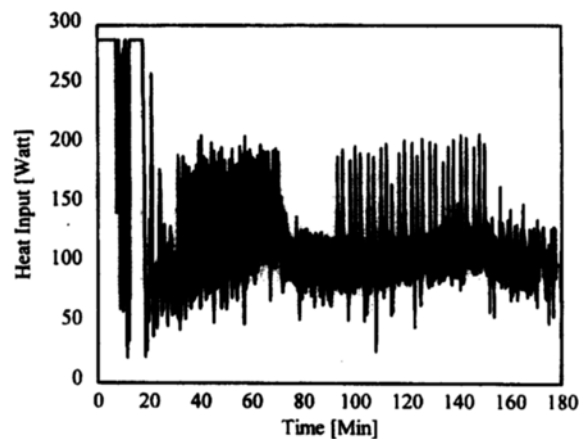Fig. 5. Comparison of setpoint tracking performances.

Fig. 6. Control input of PID controller.

that the IOLIN controller reduces overshoot significantly compared with the PID controller during the initial startup stage and gives more tight temperature control throughout the reaction. Figs. 6 and 7 show the control input of the PID and IO-LIN controller, respectively. It is shown that the IOLIN controller makes stronger action than the PID controller.

3. Disturbance Rejection Performance

During the high temperature stage (especially above EG boiling point; 197 °C) EG is vaporized and the top temperature of
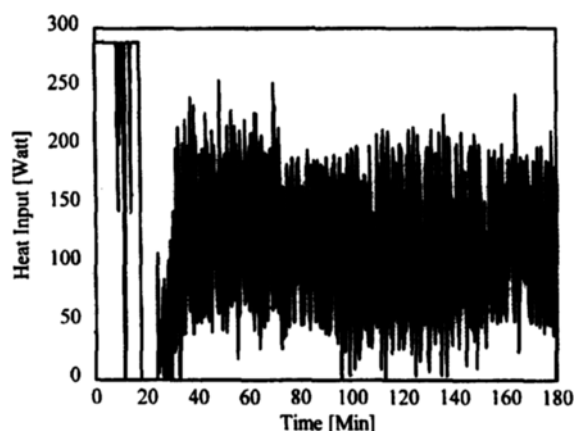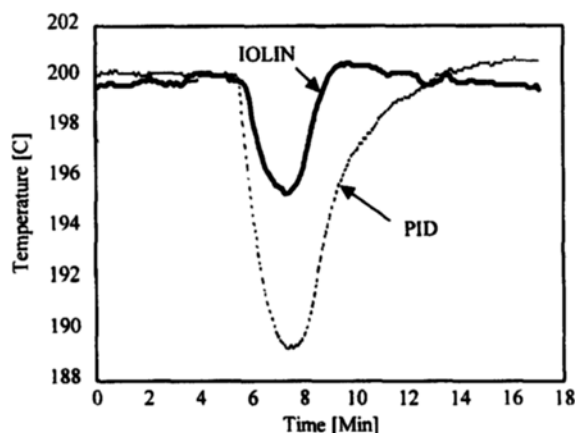
Fig. 7. Control input of IOLIN controller.

Fig. 8. Comparison of disturbance rejection performance between IOLIN controller and PID controller.
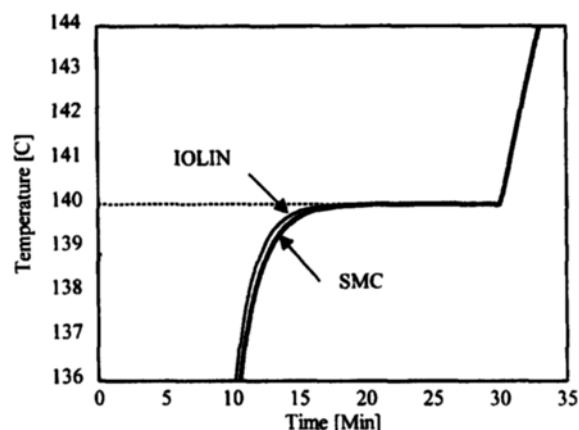

Fig. 9. IOLIN and sliding mode controller (SMC) performance with no model uncertainty.

ficient. The variation of the heat transfer coefficient is a dominant factor which affects the plant-model mismatch seriously and degrades the performance of the model-based controller like IOLIN if the variation is not modeled properly. Therefore, the nonlinear control algorithm is modified to deal with the variation of model parameters with the sliding mode control algorithm.

By simulation the sliding mode controller, if there is no change in the parameters, shows little difference in control performance from that of the IOLIN controller as we can see in Fig. 9. But if the heat transfer coefficient is assumed to vary 30%, the sliding mode controller shows better performance in reducing the overshoot during the startup stage against the IOLIN controller as in Fig. 10.

CONCLUSION

Nonlinear control algorithms using the feedback input/output linearization technique and sliding mode control are applied to the lab scale batch ester-interchange reaction system. These techniques can treat a nonlinear system as a linear one in view of the input/output relation. A linear controller is set up under the linearized input/output relation and mapped into the original nonlinear phase, making the nonlinear controller. Through experimen-

the distillation column increases beyond the methanol boiling point. Then reflux of condensed methanol is required to keep EG from escaping from the reactor. When reflux proceeds, condensed methanol flows into the reactor and lowers the reaction temperature, imposing a load disturbance to the reaction temperature of the system. Fig. 8 shows how the IOLIN controller and the PID controller reject this disturbance. The IOLIN controller shows better disturbance rejection performance than the conventional PID controller.

4. Robustness on the Model Uncertainty

Modeling any real system requires many assumptions and simplifications; only the dominant factors or dynamics are modeled mathematically. In modeling the batch ester-interchange reaction system many factors such as the variation of catalysts activities, the explicit heat loss of the reactor to the surroundings, and side reactions are neglected and are not dealt with in dynamic modeling. The performance of the IOLIN controller, which is based on the state space model, shows that those assumptions are appropriately made.

For real batch operation, however, cleaning of the batch reactor does not certainly follow after every batch cycle. In industry, cleaning is done only after every 5 or 7 batches. This occasional cleaning causes any products to stick to the wall of the reactor and thus leads to a change of the heat transfer coef-
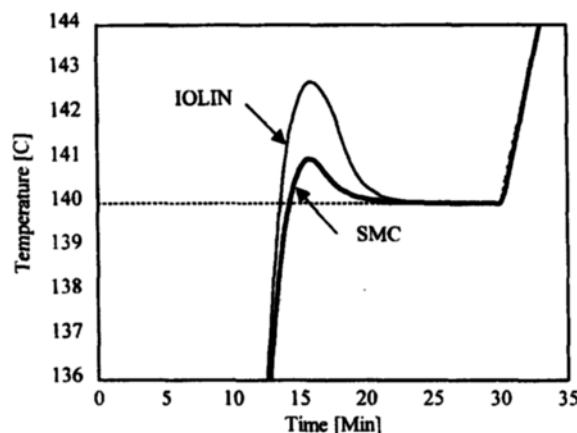

Fig. 10. IOLIN and sliding mode controller (SMC) performance with 30% variation of heat transfer coefficient.

tation we have shown that the nonlinear controller improves control performance against the conventional PID controller both in setpoint tracking and disturbance rejection.

Careful consideration, however, is needed to use the input/output linearization technique because there is no concern on the internal dynamics which is excluded from the input/output relation. For this reason the input/output linearization technique is accepted only when the internal dynamics is stable.

Another point mentioned is that we cannot guarantee the robustness of the nonlinear controller when there are mismatches between the plant and the model. Modification of the control algorithm is needed to enhance the robustness. Sliding mode control is studied and is constructed on the input/output linearization technique. The simulation result shows that sliding control improves robustness, maintaining good control performance.

NOMENCLATURE

A   : heat transfer area between reactor and jacket [m^2]
A$_\infty$: heat transfer area between jacket and ambient atmosphere [m^2]
C   : number of moles of methyl groups per mass of mixture [moles/kg]
C$_p$: heat capacity of reaction medium [J/kg]
C$_{pj}$: heat capacity of jacket medium [J/kg]
k$_0$: preexponential factor [mole$^{1.5}$/Kg$^{1.5}$ sec]
E   : activation energy [J/mole]
ΔH$_{rxn}$: heat of reaction [J/mole]
m   : mass of reaction medium [Kg]
M$_j$: mass of jacket medium [Kg]
Q   : heat input [Watt]
R   : gas constat [J/mole·K]
T   : reaction tempereture [K]
T$_j$: jacket temperature [K]
T$_\infty$: ambient temperature [K]
U   : overall heat transfer coefficient between reactor and jacket [W/m^{2}K]
U$_\infty$: overall heat transfer coefficient between jacket and ambient atmosphere [W/m^{2}K]
X   : extent of reaction
y$_d$(t)   : desired output variable as a function of time
y(t)   : system output variable as a function of time

Greek Letters

α_i : process parameters (i=1,..7) or parameters for Hurwitz polynomial
β_1, β_2 : parameters of the error dynamics
γ : parameter of the sliding mode control representing model uncertainty
R   : real space
δ, λ : parameters of the sliding mode control
ζ_1, ζ_2, η : transformed state variables for the normal form
x   : state vector

Φ : width of the boundary layer of the sliding surface

REFERENCES

Bonvin, D. and Saner, Urs, "Online Procedures for Supervising the Operation of Batch Reactors," *Comput. chem. Engng.*, **12**, 371 (1988).

Choi, K. and Khan, A. A., "Optimal State Estimation in the Transesterification Stage of a Continuous Polyethylene Terephthalate Condensation Polymerization Process," *Chem. Eng. Sci.*, **43**, 749 (1988).

Datye, K. V. and Raje, H. V., "Kinetics of Transesterification of Diethylene Terephthalate with Ethylene Glycol," *J. Appl. Polym. Sci.*, **30**, 205 (1985).

Fernandez, B. R. and Hedrick, J. K., "Control of Multivariable Nonlinear Systems by the Sliding Mode Method," *Int. J. Control*, **46**, 1019 (1987).

Hoo, K. A. and Kantor, J. C., "An Exothermic Continuous Stirred Tank Reactor is Feedback Equivalent to a Linear System," *Chem. Eng. Commun.*, **37**, 1 (1985).

Hunt, L. R., Su, R. and Meyer, G., "Global Transformations of Nonlinear Systems," *IEEE Trans. Automat. Contr.*, **AC-28**, 24 (1983).

Isidori, A., "Nonlinear Control Systems," 2nd ed., Springer-Verlag (1989).

Kumar, A., Sukthankar,V. K., Vaz, C. P. and Gupta, S. K., "Optimization of the Trans-esterification Stage of Polyethylene Terephthalate Reactors," *Polymer Eng. Sci.*, **24**, 185 (1984).

Kravaris, C. and Chung, C. B., "Nonlinear State Feedback Synthesis by Global Input/Output Linearization," *AIChE J.*, **33**, 592 (1987).

Kravaris, C. and Kantor, J. C., "Geometric Methods for Nonlinear Process Control. 1. Background," *Ind. Eng. Chem. Res.*, **29**, 2295 (1990).

Kravaris, C. and Kantor, J. C., "Geometric Methods for Nonlinear Process Control. 2. Controller Synthesis," *Ind. Eng. Chem. Res.*, **29**, 2311 (1990).

Kravaris, C., Wright, L. A. and Carrier, J. F., "Nonlinear Controllers for Trajectory Tracking in Batch Processes," *Comput. Chem. Eng.*, **13**, 73 (1989).

Perry, R. H. and Green, D., "Perry's Chemical Engineers' Handbook," 6th ed. McGraw-Hill (1984).

Ravindranath, K. and Mashelkar, R. V., "Modeling of Poly(ethylene Terephthalate) Reactors-I. A Semibatch Ester Interchange Reactor," *J. Appl. Polym. Sci.*, **26**, 3179 (1981).

Reid, R. C., Prausnits, J. M. and Poling, B. E., "The Properties of Gases and Liquids," 4th ed., McGraw-Hill (1988).

Slotine, J. and Weiping, Li, "Applied Nonlinear Control," Prentice-Hall (1991).

Soroush, M. and Kravaris, C., "Nonlinear Control of a Batch Polymerization Reactor: An Experimental Study," submitted to *AIChE J.* (1992).

Utkin, V. I., "Sliding Modes and Their Application in Variable Structure Systems," MIR Publishers (1978).