NONLINEAR-STATE FEEDBACK CONTROLLER DESIGN FOR NONLINEAR PROCESSES

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The control performance and robust behaviour of model-based control algorithms have been proved better than those of the traditional control algorithms. However, when the processes have highly nonlinear behaviour, use of linear model-based control strategies alone does not quite provide good control performance. Therefore, in this study a nonlinear-state feedback control (NSFC) strategy is developed to overcome such nonlinear process control problems. The basic structure of the NSFC strategy is coupled with a steady-state model and a nonlinear-state feedback controller derived from the nonlinear process model. We then apply the NSFC concept to establish an nonlinear inferential control system to control the packed-bed reactor. Simulation results have shown that the control performances of the NSFC scheme are much better than those of the internal model control (IMC) scheme and the generic model control (GMC) scheme.

Introduction

In recent years, several model-based control algorithms (e.g., Dynamic Matrix Control, Model Algorithmic Control and Internal Model Control) have attracted considerable interest as powerful and versatile frameworks for process control system designs. All of these controllers employ a linear model to represent the process. However, for the regulation of severely nonlinear chemical processes, the performance of a linear model-based control structure tends to degrade. Therefore, nonlinear model-based control strategies were developed to overcome this problem. Although many nonlinear control strategies[7,9,11,12] have been proposed to accomplish the control of nonlinear systems they all present methods for transforming a nonlinear process into a completely or partially linear system.

A major contribution of this paper is a nonlinear-state feedback control (NSFC) configuration, proposed to control nonlinear chemical processes. The control structure of NSFC focuses attention on three points:

1. predicting steady-state output by a steady-state model
2. designing the nonlinear controller by a reduced-order, nonlinear process model
3. developing a compensation function to improve the steady-state output which is affected by modeling errors and measurement noise

The concept of synthesis of nonlinear state feedback controller is used to establish a nonlinear inferential

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control system to control the packed-bed reactor. For control of the packed-bed reactor, we use the inlet temperature as the manipulated variable in controlling the exit conversion.

1. Nonlinear State Feedback Control

In most of the course of theoretical development and application of feedback control, only linear systems have been considered. There are, however, no inherent linear limitations in feedback control. Since chemical reactors are usually nonlinear, the effectiveness of control should be improved by including nonlinearities in the design of feedback controllers. Thus here the NSFC strategy is developed, the structure of which is illustrated in **Fig. 1.** The basic structure of the NSFC strategy consists of a nonlinear controller, modeling error observer, modeling error compensator, and steady-state model. The observer is used to measure modeling errors in the process. The compensator is used to improve the desired trajectory output and steady-state output, which are affected by modeling errors and measurement noise. The steady-state model is used to predict the steady-state output when the control law makes changes in the manipulated variable.

A given real process (i.e., a plant) can be described by the following equations:

$$\dot{x}=g(y, x, m, u, t) \tag{1}$$

$$\dot{y}=f(y, x, m, u, t) \tag{2}$$

where y is the output, x is the state variable vector, m is the manipulated variable, and u is the disturbance vector. The steady-state model in the structure of NSFC (as shown in Fig. 1) is defined as

$$g(y_s, x_s, m_s, u_s)=0 \tag{3}$$

$$f(y_s, x_s, m_s, u_s)=0 \tag{4}$$

where y_s, x_s, m_s, and u_s are the process output, state variable vector, manipulated variable, and disturbance vector at steady state, respectively. By using this prediction concept in the NSFC strategy, control performance can be improved effectively[3]. But if modeling errors and measurement noise exist in the control system, the steady-state model must be modified to eliminate the effect of modeling errors and measurement noise. This can be accomplished by adding the modeling error observer and modeling error compensator to the NSFC structure. The modeling error observer and compensator can be described as

$$x_\varepsilon(t)=x(t)-x_s(t) \tag{5}$$

$$y_\varepsilon(t)=y(t)-y_s(t) \tag{6}$$

$$x_{cs}(t)=x_{cs}(t-\Delta t)+x_\varepsilon(t) \tag{7}$$

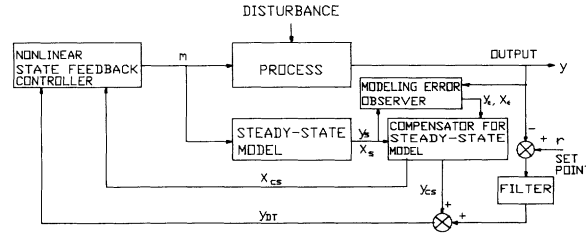

Fig. 1. Structure of nonlinear state feedback control (NSFC)

$$y_{cs}(t)=y_{cs}(t-\Delta t)+y_\varepsilon(t) \tag{8}$$

where $x_\varepsilon(t)$ and $y_\varepsilon(t)$ are the modeling errors resulting from the difference between the process and the steady-state model at time t, and $x_{cs}(t)$ and $y_{cs}(t)$ are the compensated state variables and output of the steady-state model at time t.

The control critertion is chosen to keep y at its set-point value, r, i.e.,

$$y=r=y_s \tag{9}$$

It is clear that

$$\frac{dx}{dt}=\frac{dy}{dt}=0 \tag{10}$$

If the process is away from its set-point r, we would like the rate of change of y to be such that the process is returning toward the set-point. Therefore, the desired trajectory output y_{DT} can be obtained as

$$y_{DT}=y_{cs}+(r-y)f_1 \tag{11}$$

where f_1 is a first-order filter. By substituting Eqs. (9)–(11) into the steady-state output model Eq. (4), the control law of the nonlinear state feedback control structure is

$$f(y_{DT}, x_{cs}, m_s, u_s)=0 \tag{12}$$

where x_{cs} is the compensated state variables obtained from the modeling error compensator. The concept of using the steady-state model to synthesize the nonlinear feedforward controller was proposed by Luyben[13].

2. Application of NSFC Algorithm to Nonlinear Inferential Control System

There are many chemical processes that have highly nonlinear behavior and whose primary output variable to be controlled is not easily measured or cannot be measured directly. Consequently, feedback control or any other configuration which necessitates direct measurement of the controlled variable connot be used. If the disturbances that create the control problems can be measured and an adequate process model is available, feedlorward control can be used to keep the unmeasured output at its desired value. However, when the disturbances cannot be measured,

inferential control is the only method of overcome the above problems. Inferential control strategy, proposed by Joseph and Brosilow in 1978, utilizes easily available secondary measurements, such as temperature, pressure and flow, to estimate and hence control product quality. In 1991, an adaptive inferential control strategy using a nonlinear controller was proposed by Chen and Sun[3] to solve the control problems of a nonlinear and nonstationary process. In this section, three types of inferential control strategies are studied, and their control performances on the packed-bed reactor are examined: the nonlinear state feedback control (NSFC) scheme, internal model control (IMC) scheme[6], and generic model control (GMC) scheme.[11,12]

2.1 Process description

Phthalic anhydride is of great commercial importance. It finds much use in the menufacture of plasticizers and of polyester and alkyl resins, and also as an intermediate in the preparation of dyes. The phthalic anhydride (PA) reactor consists of 2,500 tubes of 2.5 cm diameter, packed with V_2O_5 catalyst and surrounded by molten salt for cooling. The feed stream is *o*-xylene and air, with air in great excess to avoid explosion limits and suppress the temperature rise. The structure of a single-tube reactor for phthalic anhydride synthesis is illustrated in **Fig. 2**.

A number of PA reactor models have been presented by Froment[5], Stewart and Sorensen[14], and Chen and Sun[2]. For the purpose of control studies in our work, a discretized reactor model is developed in which intraparticle temperature and concentration gradients are neglected (Carberry and White.[1]) because the particle size of industrially used V_2O_5/Sb_2O_3 catalyst is very small (from 0.5 to 0.0065 cm). The reaction scheme reported by Froment[5] consists of one parallel and two consecutive reactions (see **Fig. 3**). Owing to the large excess of oxygen, the reaction kinetics may be considered to be pseudo-first order. Rate equations for the reaction are

$$r_a = -k'_1 \exp(-E_1/R_gT^*)C_a^* - k'_3\exp(-E_3/R_gT^*)C_a^* \tag{13}$$

$$r_b = k'_1 \exp(-E_1/R_gT^*)C_a^* - k'_2 \exp(-E_2/R_gT^*)C_b^* \tag{14}$$

To obtain a discretized reactor model, the pseudo-homogeneous reaction model of the phthalic anhydride reaction is discretized in the axial direction using orthogonal collocation. The collocation method is briefly explained in Appendix A. The collocation points are chosen as the roots of Legendre polynomials. The axial derivatives are approximated as:

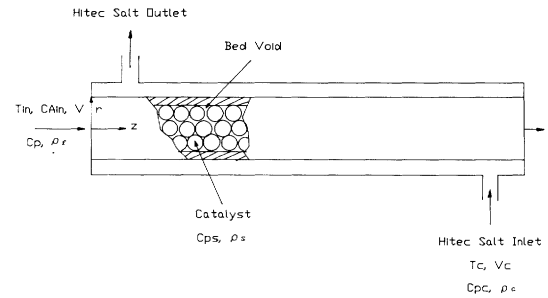

Fig. 2. Packed-bed reactor for oxidation of *o*-xylene to phthalic anhydride

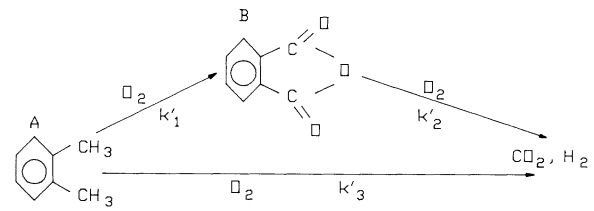

Fig. 3. Kinetic scheme for oxidation of *o*-xylene

$$\left.\frac{dC_a}{d\xi}\right|_i = \sum_{j=1}^{N+2} A_{ij}C_{aj}, \quad \left.\frac{dC_b}{d\xi}\right|_i = \sum_{j=1}^{N+2} A_{ij}C_{bj}$$
$$\left.\frac{dT}{d\xi}\right|_i = \sum_{j=1}^{N+2} A_{ij}T_j, \quad \left.\frac{dT_c}{d\xi}\right|_i = \sum_{j=1}^{N+2} A_{ij}T_{cj} \tag{15}$$

where

$$C_{a1} = C_{ain},\ C_{b1} = 0,\ T_1 = T_{in},\ T_{cN+2} = T_{cin}$$

The discretized reactor model is obtained as

$$\varepsilon\frac{dC_{ai}}{dt} = -\sum_{j=1}^{N+2} A_{ij}C_{aj} + \mu(1-\varepsilon)\left[-\psi_1\exp\left(-\frac{\gamma_1}{T_i}\right) - \psi_3\exp\left(-\frac{\gamma_3}{T_i}\right)\right]C_{ai} \tag{16}$$

$$\varepsilon\frac{dC_{bi}}{dt} = -\sum_{j=1}^{N+2} A_{ij}C_{bj} + \mu(1-\varepsilon)\left[\psi_1\exp\left(-\frac{\gamma_1}{T_i}\right)C_{ai} - \psi_2\exp\left(-\frac{\gamma_2}{T_i}\right)C_{bi}\right] \tag{17}$$

$$\frac{dT_i}{dt} = -\tau\sum_{j=1}^{N+2} A_{ij}T_j + \left\{\mu(1-\varepsilon)\left[\psi_1K_1\exp\left(-\frac{\gamma_1}{T_i}\right)C_{ai} + \psi_2K_2\exp\left(-\frac{\gamma_2}{T_i}\right)C_{bi} + \psi_3K_3\exp\left(-\frac{\gamma_3}{T_i}\right)C_{bi}\right]\right\} - \Omega(T_i - T_{ci}) \tag{18}$$

$$\frac{dT_{ci}}{dt} = Q'\sum_{j=1}^{N+2} A_{ij}T_{cj} + \beta(T_i - T_{ci}) \tag{19}$$

where

N = number of collocation points

$i = 1, 2, 3, \ldots, N+2$

Numerical values for the parameters and the

steady-state operating conditions of the PA reactor are given in **Table 1** and **Table 2** respectively. The steady-state simulation and the parametric sensitivity analysis of the packed-bed reactor, such as inlet and coolant temperatures, inlet concentration, catalyst activity, overall heat-transfer coefficient, coolant flow velocity, and gas flow velocity, were studied by using the PA reactor model[2].

2.2 The structure of nonlinear inferential control

For the PA reactor, the primary output is not easily measured, so in the internal model control (IMC), generic model control (GMC), and nonlinear state feedback control (NSFC) structures we add the concept of inferential control (i.e., a state estimator) to the make-up of the IMC scheme, GMC scheme, and NSFC sheme. The IMC scheme makes use of a process model to infer the effect of unmeasured disturbances on the process output, and then counteracts that effect. The IMC controller is composed of an inverse of the process model and a filter with adjustable parameters. For the GMC scheme, a nonlinear process model is added to the control structure directly. The GMC controller with an exact process model[11,12] can be described as

$$f(y, m, u, t) - K_1(y^* - y) - K_2 \int_0^t (y^* - y)dt = 0 \quad (20)$$

where y^* is the desired steady-state value of the process, and K_1 and K_2 are adjustable parameters. The detailed control theory of IMC and GMC can be found in the orginal papers. The structure of the scheme consists of the nonlinear state feedback controller and a steady-state model that predicts the steady-state output when the control law makes changes in the manipulated variable. Also, compensation parts[3] are used to improve the estimated state variable and steady-state output which are affected by modeling errors and measurement noise. The structure of nonlinear inferential control (NSFC scheme) is illustrated in **Fig. 4.** Here, the modeling error observer and compensator respectively are used to measure and compensate the modeling error resulting from not only the difference between the process output and the steady-state output but also that between the process output and the estimated output. The nonlinear estimator, proposed by Chen and Sun[3] in 1991, is used to estimate the state variables of the process. The nonlinear estimation theory is described in Appendix B.

The nonlinear estimator of the process can be described as follows:

$$\hat{y} = \hat{f}(\hat{x}, m, u, \theta) \quad (21)$$

where $\hat{y}$ is the estimated output and θ is the secondary measurement vector. Here we want the estimated output $\hat{y}$ to describe the process output y completely,

Table 1. Numerical values for parameters of the PA reactor

$L = 4$ m	$\rho_c = 1{,}851.456$ kg/m^3
$\varepsilon = 0.35$	$\rho_f = 0.582$ kg/m^3
$k_1' = 2.418 \times 10^9$ s^{-1}	$\rho_s = 2{,}000$ kg/m^3
$k_2' = 2{,}706 \times 10^9$ s^{-1}	$C_{pc} = 483.559$ J/kg-K
$k_3' = 1.013 \times 10^9$ s^{-1}	$C_{ps} = 836.0$ J/kg-K
$E_1 = 1.129 \times 10^8$ J/kmol	$C_{pf} = 1{,}045$ J/kg-K
$E_2 = 1.313 \times 10^8$ J/kmol	$r_0 = 0.0125$ m
$E_3 = 1.196 \times 10^8$ J/kmol	$r_1 = 0.0225$ m
$\Delta H_1 = -1.285 \times 10^9$ J/kmol	$U = 96.02$ J/m^2-s-K
$\Delta H_2 = -3.276 \times 10^9$ J/kmol	$v = 2.06$ m/s
$\Delta H_3 = -4.561 \times 10^9$ J/kmol	$v_c = 2.0$ m/s
$C_{ref} = 0.0001811$ kmol/m^2	$T_{ref} = 628.0$ K

Table 2. Base steady-state input variables and operating conditions

Inlet o-xylene concentration (oxygen in excess) = 0.0001811 kmol/m^3
Reactor pressure = 27–29 psig
Gas flow rate = 2.06 m/s
Coolant flow rate = 2.0 m/s
Feed inlet temperature (T_{in}^*) = 628.0 K
Coolant inlet temperature (T_{cin}^*) = 628.0 K

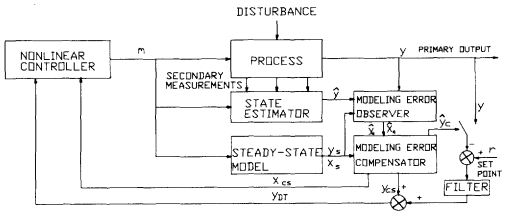

Fig. 4. Structure of nonlinear inferential control (NSFC scheme)

but if modeling errors and measurement noises exist in the inferential control system, the estimated output $\hat{y}$ will differ from the process output y. Thus, we must modify the estimated output $\hat{y}$ to approximate the process output y as much as possible. The compensator used to compensate the estimated output $\hat{y}$ can be described as follows.

The process output y can be obtained from instrumental analysis (such as gas chromatography). However, it may take one or two hours, or even longer. Since we obtain the process output y after a period of time, then at any sampling time (i.e., $t = nT_s$), the compensation for the estimated output y can be described as

$$\hat{y}_c(t)\Big|_{t=nT_s} = y(t) \quad (22)$$

where $\hat{y}_c$ is the compensated output.

Since the process output y cannot be obtained in a short period, before the next process output y obtained through instrumental analysis (i.e., between two

sampling times), the process output y must thus be replaced by the estimated value $\hat{y}$ from the state estimator. In addition, the estimated output $\hat{y}$ will be influenced by modeling errors and measurement noise. This can be dealt with by adding a modeling error observer and compensator for the estimated output and the steady-state output to the nonlinear inferential control structure:

$$\begin{aligned} \hat{y}_c(t) &= \hat{y}_c(t-\Delta t) + \hat{y}_\varepsilon(t) \\ y_{cs}(t) &= y_{cs}(t-\Delta t) + \hat{y}_\varepsilon(t) \end{aligned} \tag{23}$$

where

$$\hat{y}_\varepsilon(t) = \hat{y}_c(t-\Delta t) - y_s(t)$$

For the o-xylene oxidation reactor, we wish to use the inlet temperature (T_{in}) as the manipulated variable in controlling the exist concentration (C_{aN+2}) of the reactor. The control criterion is chosen to keep C_{aN+2} to its steady-state value, C_{as}, i.e.,

$$C_{aN+2} = C_{as} \tag{24}$$

It is clear that

$$\left.\frac{dC_{ai}}{dt} = \frac{dC_{bi}}{dt} = \frac{dT_i}{dt} = \frac{dT_{ci}}{dt}\right|_{i=N+2} = 0 \tag{25}$$

By substituting eqs (24) and (25) into the discretized reactor model Eqs. (16)—(19), and then using Eq. (12), the nonlinear-state feedback controller can be obtained as

$$\begin{aligned} T_{in} = \Bigg\{ \Bigg\{ \frac{1}{\tau} \Bigg\{ \mu(1-\varepsilon) \Bigg[\psi_1 K_1 \exp\left(-\frac{\gamma_1}{T_{N+2}}\right) C_{aN+2} \\ + \psi_2 K_2 \exp\left(-\frac{\gamma_2}{T_{N+2}}\right) C_{bN+2} \\ + \psi_3 K_3 \exp\left(-\frac{\gamma_3}{T_{N+2}}\right) C_{aN+2} \Bigg] \Bigg\} - \Omega(T_{N+2} - T_{c0}) \Bigg\} \\ - \sum_{j=2}^{N+2} A_{N+2j} T_j \Bigg\} \Bigg/ A_{N+2,1} \,. \end{aligned} \tag{26}$$

The state variables of the nonlinear-state feedback controller equation can be obtained from the state estimator and steady-state model.

3. Simulation Results

To test the control performance of the proposed NSFC scheme which is applied to the inferential control system, the changes in load disturbances, set point, and adjustable parameters of the controllers have been included in the precess control simulation. These simulation results are presented in Fig 5–13.

Figure 6 compares the control performances of the NSFC scheme, IMC scheme, and GMC scheme when the feed flow rate of the process is changed (as shown in **Fig. 5**). **Figure 8** makes the same comparison when

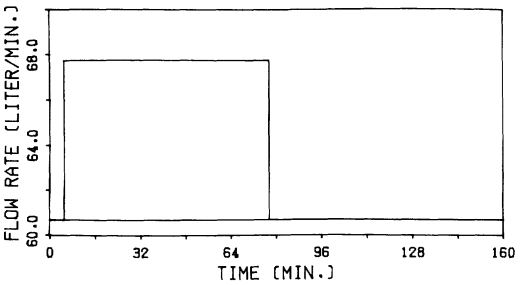

Fig. 5. Step change in feed flow rate from 60.67 l/min to 67.74 l/min

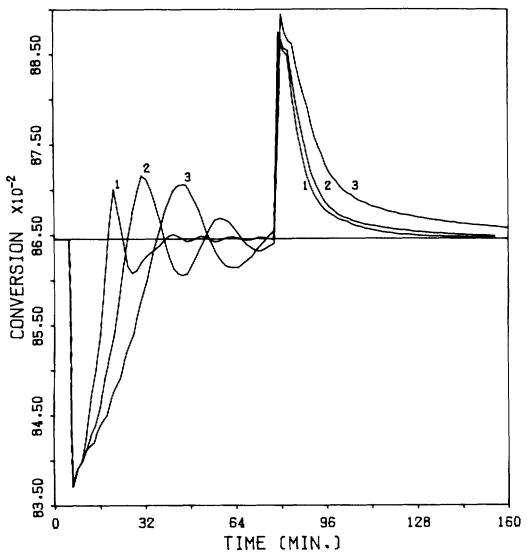

Fig. 6. Control performances of inferential control under feed flow rate change given in Figure 5. (1) SFC ($T_f = 2.0$), (2) IMC ($T_f = 2.0$), (3) GMC ($K_1 = 0.00025$, $K_2 = 0.00005$)

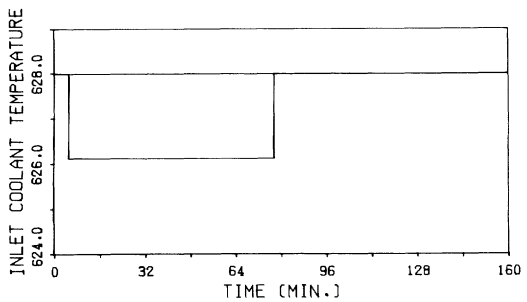

Fig. 7. Step change in inlet coolant temperature from 626 K to 628 K

the inlet coolant temperature of the process is changed (as showen in **Fig. 7**). And **Fig. 9** shows the same comparison as the set-point changes. From the simulation results, we can find that the control performances of the NSFC scheme are better than those of the IMC scheme and GMC scheme because the nonlinear-state feedback controller is directly made up by the nonlinear PA reactor model. And the steady-state model in the NSFC scheme can predict the steady-state output when the controller generates

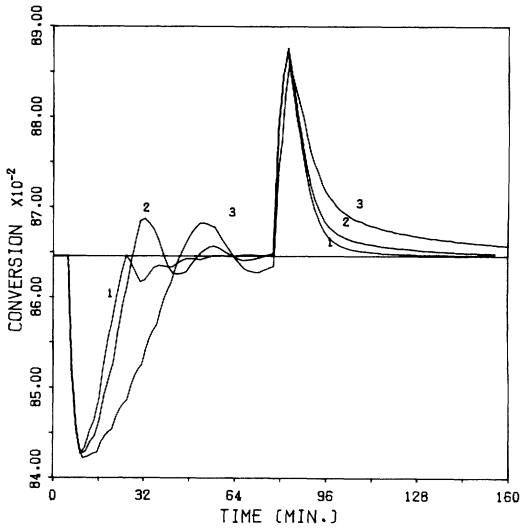

Fig. 8. Control performances of inferential control under inlet coolant temperature change given in Fig. 7. (1) SFC ($T_f=2.0$), (2) IMC ($T_f=2.0$), (3) GMC ($K_1=0.00025$, $K_2=0.00005$)

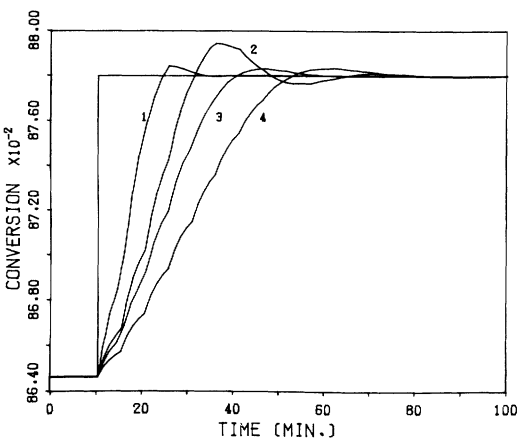

Fig. 9. Control performances of inferential control as the set point changes. (1) SFC ($T_f=2.0$), (2) IMC ($T_f=2.0$), (3) GMC ($K_1=0.00025$, $K_2=0.00005$), (4) GMC ($K_1=0.0001$, $K_2=0.00005$)

changes in the manipulated variable of the process. With this prediction concept and the nonlinear controller in the NSFC scheme, a better control performance can be obtained. As for the GMC scheme, although there is a nonlinear function term in the controller, the control algorithm is not a completely nonlinear system, but is actually a partially linear system. Therefore, the control performances of the GMC scheme are not as good as what we would expect.

Figures 10–13 indicate the control performances of the process when the adjustable parameters (i.e., K_1, K_2, and filter time constant) of the controllers change. **Figure 10** shows that for the NSFC scheme a change in the filter time constant will affect only the percentage overshoot of the response but does not obviously affect the settling time. In **Figs. 11–13**, however, we see that

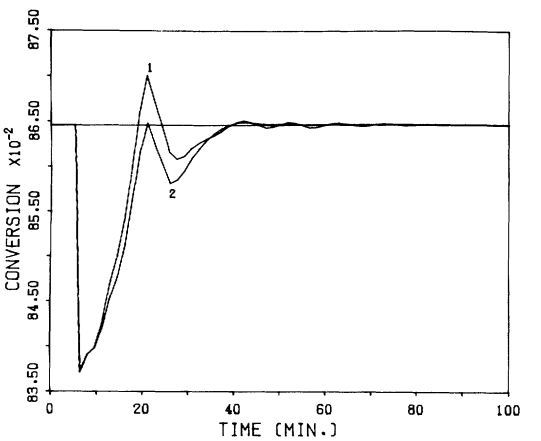

Fig. 10. Control performances of the NSFC scheme as filter time constant changes with feed flow rate change given in Fig. 5. (1) $T_f=2.0$, (2) $T_f=3.5$

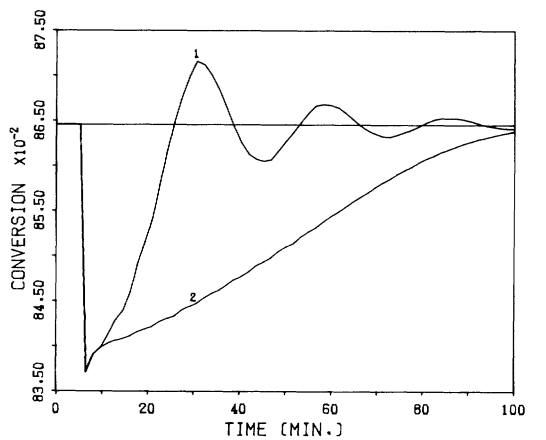

Fig. 11. Control performances of the IMC scheme as the filter time constant changes with feed flow rate change given in Fig. 5. (1) $T_f=2.0$, (2) $T_f=3.5$

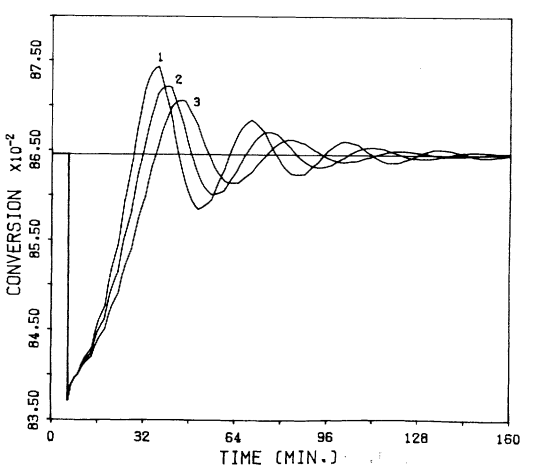

Fig. 12. Control performances of the GMC scheme as K_2 changes under feed flow rate change given in Fig. 5 and $K_1=0.00025$. (1) $K_2=0.0001$, (2) $K_2=0.00005$, (3) $K_2=0.000005$

for the IMC scheme and the GMC scheme the changes in the adjustable parameters of controllers will affect both. From the results above it is seen that, when the

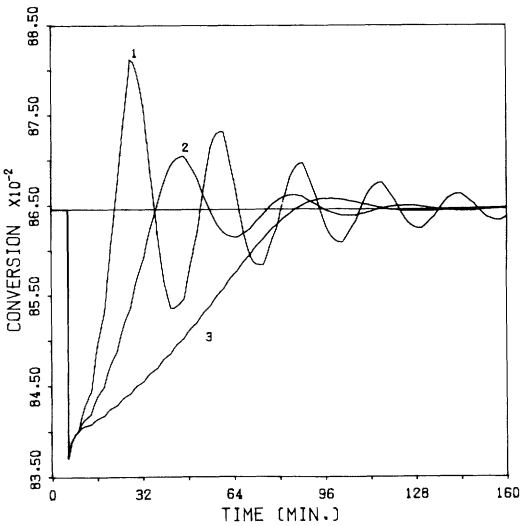

Fig. 13. Control performances of the GMC scheme as K_1 changes with feed flow rate change given in Fig. 5 and $K_2=0.0$. (1) $K_1=0.0005$, (2) $K_1=0.00025$, (3) $K_1=0.0001$

process is undergoing large disturbances, proper adjustment of the filter time constant is necessary to obtain stable control.

Conclusion

In this paper, we develop the NSFC strategy to improve the control performances of nonlinear chemical processes. From simulation results we find that the control performances of the NSFC scheme are superior to those of the IMC scheme and the GMC scheme. Here, we use a compensation part which eliminates the effects of modeling errors and measurement noise, a nonlinear state feedback controller, and a steady-state model to develop the NSFC strategy. Since the process model is very important in describing the characteristics of a real process for a model-based control, a reduced-order, nonlinear process model was adopted for designing a controller of the NSFC strategy that improves the control performances. In the NSFC scheme, the control performances are mainly influenced by the nolinear controller, while there is no obvious influence of the filter time constant. However, the IMC scheme and the GMC scheme are completely or partially linear systems, in which the adjustable parameters of the controllers will have more influence on the control performances. So we can conclude that nonlinear chemical processes that are poorly controlled using linear or partially linear systems can be controlled well by the NSFC scheme.

Nomenclature

C_a = dimensionless concentration of A
C_a^* = concentration of A, kmol/m^3
C_b = dimensionless concentration of B
C_b^* = concentration of B, kmol/m^3
C_{pc} = heat capacity of coolant, J/(kg-K)
C_{pf} = heat capacity of fluid, J/(kg-K)
C_{ps} = heat capacity of catalyst, J/(cat. kg-K)
C_{ref} = reference concentration, kmol/m^3
E_i = activation energy of reaction i, J/kmol
$f_1(t)$ = first-order filter in time domain
ΔH_i = heat of reaction i, J/kmol
k_i' = reaction rate frequency factor, 1/s
K_i = dimensionless heat of reaction = $[C_{ref}(-\Delta H_i)]/(T_{ref}\overline{\rho C_p})$
K_1 = GMC performance specification
K_2 = GMC performance specification
L = reactor length, m
m = manipulated variables
N = number of collocation points
Q' = dimensionless variable $=v/v_c$
$r(t)$ = set point
r_0 = reactor radius, m
r_1 = coolant tube radius, m
R_g = gas constant, J/(kmol-K)
R' = dimensionless variable $=r_0[(r_1/r_0)^2-1]$
t = dimensionless variable $=t^*v/L$
t^* = time, s
T = dimensionless temperature $=T^*/T_{ref}$
T^* = reactor temperature, K
T_c = dimensionless coolant temperature T_c^*/T_{ref}
T_c^* = coolant temperature, K
T_f = filter time constant
T_{ref} = reference temperature, K
U = overall heat-transfer coefficient, J/(m^2-s-K)
u = input disturbance vector
v = fluid velocity, m/s
v_c = coolant velocity, m/s
x = state variables
x_{cs} = compensated state variables
x_s = state variables obtained from steady-state model
x_ε = modeling error, difference between x and x_s
y = process output
$\hat{y}$ = estimated output
$\hat{y}_c$ = compensation value for estimated output $\hat{y}$
y_{cs} = compensation value for steady-state output y
y_{DT} = desired trajectory output
y_s = steady-state output obtained from steady-state model
y^* = desired steady-state value
y_ε = modeling error, difference between y and y_s
$\hat{y}_\varepsilon$ = modeling error, difference between $\hat{y}_c$ and y_s
$\bar{z}$ = reactor length coordinate, m
β = dimensionless variable $=2UL/(R'\rho_c C_{pc}v)$
γ_i = dimensionless activation energy for reaction $i=E_i/(R_gT_{ref})$
ε = void volume fraction of reactor
θ = measurement vector
μ = catalyst activity
ξ = dimensionless reactor length coordinate
ρ_c = coolant density, kg/m^3
ρ_f = fluid density, kg/m^3
ρ_s = catalyst density, kg/m^3
$\overline{\rho C_p}$ = $(1-\varepsilon)\rho_s C_{ps}+\varepsilon\rho_f C_{pf}$
τ = heat capacity ratio $=(\rho_f C_{pf})/\overline{\rho C_p}$
ϕ_i = dimensionless reaction rate constant for $i=(k_i'L)/v$
Ω = dimensionless heat-treasfer coefficient = $(2UL)/(r_0\overline{\rho C_{pv}})$

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Appendix A

A detailed discussion of the collocation method is available in the textbooks of Finlayson[4] and Villadsen and Michelsen[15]. In the method of orthogonal collocation the dependent variables are expressed as polynomials in the direction of discretization. The coefficients in the polynomial approximation are then forced to satisfy the original equations at a number of selected points (collocation points). The orthogonal collocation method can be used to solve ordinary differential equations as well as partial differential equations. Consider an ordinary differential equation

$$\frac{1}{x}\frac{d}{dx}\left(x\frac{dy}{dx}\right)=f(y)$$

$$\left.\frac{dy}{dx}\right|_{x=0}=0\,,\quad y(x=1)=y_1 \tag{A1}$$

In many of these problems it is possible to prove that the solution is a symmetrical function of x, i.e., a function of only even powers of x, excluding all odd powers. In such a case it is our prerogative to include that information in the choice of trial functions (or perturbation functions). To do this we construct orthogonal polynomials that are functions of x^2. One choice is

$$y(x^2)=y(1)+(1-x^2)\sum_{j=1}^{n}a_jP_{j-1}(x^2) \tag{A2}$$

Equivalent choices are

$$y(x^2)=\sum_{j=1}^{N}b_jP_{j-1}(x^2)=\sum_{j=1}^{n}d_{jx}^{2j-2} \tag{A3}$$

We define the polynomials to be orthogonal with the condition

$$\int_0^1 w(x^2)P_k(x^2)P_m(x^2)x\,dx=0\,,\quad k<m-1 \tag{A4}$$

We take the first coefficient of the polynomial as one, as that the choice of the weighting function $W(x^2)$ completely determines the polynomial, and hence the trial function and the collocation points. Taking the derivative of (A2) yields

$$\frac{dy}{dx}=\sum_{j=1}^{N+1}d_j(2j-2)x^{2j-3} \tag{A5}$$

We take as collocation points the N interior points ($0\le x_i<1$ and one boundary point $x_{N+1}=1$. The point $x=0$ is not included because the symmetry condition requires that the first derivative be zero at $x=0$ and that condition is already built into the trial function. The derivatives are evaluated at the collocation point to give

$$y(x_i)=\sum_{j=1}^{N+1}x_i^{2j-2}d_j$$

$$\frac{dy}{dx}(x_i)=\sum_{j=1}^{N+1}x_i^{2j-3}(2j-2)d_j \tag{A6}$$

or in matrix notation

$$\boldsymbol{y}=\boldsymbol{Qd} \tag{A7}$$

$$\dot{\boldsymbol{y}}=\boldsymbol{Cd} \tag{A8}$$

where

$$Q_{ij}=x_i^{2j-2}$$

$$C_{ij}=(2i-2)x_i^{2j-3}$$

Substituting (A7) into (A8) yields

$$\dot{\boldsymbol{y}}=\boldsymbol{CQ}^{-1}\boldsymbol{y}=\boldsymbol{Ay} \tag{A9}$$

The collocation matrix $\boldsymbol{A}=\boldsymbol{CQ}^{-1}$ can therefore be calculated for gny given order of polynomial and location of the collocation points.

Appendix B

The general steady-state, nonlinear estimation problem can be stated as follows.

Here is a process described by

$$f(\boldsymbol{x},\boldsymbol{u})=0 \tag{B1}$$

We shall estimate x from nonlinear measurements of the form

$$\boldsymbol{z}=\boldsymbol{h}(\boldsymbol{x})+\eta \tag{B2}$$

The least-squares estimate of $\boldsymbol{x}$ given $\boldsymbol{z}$ is defined as the value $\hat{\boldsymbol{x}}$ that minimizes the performance index

$$J=[\boldsymbol{z}-\boldsymbol{h}(\boldsymbol{x})]^{\mathrm{T}}[\boldsymbol{z}-\boldsymbol{h}(\boldsymbol{x})] \tag{B3}$$

where the weighting matrix has been chosen as an identity matrix for convenience.

Suppose that an initial estimate $\boldsymbol{x}^*$ of $\boldsymbol{x}$ is available. A necessary condition that $\boldsymbol{x}^*$ minimizes J is that

$$\left.\frac{\partial J(\boldsymbol{x})}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}=\boldsymbol{x}^*}=0 \tag{B4}$$

Thus, to determine the least-squares estimate $\hat{x}$, form

$$\left.\frac{\partial J}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}=\hat{\boldsymbol{x}}}=-2[\boldsymbol{z}-\boldsymbol{h}(\boldsymbol{x})]^{\mathrm{T}}\left.\frac{\partial \boldsymbol{h}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}=\hat{\boldsymbol{x}}}=0 \tag{B5}$$

which can be rewritten as

$$\left[\frac{\boldsymbol{h}(\hat{\boldsymbol{x}})}{\boldsymbol{x}}\right]^{\mathrm{T}}\left[\boldsymbol{z}-\boldsymbol{h}(\hat{\boldsymbol{x}})\right]=0 \tag{B6}$$

Because $\boldsymbol{h}(\boldsymbol{x})$ is nonlinear, eq. (A6) represents a set of nonlinear algebraic equations for which, in general, there is no closed-form solution. Thus, an iterative procedure for finding an approximation of the least-squares estimate is suggested. A necessary condition

for $\hat{x}$ to be the least-squares estimate is that the orthogonality condition [eq. (A6)] be satisfied (i.e., the gradient vanishes).

By using the nonlinear estimation theory, the state estimation of the PA reactor can be described as follows: Reactor model

$$A_{i1}C_{a1}+\sum_{j=2}^{N+1}A_{ij}C_{aj}=\mu(1-\varepsilon)\left[-\psi_1\exp\left(\frac{-\gamma_1}{T_i}\right)-\psi_3\exp\left(\frac{-\gamma_3}{T_i}\right)\right]C_{ai} \tag{B7}$$

$$A_{i1}C_{b1}+\sum_{j=2}^{N+2}A_{ij}C_{bj}=\mu(1-\varepsilon)\left[\psi_1\exp\left(\frac{-\gamma_1}{T_i}\right)C_{ai}-\psi_2\exp\left(\frac{-\gamma_2}{T_i}\right)C_{bi}\right] \tag{B8}$$

$$A_{i1}T_1+\sum_{j=2}^{n+2}A_{ij}T_j=\frac{1}{\tau}\left\{\mu(1-\varepsilon)\left[\psi_1K_1\exp\left(\frac{-\gamma_1}{T_i}\right)C_{ai}+\psi_2K_2\exp\left(\frac{-\gamma_2}{T_i}\right)C_{bi}+\psi_3K_3\exp\left(\frac{-\gamma_3}{T_i}\right)C_{ai}\right]\right\}-\Omega(T_i-T_{ci})\quad i=2,3,\cdots,N+2 \tag{B9}$$

$$\sum_{j=1}^{N+1}A_{ij}T_{cj}+A_{i,N+2}T_{cN+2}=-\frac{\beta}{Q'}(T_i-T_{ci}),\quad i=1,2,\cdots,N+1 \tag{B10}$$

where

$$C_{a1}=C_{ain},\quad C_{b1}=C_{bin},\quad T_1=T_{in},\quad T_{cN+2}=T_{cin}$$

Define

$$\boldsymbol{x}=[T_2,T_3,\cdots,T_{N+2},C_{a2},C_{a3},\cdots,C_{aN+2},C_{b2},C_{b3},\cdots,C_{bN+2},T_{c1},T_{c2},\cdots,T_{cN+1}]^T$$

$$\boldsymbol{u}=[C_{ain},T_{in},v,v_c]^T$$

Then the equations can be reduced to the form

$$f(x,u)=0 \tag{B11}$$

If the observations are taken along the collocation proints, then the observation vector is

$$z=[T_2,T_3,\cdots,T_{N+2}] \tag{B12}$$

The problem is to estimate the conversion

$$\text{conversion}=\frac{C_{ain}-C_{aN+2}}{C_{ain}} \tag{B13}$$

GRG2 (Lasdon *et al.*[10]), a computer package for implementing the generalized reduced-gradient method for constrained optimization problems, is used to solve the above equations.