On-Line Optimizing Control of a Nonadiabatic Fixed Bed Reactor

A scheme of on-line optimizing control is presented for a nonadiabatic fixed bed reactor which experiences a highly exothermic reaction. The control scheme has been devised to perform adaptive control of bed temperature and on-line steady state optimization simultaneously.

Experiments were conducted with a pilot scale fixed bed reactor where partial oxidation of *n*-butane to maleic anhydride occurs. The reactor system was interfaced with a microcomputer for real-time control and optimization. With an objective function consisting of a net profit by producing maleic anhydride plus a penalty term on high bed temperature, it was clearly shown that the reaction conditions were driven to the expected optimum region.

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SCOPE

The rising costs of energy and raw materials have afforded a strong incentive to chemical engineers to develop a well-posed control scheme which gives greater economic return in operating a process. Optimizing control has been accepted as one of the promising ways to fulfill the above requirement and now attracts much attention (Latour, 1979a,b).

As was reviewed by Arkun and Stephanopoulos (1980), various optimizing control methods have been proposed up to now. Many of the schemes devised, however, have been based on the steady state behavior of a process (e.g., Box and Draper, 1969; Edler et al., 1970; Haimes and Wismer, 1972; Roberts and Williams, 1981). Two major drawbacks of these methods are that they are slow, and that if the process is subject to persistent disturbances which prevent it from reaching any steady state, they will not be sufficient.

Bamberger and Isermann (1978) presented a new optimizing control method where a nonlinear dynamic model of a process is identified using a recursive identification method. Their scheme has many outstanding features, such as noise insensitivity and fast convergence to the optimum point. These features were illustrated by experimentally implementing the method on a thermal pilot process. This idea recently was extended to a large-scale system with many interconnected subprocesses by Garcia and Morari (1981).

In this paper, we are concerned with on-line optimizing control of a fixed bed reactor with exothermic reaction. Aside from economic benefit, the study of on-line optimizing control of the reactor is well-justified because modeling difficulty and time-varying characteristics due to catalyst deactivation do not allow advance determination of long-term optimum operating conditions.

In a fixed bed reactor with exothermic reaction, control of bed temperature is required in addition to on-line optimization. In this work, we propose an on-line optimizing control scheme which can achieve the above two requirements simultaneously in a fully adaptive manner. This scheme is developed by combining an adaptive control loop for bed temperature with the optimizing control loop of Bamberger and Isermann (1978). In the optimizing control loop, identification of a reactor model and steady state optimization are conducted. The objective function for optimization is taken to be the sum of a net profit by producing a desired product and a penalty term on high bed temperature. To evaluate practical applicability of the proposed scheme, experimental studies are performed in a pilot-scale fixed bed reactor which produces maleic anhydride from *n*-butane.

CONCLUSIONS AND SIGNIFICANCE

The method of on-line optimizing control developed by Bamberger and Isermann (1978) was modified for application to a nonadiabatic fixed bed reactor by incorporating an adaptive control loop for bed temperature within an on-line optimization loop. The proposed scheme was successfully implemented using a microcomputer in a pilot-scale reactor system for partial oxidation of *n*-butane to maleic anhydride. The optimizing control scheme was designed to perform two functions concurrently: adaptive control of a bed temperature, and on-line identification and optimization. The adaptive control loop prevents excessive bed temperature caused by unknown disturbances. In this loop, a temperature in the region where a hot spot occurs under normal reaction conditions was controlled. In the identification loop, the relation between maleic anhydride and reaction conditions was approximated by a nonlinear second-order Hammerstein model and its parameters were identified using the recursive instrumental variable method. The random search method was used to solve the optimization problem.

The on-line optimizing controller drove the reactor from an initial condition of low productivity and high bed temperature to the expected optimum operating region. The control scheme required the least amount of information on the process for its implementation due to its fully adaptive mode of operation. The

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use of the second-order Hammerstein model in the scheme with a recursive identification method was reliable enough to represent nonlinear behavior of the reactor even in a limited operating range.

In this work, emphasis has been placed on the practical implementation of advanced control theories. Methods to further reduce the total time for on-line optimization and to assure the optimum point will improve the overall scheme. Nevertheless, based on very encouraging experimental results, the on-line optimizing control scheme in its present form is believed to be applicable to an industrial reactor to yield a greater economic return.

EXPERIMENTAL REACTOR SYSTEM

The reaction considered here is partial oxidation of n-butane to maleic anhydride (MA), a highly exothermic reaction carried out over vanadium phosphorous catalyst. It is one of the typical industrially important partial oxidation reactions where selectivity of the intermediate product is important. The reaction path is represented as follows:

$$\begin{aligned} n\text{-}C_4H_{10} + O_2 &\rightarrow C_4H_2O_3 + H_2O \\ n\text{-}C_4H_{10} + O_2 &\rightarrow CO + CO_2 + H_2O \\ C_4H_2O_3 + O_2 &\rightarrow CO + CO_2 + H_2O \end{aligned} \quad (1)$$

A schematic diagram of the reactor system is shown in Figure 1a. The reactor consists of a single stainless steel tube of 2.54 cm ID and 70 cm length, of which a total bed length of 55 cm is packed with catalyst. Nine thermocouples are positioned along the central axis of the bed to monitor bed temperatures. The reactor tube is immersed in a vigorously stirred molten salt bath which is enclosed by insulating walls. Unlike industrial reactors with five thousand or more reactor tubes, reaction heat in our reactor system is small compared to heat loss through insulating walls. Thus an immersion-type electric heater is furnished to supplement the heat loss.

The reactor system is equipped with three actuators, two control valves for air and n-butane flow rates, and an electric heater for adjustment of salt bath temperature. Analog PID controllers are connected to these three actuators, and their set points are supplied by the on-line microcomputer system. A microcomputer system (Cromemco, CS-3) with Z-80 microprocessor interfaced with the reactor system provides real-time data acquisition, control, and optimization.

Exit concentrations of CO, CO_2, and O_2 are continuously measured with an infrared gas analyzer (Infrared, IR-702) and a membrane electrode oxygen analyzer (Beckman, 7003) after capturing MA in a seven-stage ice trap. Maleic anhydride yield is then calculated in the computer system through material balances. Since the gas concentrations are measured in flowing condition, a wrong MA yield might result from the difference in measurement dynamics between the two gas analyzers, but by choosing a sampling time of 1 min. this problem could be resolved. The sampling time chosen is sufficiently long for the gas analyzers to reach steady states and also short enough compared to time constant of the reactor system: 10 to 15 min., depending on reaction conditions.

In this reactor system, three variables—coolant temperature (or salt bath temperature), contact time (defined by bed volume/feed flow rate at reaction condition), and feed concentration—are available as manipulated variables. The feed concentration is, however, maintained constant (n-butane/air = 1.1%) to avoid acceleration of catalyst deactivation (Varma and Saraf, 1978) and possible hazard when it exceeds the explosion limit (about 1.8% at 450°C).

Among bed temperatures at various positions, only one around which a hot spot occurred most frequently under normal operations is chosen as a controlled variable. This temperature measurement is located at a normalized axial position of $z = 0.136$ and denoted by T^*. Since a fixed bed reactor has a characteristic of the distributed parameter system, control of a temperature at the fixed position alone cannot result in the regulation of the whole temperature distribution at any desired state. However, from the standpoint that the role of the temperature control loop is to prevent excessive bed temperature caused by unknown disturbances, control of a bed temperature at the fixed position can be justified.

The overall reactor system becomes a 2 × 2 multiinput multioutput (MIMO) system as illustrated in Figure 1b. The control inputs are, in fact, the set points of contact time and coolant temperature. But throughout this paper, "contact time" and "coolant temperature" are used instead of "set point of . . ." unless there arises any confusion between them.

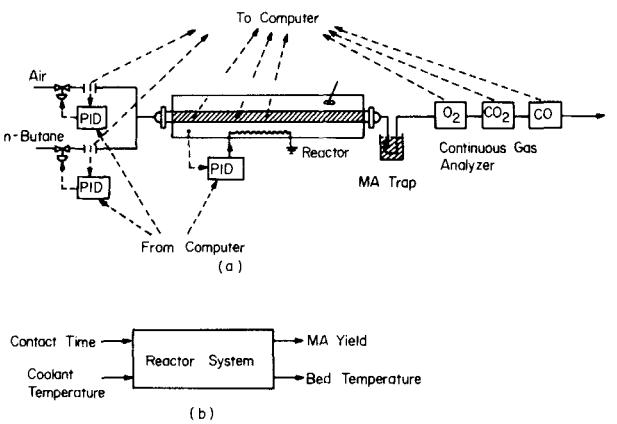


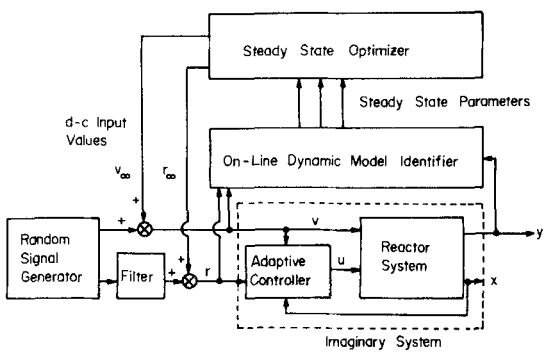
Figure 1. Experimental reactor system.

ON-LINE OPTIMIZING CONTROL SCHEME

Based on the method of Bamberger and Isermann (1978), an on-line optimizing control scheme was designed to perform the following functions simultaneously.

1. Adaptive control of the bed temperature, T^*, using coolant temperature as a control input.
2. On-line identification of a dynamic model of the reactor system.
3. Steady-state optimization using system parameters supplied by the on-line identifier.

The proposed optimizing control scheme is shown in Figure 2. It is composed of two loops, the inner loop where adaptive control of the bed temperature T^* is performed, and the outer loop where identification and steady state optimization are conducted. The adaptive control loop for bed temperature was incorporated within the scheme to satisfy an additional requirement of a fixed bed reactor with exothermic reaction. Since the steady state part of a dynamic model of the process is used to determine the current optimum and the direction of movement for the control inputs, the 2 × 2 MIMO system shown in Figure 1b should be identified before



u = Δ Coolant Temperature
v = Δ Contact Time
x = Δ Bed Temperature, T^*
y = Δ MA Yield

Figure 2. On-line optimizing control scheme for a nonadiabatic fixed bed reactor.

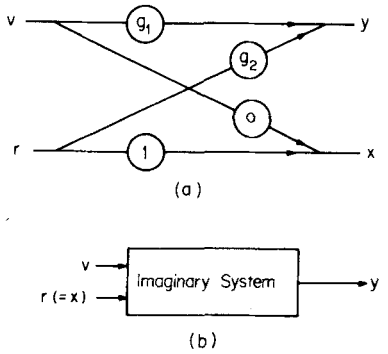


Figure 3. Input-output relation of imaginary system.

the optimization phase is executed. Even for a 2 × 2 system, the amount of calculation for MIMO system identification is usually large. To reduce the computational load and consequently to improve the parameter convergence rate, an imaginary system was conceived by adding a feedforward mode in the adaptive loop as shown in Figure 2.

The imaginary system has two inputs, contact time and set point of T^*, and two outputs, MA yield and T^*. When T^* follows its set point perfectly in the adaptive control loop, the input-output relation of the imaginary system can be altered as illustrated in Figure 3a, and equivalently the imaginary system becomes a 2-input 1-output system as shown in Figure 3b where only one output, MA yield, is significant. Through this reduction, the system to be identified is much simplified and the objective function in the optimizer becomes an explicit function of input variables only, v and r of the imaginary system.

The procedure of identification and optimization is illustrated in Figure 4, where the contour represents a constant profit function obtained from computer simulation work with the reactor model. Initially the reactor is under an arbitrary condition, say, point A. Random inputs, pseudorandom binary sequences (PRBS) here, are superimposed on steady state input values and activate the imaginary system. Its input and output signals are sampled by the on-line identifier and parameters of a dynamic model of the imaginary system are estimated recursively. After the dynamic model has been identified to some extent, the optimizer takes steady state gains of the identified model, and determines new optimum *d-c* input values from the constrained region where the identification has been done. This new optimum point is denoted by point *B* in Figure 4. This procedure is repeated until no further improvement is obtained.

In the adaptive control loop for bed temperature, tracking should be done since the set point of T^* varies continuously due to the PRBS. In this work, coolant temperature was manipulated for this tracking. It is noteworthy that contact time was not found appropriate as a control input, since its only effect is to contract or to expand the bed temperature profile along the axial direction. Moreover, bed temperature around the hot spot may show an inverse response when there is a step change in contact time (Lee, 1983). The inverse response is often characterized as a nonminimum phase behavior and makes the adaptive control difficult. The coolant temperature, however, always gave a minimum phase behavior and rather linear response to bed temperatures over a wide range of variations. Additional time lag due to the capacity of the molten salt bath is thought to be a drawback as a control input. But this effect can be compensated by its high steady state gain to bed temperatures. By taking coolant temperature as the control input, the contact time acts as a known disturbance to the imaginary system since it varies according to the predefined PRBS. Thus, it is necessary to compensate for this known disturbance by adding a feedforward mode to the adaptive control loop.

In the following sections each functional block in Figure 2 will be described.

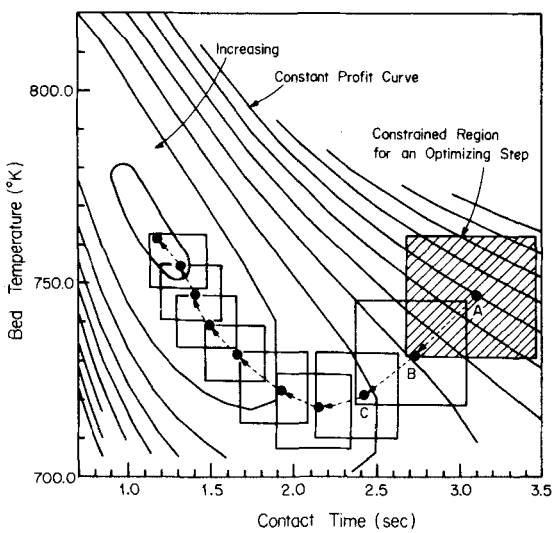


Figure 4. Procedure of optimizing control.

Nonlinear Process Model for the Imaginary System

By the characteristics of a series-parallel reaction, a maximum MA yield exists over the reaction conditions. A simulated result of the relation between steady state MA yield and reaction conditions is given in Figure 5. Convexity is noted between them, especially between MA yield and contact time. Such a nonlinearity may be approximated by a quadratic-type function of reaction conditions, even in a limited region. By extending this idea, the following nonlinear model was assumed to represent the dynamics of the imaginary system:

$$D(q^{-1})y(k) = E_v(q^{-1})v(k-d_v) + E_r(q^{-1})r(k-d_r) + E_{v^2}(q^{-1})v(k-d_v)^2 + E_{r^2}(q^{-1})r(k-d_r)^2 + E_{vr}(q^{-1})v(k-d_v)r(k-d_r) + D_I \quad (2)$$

where

$$D(q^{-1})y(k) = y(k) + d^1y(k-1) + \ldots$$
$$E_v(q^{-1})v(k) = e_v^0 v(k) + e_v^1 v(k-1) + \ldots$$
$$E_{v^2}(q^{-1})v(k)^2 = e_{v^2}^0 v(k)^2 + e_{v^2}^1 v(k-1)^2 + \ldots$$
$$\vdots \quad (3)$$

and D_I is a bias term.

Variables, $y(k)$, $v(k)$, and $r(k)$ correspond to deviation variables of MA yield, contact time, and the bed temperature T^* from those at initial steady state, say, point A in Figure 4. Equation 2 is really a second-order Hammerstein model, a special form of Uryson series (Sternby, 1980) which is used to represent a nonlinear system in discrete time.

At steady state, Eq. 2 becomes

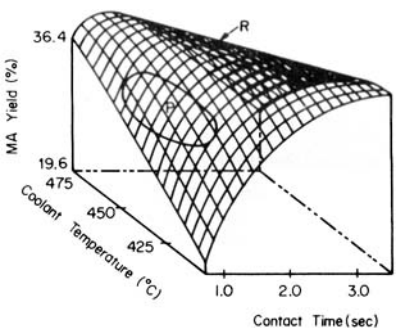


Figure 5. Maleic anhydride (MA) yield at various reaction conditions obtained from reactor simulation.

$$y_\infty = G_v v_\infty + G_r r_\infty + G_{v^2} v_\infty^2 + G_{r^2} r_\infty^2 + G_{vr} v_\infty r_\infty + G_I \tag{4}$$

where

$$G_v = E_v(1)/D(1)$$
$$\vdots$$
$$G_I = D_I/D(1) \tag{5}$$

These steady state gains are used by the steady state optimizer to find a new optimum condition.

On-line Identifier

Various recursive methods have been reported for identification of a dynamic model such as Eq. 2 which is linear in parameters. Among them, the instrumental variable method (Wong and Polak, 1967; Young, 1970; Söderström and Stoica, 1981) which gives unbiased estimates in a noisy environment was adopted in this work. Other unbiased estimators (Söderström et al., 1978; Goodwin and Payne, 1977) such as recursive maximum likelihood, recursive generalized least squares, and recursive extended least squares methods can be considered. But additional parameters on noise dynamics, which are not needed for our work, are identified in these methods, resulting in much computational burden and a slow convergence rate. Nonparametric methods such as correlation analysis may be useful when there is a significant noise effect. In the work by Isermann et al. (1974) comparing various parameter estimation methods, the recursive instrumental variable method always gave the most accurate results and required less computation time than others but showed it might diverge in some cases. For the most part, however, this divergence can be resolved with the help of a recursive least squares method at initial identification steps.

The instrumental variable method is a modification of the least squares method to eliminate the parameter bias problem by introducing the so-called instrumental variable. Its recursive form for the nonlinear system, Eq. 2 is as follows.

Define the process variable vector $\theta(k)$, the instrumental variable vector $\bar{\theta}(k)$ and the parameter vector $\hat{\psi}(k)$ to be

$$\theta^T(k) = [-y(k-1), -y(k-2), \ldots, v(k-d_v), \ldots, r(k-d_r), \ldots v(k-d_v)^2, \ldots, r(k-d_r)^2, \ldots, v(k-d_v)r(k-d_r), \ldots, 1] \tag{6}$$

$$\bar{\theta}^T(k) = [-\bar{y}(k-1), -\bar{y}(k-2), \ldots, v(k-d_v), \ldots, r(k-d_r), \ldots v(k-d_v)^2, \ldots, r(k-d_r)^2, \ldots, v(k-d_v)r(k-d_r), \ldots, 1] \tag{7}$$

$$\hat{\psi}T_{(k)} = [\hat{d}^1(k), \hat{d}^2(k), \ldots, \hat{e}_v^0(k), \ldots, \hat{e}_r^0(k), \ldots, \hat{e}_{v2}^0(k), \ldots \hat{e}_{r2}^0(k), \ldots, \hat{e}_{vr}^0(k), \ldots, \hat{D}_I] \tag{8}$$

where

$$\bar{y}(k) = \hat{\psi}^T(k)\,\bar{\theta}(k). \tag{9}$$

Then the recursive parameter estimation is done by

$$\hat{\psi}(k) = \hat{\psi}(k-1) + F(k)\,\bar{\theta}(k)\left[\frac{y(k) - \hat{\psi}^T(k-1)\,\theta(k)}{1 + \theta^T(k)\,F(k)\,\bar{\theta}(k)}\right] \tag{10}$$

$$F(k+1) = \left[F(k) - \frac{F(k)\,\bar{\theta}(k)\,\theta^T(k)\,F(k)}{\lambda(k) + \theta^T(k)\,F(k)\,\bar{\theta}(k)}\right] \Big/ \lambda(k) \tag{11}$$

where $0 < \lambda(k) \leq 1$, $F(0) > 0$, $\hat{\psi}(0) = \psi_0$ and $\bar{y}(0) = \bar{y}(-1) = \ldots = 0$.

Equation 9 is called the bootstrap technique. $\hat{\psi}(k)$ in Eq. 9 should be replaced by the true system parameter vector $\psi(k)$. In this case, it has been shown by Söderström et al. (1978) that the estimates $\hat{\psi}(k)$ converge to true parameters with a probability of one if the identification is done in open loop condition. True parameters, however, are not known a priori, thus $\bar{y}(k)$ is generated using the bootstrap technique. Since the imaginary system in the proposed optimizing control operates in open loop condition, consistent estimates can be obtained if they converge.

Random Signal Generator

To enhance the efficiency of identification, the imaginary system should be activated by randomly disturbed inputs. Most preferably, the inputs should have all frequency components with the same power. Such a signal, namely white noise, is not physically realizable so here the maximum-length null sequences (Graupe, 1972), one kind of PRBS of order 6 and 7, were used for $r(k)$ and $v(k)$, respectively.

For $r(k)$, the PRBS was low-pass filtered (see Figure 2). Otherwise, the bed temperature T^* cannot follow an abrupt transition of the PRBS due to limited power of the control input, the coolant temperature, and then the input-output relation of the imaginary system shown in Figure 3 cannot be realized. As far as the input $r(k)$ is concerned, the imaginary system acts as a low-pass filter. Thus $r(k)$ does not need to have high frequency components, and it will be sufficient to use the low-pass filtered input as a disturbing signal for identification of the imaginary system.

Feedback-Feedforward Adaptive Control

In designing the adaptive control loop, it was necessary to eliminate the effect of contact time through addition of a feedforward loop by regarding the contact time as a known disturbance. For this purpose, the following linear relation was used to represent a dynamic model between bed temperature and coolant temperature:

$$A(q^{-1})x(k) = B(q^{-1})u(k - d_u) + C(q^{-1})v(k - d_v') + D_c \tag{12}$$

where

$$A(q^{-1})x(k) = x(k) + a_1 x(k-1) + \ldots + a_{n_A} x(k - n_A)$$
$$B(q^{-1})u(k) = b_0 u(k) + b_1 u(k-1) + \ldots + b_{n_B} u(k - n_B), \quad b_0 \neq 0 \tag{13}$$
$$C(q^{-1})v(k) = c_0 v(k) + c_1 v(k-1) + \ldots + c_{n_C} v(k - n_C), \quad c_0 \neq 0$$

and D_c is a bias term. Control input $u(k)$ is determined for $x(k)$ to follow its reference output sequence $r(k)$ as k increases.

For the derivation of control law, first consider the following polynomial identity

$$1 = A(q^{-1})S(q^{-1}) + q^{-d_u}R(q^{-1}) \tag{14}$$

where

$$S(q^{-1}) = 1 + s_1 q^{-1} + \ldots + s_{n_S} q^{-n_S}, \; n_S = d_u - 1$$
$$R(q^{-1}) = r_0 + r_1 q^{-1} + \ldots + r_{n_R} q^{-n_R}, \; n_R = n_A - 1 \tag{15}$$

Multiplication of $x(k + d_u)$ on both sides of Eq. 14 yields

$$x(k + d_u) = P(q^{-1})u(k) + H(q^{-1})v(k + d_u - d_v') + R(q^{-1})x(k) + D_c' \tag{16}$$

where

$$P(q^{-1}) = S(q^{-1})B(q^{-1}) = p_0 + p_1 q^{-1} + \ldots + p_{n_p} q^{-n_P}, \quad n_P = d_u + n_B - 1$$
$$H(q^{-1}) = S(q^{-1})C(q^{-1}) = h_0 + h_1 q^{-1} + \ldots + h_{n_H} q^{-n_H}, \quad n_H = d_u + n_C - 1 \tag{17}$$
$$D_c' = D_c S(1)$$

For $x(k + d_u)$ to be equal to $r(k + d_u)$, $u(k)$ should be:

$$u(k) = [r(k + d_u) - p_1 u(k-1) - \ldots - p_{n_p} u(k - n_P) - h_0 v(k + d_u - d_v') - \ldots - h_{n_H} v(k + d_u - d_v' - n_H) - r_0 x(k) - \ldots - r_{n_R} x(k - n_R) - D_c']/p_0 \tag{18}$$

In the adaptive control, coefficients in the polynomials $P(q^{-1})$, $H(q^{-1})$, $R(q^{-1})$, and the bias term D_c' are assumed to be unknown. Very often they are estimated and updated at every sampling time using the recursive least squares method. Then the overall algorithm is as follows:

Define $\phi^T(k) = [u(k-d_u), \ldots, u(k-d_u-n_p), v(k-d_v'), \ldots, v(k-d_v-n_H), x(k-d_u), \ldots, x(k-d_u-n_R), 1] \triangleq [u(k-d_u):\phi_0^T(k)]$ (19)

$\hat{\alpha}^T(k) = [\hat{p}_0(k), \ldots, \hat{p}_{np}(k), \hat{h}_0(k), \ldots, \hat{h}_{nH}(k), \ldots \hat{r}_0(k), \ldots, \hat{r}_{nR}(k), \hat{D}_c'(k)] \triangleq [\hat{p}_0(k):\hat{\alpha}_0^T(k)]$ (20)

The parameters are updated by the recursive least squares algorithm.

$$\hat{\alpha}(k) = \hat{\alpha}(k-1) + \Gamma(k)\phi(k)\left[\frac{x(k) - \hat{\alpha}^T(k-1)\phi(k)}{1 + \phi^T(k)\Gamma(k)\phi(k)}\right] \quad (21)$$

$$\Gamma(k+1) = \left[\Gamma(k) - \frac{\Gamma(k)\phi(k)\,\phi^T(k)\,\Gamma(k)}{\lambda(k) + \phi^T(k)\Gamma(k)\phi(k)}\right] \Big/ \lambda(k) \quad (22)$$

where $0 < \lambda(k) \leq 1$, $\Gamma(0) > 0$, $\hat{\alpha}(0) = \alpha_I$.

Control input $u(k)$ is determined by

$$u(k) = [r(k+d_u) - \hat{\alpha}_0^T(k)\phi_0(k)]/\hat{p}_0(k) \quad (23)$$

Goodwin et al. (1980) and also Landau and Lozano (1981) have proposed various algorithms of adaptive control and have proved that the control error in their schemes converges to zero as k goes to infinity. In the stochastic version of adaptive control, the self-tuning regulator (Åström et al., 1977), it has been shown by Ljung (1977) that the estimated parameters using the least squares method converge to the parameters for minimum variance control strategy (Åström, 1970) with a probability of one if positive realness, which is satisfied in our scheme, is assured. Although the above algorithm contains a feedforward mode, it has essentially the same features as those by the previous researchers and the convergence can be proven in the same way as in Landau and Lozano (1981) or others.

Inclusion of the bias term D_c is needed since precise values of steady state input and output variables are not usually known. Instead of using the bias term D_c, control input $u(k)$ can be replaced by an incremental variable such as $\Delta u(k) = u(k) - u(k-1)$, but it was revealed from preliminary simulation work that more oscillatory transient response as well as excessive control action resulted with the incremental control input.

Steady State Optimizer

In the steady state optimizer, a profit function of the form

$$J = J_{MA} - J_T \quad (24)$$

where $J_{MA} = [\alpha(y_\infty + MA_I) - 100]/(v_\infty + \tau_I)$

$$J_T = \beta(r_\infty + T_{HI} - T_{HB})^2 \quad (25)$$

was used. Here, J_{MA} is the net profit per unit time by producing MA from n-butane, where α, MA_I and τ_I are the cost ratio of MA to n-butane on molar basis, initial values of MA yield (%), and contact time at point A in Figure 4, respectively. J_T is the penalty term on high bed temperature, where β, T_{HI} and T_{HB} are the penalty cost, an initial bed temperature, and a base temperature below which the depreciation due to catalyst deactivation is negligible compared to the profit J_{MA}. The value of α was chosen to be 5, which was the cost ratio in Korea in 1982. The functional form of J_T and its parameters were chosen arbitrarily but to be subjected to larger penalty as the bed temperature deviates more from T_{HB}.

Substitution of y_∞ in Eq. 4 into Eq. 24 yields

$$J = f(r_\infty, v_\infty) \quad (26)$$

and then the profit becomes an explicit function of the input variables of the imaginary system.

Since the steady state model given by Eq. 4 is valid only in a constrained region where the identification has been performed, the problem in the steady state optimizer becomes a constrained parameter optimization to find r_∞ and v_∞ which give the maximum profit.

There are many techniques of handling a constrained optimization. In this work we used the random search method. This method can easily be applied to a constrained optimization and always gives a reliable result. Slow convergence is often pointed out as its drawback, but it does not matter in our case, where only two parameters are involved in the explicit function. Hill-climbing methods can be used for a fast convergence rate, but they become very complicated in the constrained optimization. Recently, Bhattacharya and Joseph (1982) used the method of successive linear programming to solve the constrained optimization problem for optimizing control of a chemical process. Such a method would be suitable for a case with a large number of parameters to be optimized.

EXPERIMENT

The proposed scheme of on-line optimizing control was implemented on the reactor system using a microcomputer. Parameters used in the on-line optimizing controller are listed in Table 1. The initial reaction condition was chosen arbitrarily but to be far away from the industrially proved optimum operating region, contact time of 1–1.5 s, and coolant temperature of 400–500°C. A sampling time of one minute was used throughout the experiments. This value was determined by considering the response dynamics of gas analyzers as well as the time constant of the reactor system.

The experimental procedure was divided into two stages; initiation and advance. Through 30 minutes of steady state run, initial steady state values of the reactor variables were taken, and then the adaptive control and identification were performed during 300–400 sampling steps to get the optimizing control loop started. The first optimization was done just after this initiation period, and optimum d-c input values of the imaginary system were determined in a constrained region bounded by amplitudes of the PRBS's. In the advance stage, optimization was performed once every 100 sampling steps, while the identification scheme was operated at every sampling step. This procedure was repeated until no further improvement was obtained.

The periods of initiation and each advance stage were determined based on preliminary experiments. With sampling steps of 100 and 30 for the initiation and the advance stages in the experiments, the reaction conditions tended to move toward the optimum operating region in almost all cases. During the initial transients, however, movements of the reaction conditions were nearly unpredictable, and the optimizing controller took the reactor to a high temperature region depending on initial assumption of the parameter vector $\hat{\psi}(k)$. This high temperature may damage the reactor and/or accelerate catalyst deactivation. For the sake of safe operation, the periods for initiation and each advance stage were chosen to be somewhat conservative.

In the adaptive control loop, constraints were placed on the minimum and maximum values of the control input. Without adding constraints, the linear relation of Eq. 12 may be violated when a large amount of the control action $u(k)$ is generated during the initial transients. In addition, due to a limited heat generation by the electric heater, the coolant temperature exhibits a velocity limit. All these effects may cause the adaptive controller

TABLE 1. PARAMETERS OF ON-LINE OPTIMIZING CONTROLLER

Experiment	n-butane/air = 1.1% Sampling time = 1 min. T^* = bed temperature at $z = 0.136$
Adaptive Controller	$n_A = 2$, $n_B = n_C = 1$, $d_u = 2$, $d_v' = 1$ $\lambda(k) = 0.99$, $\Gamma(0) = 100I$ $\lvert u(k) - \bar{u} \rvert < 7.0$°C
On-Line Identifier	$n_D = 2$, $n_{E_0} = \ldots = n_{E_{0r}} = 1$, $d_v = 1$, $d_r = 2$, $\lambda(k) = 0.99$, $F(0) = 100I$
Random Signal Generator	Maximum-length null sequences $v(k)$: order 7, $r(k)$: order 6
Steady State Optimizer	$\alpha = 5$, $\beta = 0.003$ $T_{HB} = 420$°C
Filter	$G_F(q^{-1}) = \dfrac{0.04}{1 - 1.6\,q^{-1} + 0.64\,q^{-2}}$

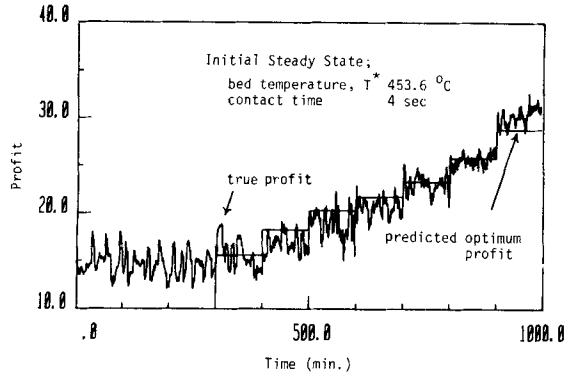


Figure 6. Improvement of profit function during first run.

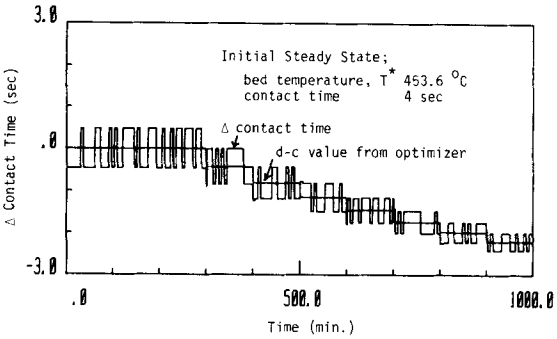


Figure 8. Variation of contact time during first run.

not to work and only to diverge. In simulation studies, adding constraints on the control input always proved to improve control performance by moderating transient response during the initial adaptation.

All necessary computer programs were written in FORTRAN IV except that Z-80 Assembler language was used to write programs for data conversion and input/output with external devices. The resulting assembled program occupies a memory space of 26K bytes.

EXPERIMENTAL RESULTS

First Run

Figures 6 through 9 show the results of the first experiment when the reactor was initially operated at the coolant temperature of 445°C and the contact time of 4 seconds. At this condition the bed temperature T^* was 453.6°C. This experiment was performed for a total duration of 1,000 sampling steps of which 300 were used for the initiation stage and 700 steps for the advance stage. In the advance stage, optimization was done once every 100 sampling steps. The amplitudes for the PRBS were set to 5°C for $r(k)$ and 12% of d-c value for $v(k)$ and not readjusted throughout the optimization. Being one of the preliminary runs, the automatic adjustment of PRBS amplitudes was not considered in this run.

The improvement of the profit is given in Figure 6. Relatively good agreement between the predicted and the measured values of the profit can be seen, indicating that good parameter estimates were obtained with the recursive instrumental variable method.

The result of the adaptive control as well as the d-c value for $r(k)$ supplied by the steady state optimizer are shown in Figure 7. As can be seen, the bed temperature followed its reference output very closely. The d-c value for the bed temperature shows an overall tendency to decrease, which is caused by the penalty term on high bed temperature in the profit function.

Variation of the contact time during the optimizing control is presented in Figure 8. The straight line during each optimization step denotes the d-c value supplied by the steady state optimizer while the uneven line is the PRBS superimposed on the d-c value. It can be observed that the contact time decreased continuously with time. This is also the anticipated result because the contact time was initially set to a large value which is far from the optimum region.

In Figure 9, variations of steady state gains of the imaginary system are given. All the parameters are seen to vary significantly during the first 500 sampling steps, meanwhile the advance stage proceeded at three times, at the 300th, 400th, and 500th sampling steps. In other experimental work on identification of the imaginary system (Lee, 1983), it was found that most of the parameter estimates began to converge in about 150 to 200 sampling steps. In light of this fact, the drastic change of the estimates between the 300th and 500th sampling steps is thought to be caused by a serious nonlinear behavior of the imaginary system around the corresponding reaction condition (contact time of 3–4 s and coolant temperature of 440–450°C). Moreover, it is seen that smooth transitions in the parameter estimates were not made during the advance stage to a new optimum operating region, indicating that the second-order Hammerstein model may be insufficient to represent the imaginary system over a wide region of reaction conditions. After the 500th sampling step, all the estimates converged to nearly constant values. In particular, the estimates of the nonlinear terms in Eq. 4, G_{v2}, G_{r2} and G_{vr}, converged nearly to zero. This means that the imaginary system was driven to a linear region as the optimization proceeded, that is, as contact time and bed temperature decreased. The computer simulation result shown in Figure 5 supports these results even though the comparison is rather qualitative.

As can be seen in Figure 5, a serious nonlinearity is observed at long contact time. But as the contact time decreases, that is, as the reaction condition moves over the ridge R and then approaches the region P, the relation between MA yield and reaction conditions

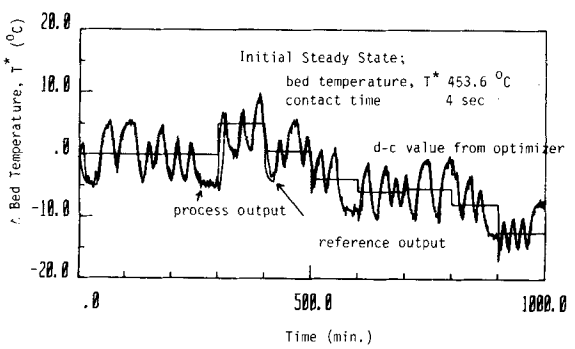


Figure 7. Adaptive control of bed temperature during first run.

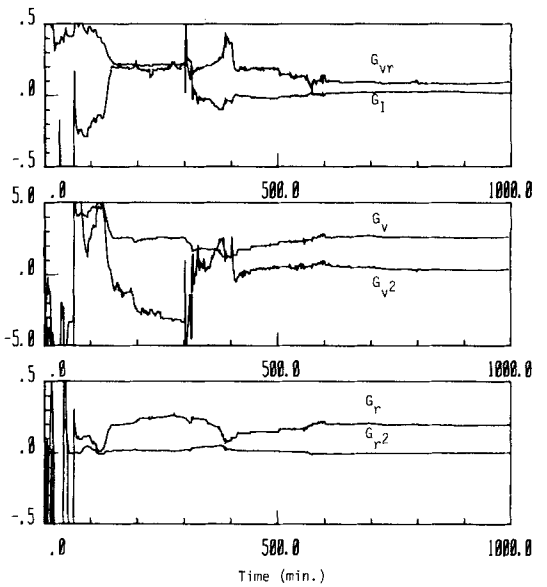


Figure 9. Results of parameter identification during first run.

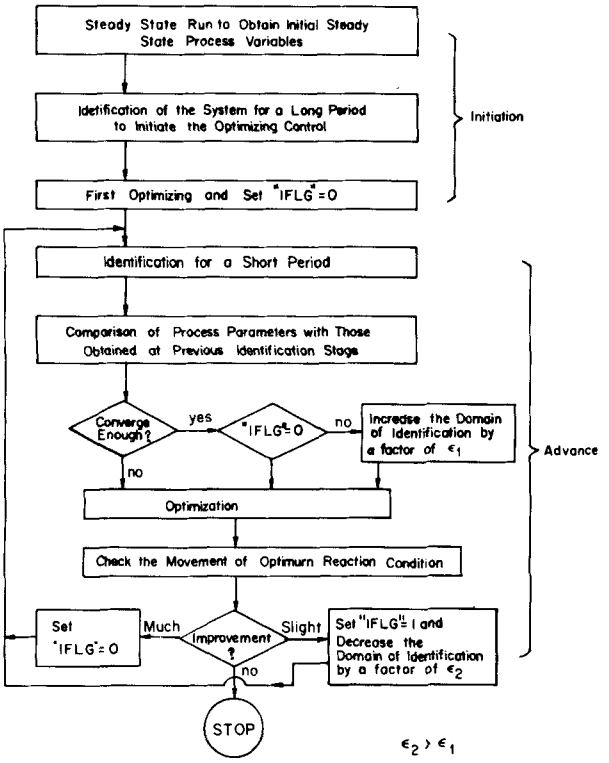


Figure 10. Implementation algorithm for second run.

become linear. It should be noted that the steady state behavior of the imaginary system differs from Figure 5 because the coolant temperature is taken as an independent variable in this figure. However, since the bed temperature changes monotonically with the coolant temperature, this plot can also be regarded as a steady state behavior of the imaginary system by simply expanding a scale of the coolant temperature. More on reactor behaviors from the reactor model can be found in Lee (1983).

Second Run

In the second run, the optimizing control experiment was carried out starting from an initial condition of 445°C and 3.5 s for the coolant temperature and the contact time, respectively, and continued until no further improvement in the profit was obtained. After 400 steps of the initiation, optimization was performed once every 100 sampling steps. In this run, amplitudes of the PRBS's were automatically adjusted depending upon convergence of the parameters and optimum condition as shown in Figure 10.

Figure 11 shows the profit improvement during the run. In this case also, a relatively good agreement between the predicted and the measured values of the profit function is observed. The discrepancy between the predicted and the true profit in the period

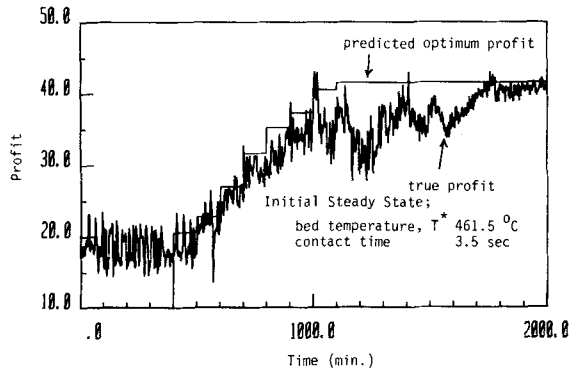


Figure 11. Improvement of profit function during second run.

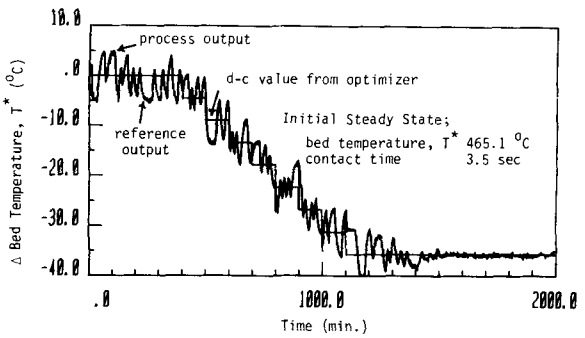


Figure 12. Adaptive control of bed temperature during second run.

of 1,100 to 1,700 sampling steps appears to be caused by a temporary drift of the oxygen analyzer but it is not clear. Nevertheless, such a discrepancy was not observed in other experiments.

Results of the adaptive control for bed temperature around each optimum *d-c* value are given in Figure 12. Good tracking performance is also obtained. As expected from its initial state, the bed temperature continuously decreased to its final value. Amplitude of the PRBS for the bed temperature was automatically readjusted to decrease as the reaction condition approached to the final optimum point.

Variation of the contact time disturbed by PRBS is shown in Figure 13 along with the *d-c* value from the optimizer. The amplitude also decreased as the optimization proceeded.

The resulting optimization path from the initial condition to the final optimum is depicted in Figure 14. Although the true optimum point was not known to us *a priori*, the final optimum point attained is thought to be in the optimum region anticipated.

DISCUSSION

Through experimental evaluation, the proposed optimizing control proved to work well in that the profit function increased continuously and also the final reaction condition attained was in the expected optimum region. Some points, however, should be discussed to clarify the aspects not tested through the experiments and also for further improvements of the proposed optimizing control.

Selection of the Bed Temperature Measurement Point

In the adaptive control loop, a bed temperature located at a fixed position was chosen as the controlled variable. Since this position is in the region where a hot spot occurred under normal operating conditions, control of the temperature at this position may also prevent other bed temperatures from being excessive. In some extreme cases, however, the hot spot may diverge while the measured temperature remains regulated. To avoid such a catastrophic case, it would be preferable to measure the true hot spot temperature if possible. The hot spot moves according to a change in re-

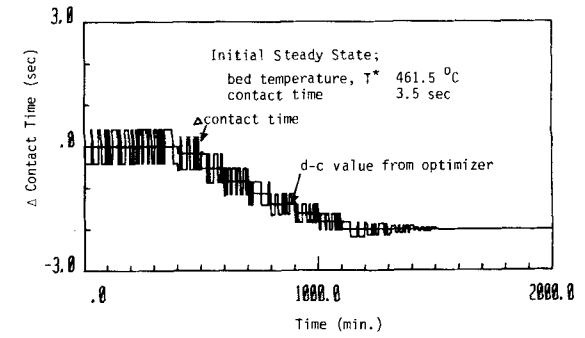


Figure 13. Variation of contact time during second run.

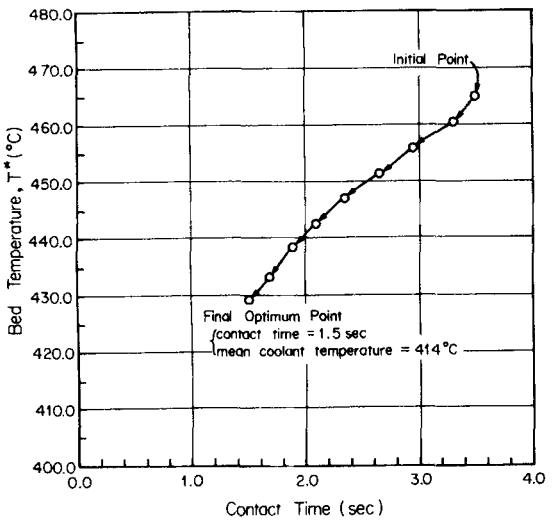


Figure 14. Optimization path during second run.

action condition, especially to a change in contact time. One of the methods to locate the hot spot is to obtain an interpolating curve of the bed temperature profile from measurements at various points with larger weight around the hot spot region, followed by its differentiation. This additional elaboration would refine the proposed optimizing control at the expense of a greater computational load and memory requirement.

Parameter Sensitivity

Since the identified model was used and the parameters of the objective function were chosen arbitrarily in the optimizing control scheme, the parameter sensitivity of the performance of the optimizing controller should be discussed, that is, how accurate the on-line identifier must be to obtain acceptable control and also what happens when the parameters α and β in the objective function are modified.

On the first question, the most important prerequisite is how accurately a dynamic model like Eq. 2 can describe the reactor behavior over a wide region of reaction conditions with a single set of parameter values. If the model is not accurate, the parameters will have a unique set of values for each region where the imaginary system is identified. In this case, parameters obtained over a region may be of no help to parameter estimation over the next region. In addition, identification should be accurate for each region. Results of some preliminary experiments related to this problem will be discussed in the following section.

On the second question, computer simulations were made concentrating on how the profit contour in Figure 4 varies as the parameters α and β in Eq. 25 are modified. With a pseudohomogeneous two-dimensional reactor model, the contours always have only one local maximum. Banana-shaped contours are yielded for high α/β ratio. But this type of poor conditioning is of no concern since the control objective is more to attain a high profit than to find an optimum point.

Reduction of Total Optimization Time

This problem is considered to be the most important one in improving the proposed optimizing control.

In the work by Bamberger and Isermann (1978), identification and optimization were performed concurrently at every sampling step after a certain initiation was done. As was discussed in the results of the first run, however, even the second-order Hammerstein model may be insufficient to describe the reactor behavior over a wide region of reaction conditions. This implies that more identification steps than one before each optimization are needed in practical application to avoid undesirable transients or potential divergence in some extreme cases. It is not necessary, however, to have accurate parameter estimates for each optimization; thus, fewer than 100 identification steps would be possible. In a preliminary experiment with 100 and 30 sampling steps for initiation and identification for each optimization, the optimizing controller tended to work but drove the reactor to high bed temperature at the initial transient depending upon the initial assumption of the parameter vector $\hat{\psi}(k)$. In this situation, the catalyst as well as the reactor tube may be damaged. Nevertheless, the above result shows a possibility that many fewer identification steps than 100 can be adopted in the present optimizing control if an appropriate algorithm capable of preventing the reactor from moving into a hazardous region is incorporated.

Reduction in identification time can also be achieved by optimizing the random input signals (Goodwin and Payne, 1977). Although the applicability of this method to a nonlinear dynamic system is limited, this method is thought to be full of promise in reducing the identification time. One more possibility for reducing the total optimization time is to automatically adjust the number of identification steps for each optimization according to the current reaction condition as well as the parameter convergence. As can be seen from Figure 9, there is no need to reidentify the parameters after about 700 sampling steps. This method can be implemented with the help of a priori knowledge of reactor behaviors and/or a well-organized decision algorithm on parameter convergence.

Discrepancy Between the Estimated Final and the True Optimum Conditions

In the proposed optimizing control, the optimum condition was determined only with the identified process model. So a difference between the estimated final and the true optimum points always results from the model error. One way to overcome this problem is to adopt a direct search method, which does not require any process model, after the proposed optimizing control has been completed.

There are many causes for the optimum point to be shifted. Catalyst deactivation, changes in feed, and product costs are some of them. Once a cause which shifts the optimum point occurs, the optimizing control should restart again. In this case, it is sufficient to start from the advance stage with values of the parameters obtained at the previous run. Although the feed and/or the product cost may change significantly depending on market conditions, the reactor itself changes only slightly with time. Thus, reidentification and optimization can be done in only a short time.

NOTATION

$A(\cdot),B(\cdot),C(\cdot)$ = polynomials in q^{-1} in the linear dynamic model of reactor system
a_i,b_i,c_i = coefficients of polynomials $A(\cdot)$, $B(\cdot)$, and $C(\cdot)$
D_c = bias term in the linear dynamic model of reactor system
D_c' = defined by Eq. 17
D_I = bias term in the nonlinear dynamic model of imaginary system
$D(\cdot),E(\cdot),\ldots$ = polynomials in q^{-1} in the nonlinear dynamic model of imaginary system
d^i,e_v^i,e_{v2}^i = coefficients of polynomials $D(\cdot)$, $E_v(\cdot)$, and $E_{v2}(\cdot)$
d_r,d_v = time delays of input signals $r(k)$ and $v(k)$ for imaginary system
d_u,d_v' = time delays of input signals $u(k)$ and $v(k)$ for reactor system
$F(k)$ = gain matrix in the recursive instrumental variable method
$G_F(\cdot)$ = transfer function of the low pass filter

$G_I, G_r, \ldots$ = steady state gains in the nonlinear dynamic model of imaginary system
$H(\cdot), P(\cdot), R(\cdot), S(\cdot)$ = polynomials in q^{-1} arising in derivation of adaptive control law
h_i, p_i = coefficients of polynomials $H(\cdot)$ and $P(\cdot)$
J = objective function of steady state optimizer
J_{MA} = net profit term per unit time by producing MA from n-butane
J_T = penalty term on high bed temperature
k = index of discrete time
MA = maleic anhydride
MA_I = MA yield (%) at initial steady state
$n_A, n_B, \ldots$ = orders of polynomials $A(\cdot)$, $B(\cdot)$, etc.
q^{-1} = backward shift operator defined by $q^{-1}x(k) = x(k-1)$
r = reference output of bed temperature T^*, deviation variable from initial steady state
T^* = bed temperature measured at $z = 0.136$
T_{HB} = base temperature in J_T
T_{HI} = T^* at initial steady state
u = coolant temperature, deviation variable from initial steady state
$\bar{u}$ = mean value of $u(k)$ during each optimization step
v = contact time, deviation variable from initial steady state
x = bed temperature T^*, deviation variable from initial steady state
y = MA yield, deviation variable from initial steady state
z = normalized axial distance of catalyst bed

Greek Letters

α, β = constants which describe J
$\alpha(k)$ = parameter vector defined by Eq. 20
$\Gamma(k)$ = gain matrix in adaptive control algorithm
$\lambda(k)$ = weighting factor in recursive estimation algorithms
$\phi(k)$ = signal vector defined by Eq. 19
$\theta(k)$ = signal vector defined by Eq. 6
$\psi(k)$ = parameter vector defined by Eq. 8
τ_I = contact time at initial steady state

Symbols

∞ = steady state
$\hat{}$ = estimated value

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