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Control of Constrained Multivariable Nonlinear Process Using a Two-Phase Approach

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A computer-based algorithm is presented for the control of complex process units which are characterized by difficult features such as nonlinear input/output relationships, multivariable nature, operational constraints, imprecise models, and inadequate measurements. A two-phase algorithm is proposed to deal with these difficult features in a direct manner. The algorithm makes use of approximate process models which take into account significant physical and chemical events in the process. The first phase of this algorithm consists of identifying unmeasured disturbances and the parameters and states of the approximate model using measurements from the immediate past. This identified model is then used in the second phase to predict the future behavior of the process and to select an appropriate control action. Application of the algorithm to a highly nonlinear, difficult-to-control CSTR system shows the advantages of this approach over other approaches which are based on linear models. Robustness in the presence of plant/model mismatch and immunity to measurement noises are also illustrated.

Most regulatory control problems in the process industry are handled well by the traditional PID-type feedback controllers which are relatively inexpensive and well understood. However, there are a number of complex process operations which still present challenging problems in control for a variety of reasons. The reasons most often cited in the literature (Foss, 1973) include the following.

(i) Process Nonlinearity. This limits the applicability range of controllers based on linear models.

(ii) Multivariable Nature. A unit may have more than one control variable and more than one output variable to be controlled.

(iii) Inadequate Measurements. The variables to be controlled may not be directly measurable on line. In such a case, the process must be controlled by using secondary measurements.

(iv) Process Constraints. The control system must maintain process variables within certain bounds using bounded inputs. Moreover, it must be able to deal with these constraints even when the constraints change with time.

Modern control theory, developed in the 1960s, has not found much acceptance by the process industry, primarily because the theory did not address many of the above issues which were critical to the process industry. However, the availability of on-line process computers spurred the development of many new algorithms for computer control. Examples are Dynamic Matrix Control developed at Shell (Culter and Ramaker, 1979), Model Algorithmic Control developed in France (Richalet et al., 1978), and Inferential Control (Brosilow, 1979). Garcia and Morari (1982) discussed these and similar algorithms from a theoretical point of view and coined a new name, Internal Model Control, to represent this class of algorithms.

The success of these algorithms can be attributed to the following important features: (i) relative ease in generating the process model, (ii) the ability to utilize process measurements to compensate for unmeasured disturbances and modeling errors, and (iii) the use of a filter in the feedback

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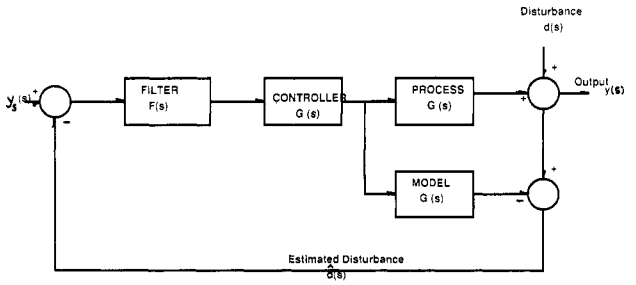

Figure 1. Block diagram for linear inferential (internal model) control.

path to increase the robustness of the controller.

The feedforward nature of these algorithms guarantees stability if the model is perfect. If not, the system may become unstable. But by introducing a filter in the feedback path, stability has been retained even with modeling errors. Indeed, the filter gives a means for a direct tradeoff between controller stability and performance.

The basics of Linear Inferential Control are discussed in the next section. The concept is generalized for the nonlinear case. The paper concludes with an application study in which the regulation of a highly nonlinear CSTR process is considered.

Linear Inferential Control

Figure 1 depicts the block diagram of a linear inferential control system. The key elements of this control system are the process model $\hat{\mathbf{G}}_p(s)$, the controller $\mathbf{G}_c(s)$ which approximates the inverse of the process, and the filter $\mathbf{F}(s)$ which slows down the feedback of information. The transfer function relationship is

$$y = \frac{(1 - \mathbf{G}_p\mathbf{G}_c\mathbf{F})d + \mathbf{G}_p\mathbf{G}_c\mathbf{F}y_s}{1 + \mathbf{G}_c\mathbf{F}(\mathbf{G}_p - \hat{\mathbf{G}}_p)} \tag{1}$$

As can be seen if $\mathbf{G}_p = \hat{\mathbf{G}}_p$ (perfect model), the denominator becomes 1 and the poles of the system are the same as the poles of the process, the controller, and the filter. Hence, if the model is perfect, the system is stable provided that the controller and filter have stable poles and the original process is stable. Also to obtain good set-point tracking, one should attempt to make $\mathbf{G}_p\mathbf{G}_c\mathbf{F}$ as close to unity as possible. In other words, choose

$$\mathbf{G}_c\mathbf{F} \approx \mathbf{G}_p^{-1} \tag{2}$$

the limitation being the invertibility of the process. Time delays and RHP zeros in $\mathbf{G}_p(s)$ will make the exact inverse unrealizable. Approximations to the inverse must be sought in such a case. Recently, some improvements of the IMC structure regarding this problem have been achieved by introducing a second feedback loop (Stephanopoulos and Huang, 1985) or by modifying the controller structure such that the poles (in the z-domain) of the system can be brought as close to the origin as possible.

In practice, most computer implementations either (i) use convolution models for representing the process or (ii) use a least-squares theory or quadratic programming to invert the process model. A typical computer implementation goes as follows.

(i) Prediction Step. Use the knowledge of past control actions to predict current and future outputs of the process.

(ii) Correction Step. Use current measurements to revise the model predictions. Usually a simple scheme such as a shift in the output is used.

(iii) Inversion Step. Solve for the control actions to be taken in the future to keep the output close to the set point. Constraints on manipulated variables and output variables are incorporated at this stage. The inversion might take the form of a least-squares problem as in DMC (Cutler and Ramaker, 1979) or of a quadratic programming problem as in MAC (Richalet et al., 1978).

Extension to Nonlinear Processes

There have been a number of attempts to extend the above internal model control algorithms and apply them to nonlinear processes. Garcia (1984) proposed an approach which uses local linearized approximations of the process. As the process operating conditions change, the linearized model is revised. Astrom and Wittenmark (1973) proposed an adaptive controller called a self-tuning regulator which uses an on-line identification scheme to update the linear model of the process. Application of adaptive control techniques to chemical processes can be found in Harris et al. (1980), Kiparissides and Shah (1983), and Zanker (1980). Here the linear parametric model of the processes is updated using a least-squares estimator.

For this algorithm a linear model of the form

$$y(k+b) = \alpha(z^{-1})y(k) + \beta(z^{-1})m(k) \tag{3}$$

is used where

$$\alpha(z^{-1}) = \alpha_0 + \alpha_1 z^{-1} + \ldots + \alpha_{n-1}z^{n-1}$$

$$\beta(z^{-1}) = \beta_0 + \beta_1 z^{-1} + \ldots + \beta_{r-1}z^{r-1}$$

and b is the dead time. On the basis of the concept of minimum variance control, the control action is given by

$$m(k) = -\frac{1}{\beta_0}[x^T(k)\theta(k)] \tag{4}$$

where

$$\theta^T(k) = [\alpha_0, \alpha_1, \ldots, \alpha_{n-1}, \beta_0, \ldots, \beta_{r+b-1}]$$

$$x^T(k) = [y(k), y(k-1), \ldots, y(k+n-1), m(k), \ldots, m(k-r-b+1)]$$

$\theta^T(k)$ is updated recursively by using a least-squares estimator.

This adaptive approach has mainly been applied to single-input/single-output systems. A major instrumentation manufacturer is now offering such a controller commercially.

An alternative approach is to use the nonlinear process models directly in the control of the process. In the past, this approach was not used mainly because of heavy computational load in such an approach. However, the computational load can be kept light by using low-order models which retain the important features and which contain enough adjustable variables (parameters) which can be estimated on-line by using current measurements. This results in a two-phase approach, which is outlined next.

The approach is based on an approximate process model of the form

$$\dot{x} = f(x,m,p,t) \tag{5}$$

where x = state variables, m = manipulated inputs, and p = unmeasured disturbances and unknown parameters.

The operational constraints are of the form

$$h(x,m,p,t) \leq 0 \tag{6}$$

In addition, a set of measurements (z) given by

$$z = g(x,m,p,t) \tag{7}$$

are also assumed to be available. These measurements

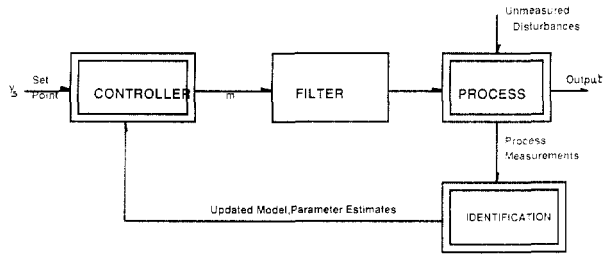

Figure 2. Structure of a regulator controller using a two-phase approach.

may be corrupted by noise. The objective of the control system is to keep a set of outputs

$$y = w(x,m,p,t) \tag{8}$$

close to their set points, y_s, while maintaining various variables within their constraints.

The two-phase algorithm can now be outlined as follows:

Phase I: Identification Phase. Determine the unmeasured states (x) and unknown variables (p) from the measurements ($\bar{z}$).

Phase II: Control Phase. By use of the process model identified above, determine the control actions, $m(t)$ to be taken to keep the predicted output, $y(t)$, close to the desired value.

Figure 2 shows the schematic of the proposed algorithm for nonlinear systems. Although represented as a block diagram, it must be remembered that normal block diagram manipulation rules will not hold in this case. The identification block serves to collect available measurements from the process and to update the current information on the variables x and p. The controller block computes the controller actions to be taken so that the output variable is brought close to the set point in the near future. The filter block slows down the control action and is used to increase the robustness of the algorithm. Each block is discussed in detail next.

Identification Block

Since the identification must be carried out on line by using discrete measurements of z, it is advantageous to formulate the problem in discrete time. The variables, p, are time varying in nature, so we focus our attention over a small time horizon in the past over which these variables can be assumed to be constant. This reduces the problem to estimating p and the value of $x(t)$ at the beginning of the time horizon.

Further, for convenience in stating the identification problem, we will assume that the measurements are taken at equidistant intervals in time although this is not necessary in the implimentation.

Let $\bar{t}$ denote the present time. Let us say that the differences between the model predictions and the current observations are large enough to indicate a change in the model parameters or the presence of some new disturbances. Measurements from the past are used to update the model and the estimates of the disturbances. We shall use the least-squares criterion to determine the goodness of fit (i.e., how good the estimates of the model parameters and disturbances are). The identification problem can be stated as follows: Given a set of observations, $\bar{z}(\bar{t})$, $\bar{z}(\bar{t}-\Delta T_i)$, ..., $z(\bar{t}-N_i\Delta T_i)$, determine x_0 and p such that

$$\sum_{j=0}^{N_i} \|\bar{z}_j - z_j\|^2 \tag{9}$$

is minimized subject to the constraints $\dot{x} = f(x,m,p,t)$, $x(t-N_i\Delta T_i) = x_0$, $z_j = g(x,m,p,t_j)$, $t_j = t - j\Delta T_i$.

This is an equality-constrained optimization problem which can be solved by a nonlinear programming method. Many efficient computer codes using generalized reduced gradients or successive quadratic programming techniques are available to solve this.

The presence of constraints in the form of ordinary differential equations will generally require a slight modification of the way in which the gradient of the objective function is evaluated. For a discussion on this and alternative approaches to identification, see Jang et al. (1986, 1987).

This approach can readily accommodate measurements that are not equidistant and measurements that may be delayed in time (due to sampling and analysis).

Since these optimization problems must be solved on line, it is advantageous to use reduced-order models which approximate the process. Poor model structures will make it difficult to match the model to the observations, and this in turn will lead to poor control. In many situations, a variety of models, of differing complexities, are available. The choice of the model involves a tradeoff between computational efficiency (i.e., cost of control) and controller performance. Past data from a plant can be used to determine the adequacy of the model used for on-line control.

Not much discussion exists in the literature regarding the use of nonlinear models for on-line estimation and control. One approach that has been suggested is the use of the extended Kalman filter for estimating states and parameters of nonlinear processes. We have made comparison between the identification approach proposed here and the extended Kalman filter, and the results are reported in Jang et al. (1987). Our findings indicate the identification method used in the two-phase approach to be superior to the extended Kalman filter.

An important issue is the frequency with which this identification must be executed. One indicator which signals the need for the execution of the identification is the difference between the model predictions and the process measurements. We used a 5% change in the variable p to trigger the identification phase. Observe that unnecessary, frequent execution of the identification phase need not lead to better performance of the control system because, when the system is relatively calm for a while, the above optimization problem tends to be ill-conditioned, thus making the yielded estimates of x_0 and p unreliable. Hence, when the system is relatively calm, identification should not be attempted. Also if ill-conditioning is detected, the identification phase should be aborted.

The Control Block

The function of the control block is to compute the manipulated input which will bring the controlled outputs closer to their set points. The approach taken here is the same as in the linear inferential control case, except the model inversion is done numerically. The control problem can be stated as

$$\min_{m(t)} \Phi = \int_{\bar{t}}^{\bar{t}+T_f} \phi \, dt \tag{10}$$

where $\phi = (y_s - y)^2$ subject to $\dot{x} = f(x,m,p,t)$, $y = w(x,m,p,t)$, and $h(x,m,p,t) \leq 0$.

Once again for implementation, a discrete formulation is necessary. Assuming that control actions are implemented every ΔT_o units of time, the control problem can be converted to

$$\min_{m_1,m_2,\ldots,m_{N_o}} \phi \tag{11}$$

subject to $\dot{x} = f(x,m,p,t)$ $x(\bar{t}) = x_0$; $y = w(x,m,p,t)$; and

$h(x,m,p,t) \leq 0$ where the initial conditions, x_0, can be obtained from the results of the identification phase. The manipulated variable, $m(t)$, is assumed to remain constant on the interval ΔT_o, i.e.,

$$m = m_j \qquad t + (j-1)\Delta T_o < t \leq t + j\Delta T_o \tag{12}$$

The number, N_o, of subintervals will determine the number of optimization variables. If a gradient-based package, such as the GRG algorithm or Powell's SQP method, is used to solve the optimization problem of expression 10, then the gradient of the objective function needs to be evaluated. In order to do so, one needs to solve a set of adjoint equations as described by the following steps. Details of its derivation are given in our previous paper (Jang et al., 1986).

Step 1. Integrate the state equations $\dot{x} = f(x,m,p,t)$ over the optimization horizon $(\bar{t},\bar{t} + N_o\Delta T_o)$.

Step 2. Solve the following adjoint differential equations backwards

$$-\frac{dq}{dt} = \left(\frac{\partial f}{\partial x}\right)^T q + \left(\frac{\partial \phi}{\partial x}\right)^T \qquad q(t+N_o\Delta T_o) = 0 \tag{13}$$

Step 3. Determine the gradient

$$\frac{\partial \phi}{\partial m_i} = \left(\frac{\partial f}{\partial m}\right)_i^T q_i + \left(\frac{\partial \phi}{\partial m}\right)_i^T \tag{14}$$

where the subscript i denotes the value determined at time $\bar{t} + i\Delta T_o$.

The evaluation of the gradient thus requires the solution of ordinary differential equations in both identification and optimization phases. Any standard method may be used to solve the ODEs. Possibilities include finite difference methods such Runge–Kutta and more complex collocation methods. An implementation using the method of collocation has been suggested by Biegler (1984). The application of this collocation algorithm is discussed in the Appendix. One disadvantage of the collocation approach is that $m(t)$ is not expressed in a discrete form suitable for computer implementation.

The Filter Block

The introduction of a filter block in order to stabilize the feedback loop was first suggested in our situation by Brosilow (1979) and later described in Garcia and Morari (1982). The simplest form for the filter is a first-order lag, which delays the feedback of information through the loop. By making the filter time constant large enough, it is often possible to delay the feedback of information sufficiently to guarantee stability. The penalty paid is usually poor control. Thus, the filter time constant provides the process operator with a tunable parameter which can be adjusted to accommodate the modeling errors.

In the two-phase approach, the filter block also serves the same purpose. The presence of modeling errors will lead to incorrect control actions. In such a case, the filter constant should be adjusted to guarantee stability even under the worst possible case. A simple form for the filter is

$$\mathbf{F}(z) = \frac{1-\alpha}{1-\alpha z^{-1}} \qquad 0 < \alpha < 1 \tag{15}$$

Lack of sufficient theory of nonlinear control precludes any quantitative analysis of the stability problem. For the linear system, Garcia and Morari (1982) provided some examples that illustrate the stabilizing nature of the filter.

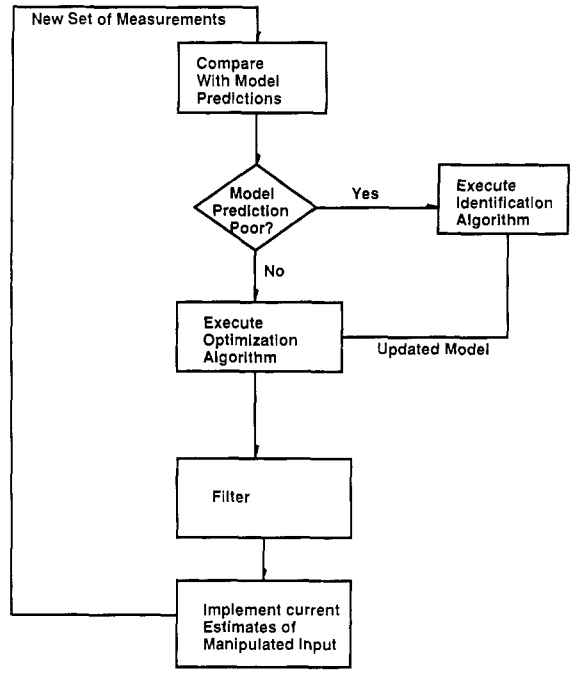

Figure 3. Schematic of proposed algorithm.

Effect of Constraints

Constraints on the manipulated variables, $m(t)$, may be directly incorporated into the above optimization problem. Constraints on process variables of the form $h(x,m,p,t) \leq 0$ are not handled as easily. A recommended approach here is to require

$$h_i = h(x_i,m_i,p,t_i) \leq 0 \tag{16}$$

that is, to require that the constraints be satisfied at the discrete time instants. Such converted constraints are readily incorporated into the optimization algorithm.

The Algorithm

Figure 3 shows the schematic of the proposed nonlinear control algorithm. The identification phase is executed whenever the difference between the model outputs and the process measurements exceeds a predetermined threshold value. This may be caused by model error, a new process disturbance, and/or a change in the process parameters. The identification phase yields a new set of parameters which are used to compute the manipulated variables. The resulting control action is implemented. After an interval of length ΔT_o, the calculations are repeated.

Please note that the above development is applicable to both simple and multivariable processes. Multiple and intermittent measurements can be readily handled. Interaction among variables is taken into account in a natural manner, eliminating the need for decouplers, etc.

Example

The following example was originally discussed by Economou and Morari (1986). The process is a CSTR as shown in Figure 4. A reversible reaction is going on in the reactor:

$$A \underset{k_-}{\overset{k_+}{\rightleftharpoons}} R$$

where the rate constants are in Arrhenius form:

$$k_\pm = C_\pm e^{-Q\pm/KT_o} \tag{17}$$

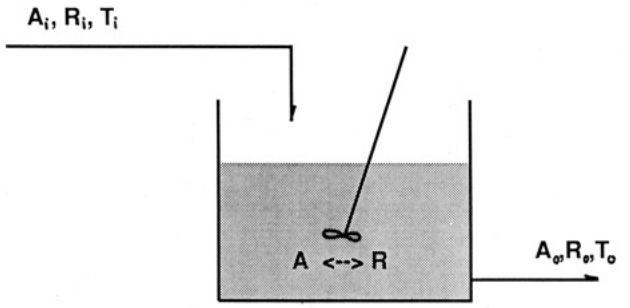

Figure 4. Continuous stirred tank reactor for the reaction A ⇄ R.

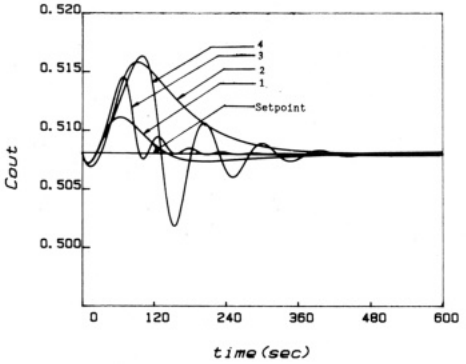

Figure 5. Comparison of different control strategies on the regulatory control of the CSTR example: (1) two-phase approach; (2) PID; (3) self-tuning control, $n = 3$, $m = 5$, $b_0 = -0.5$, $\lambda = 0.95$; (4) self-tuning control, $n = 3$, $m = 2$, $b = 4$, $b_0 = -0.8$, $\lambda = 0.97$.

Table I. Operating Conditions of the Reactor

constants	steady-state operating conditions
$\tau = 60$ s	$A_i = 1.0$ mol/L
$C_+ = 5 \times 10^3$ s^{-1}	$R_i = 0.0$ mol/L
$C_- = 1 \times 10^6$ s^{-1}	$A_o = 0.492$
$Q_+ = 10\,000$ cal mol^{-1}	$R_o = 0.508$
$Q_- = 15\,000$ cal mol^{-1}	$T_i = 427$ K
$K = 1.987$ cal mol^{-1} K^{-1}	$T_o = 430$ K
$-\Delta H_R = 5000$ cal mol^{-1}	
$R_{opt} = 0.5085$	
$T_{opt} = 434$ K	
$\rho = 1$ kg/L	
$C_p = 1000$ cal kg^{-1} K^{-1}	

The system consists of three state equations and one measurement equation

1. reactant mass balance:

$$\frac{dA_o}{dt} = \frac{1}{\tau}(A_i - A_o) - k_+A_o + k_-R_o \tag{18}$$

2. product mass balance:

$$\frac{dR_o}{dt} = \frac{1}{\tau}(R_i - R_o) + k_+A_o - k_-R_o \tag{19}$$

3. energy balance:

$$\frac{dT_o}{dt} = -\frac{\Delta H_R}{\rho C_p}(k_+A_o - k_-R_o) + \frac{1}{\tau}(T_i - T_o) \tag{20}$$

4. measurement:

$$y = R_o + \eta \tag{21}$$

where η is assumed Gaussian and zero mean.

Design data of this system are given in Table I. Note that the set point of this problem is at the maximum yield of the product for $A_i = 1$ g-mol/L. Therefore, for $A_i < 1$ g-mol/L, the set point is unreachable. In this example, the inlet concentration, A_i, is chosen as the parameter to be identified. In addition, the unknown states, A_o, and T_o are also estimated by the identification phase. The inlet stream temperature is selected as the manipulated variable of the system. The objective is to control the exit concentration of R detected as C_{out}. C_{out} was chosen as the measure variable p in conformity with the earlier work of Economou and Morari (1986).

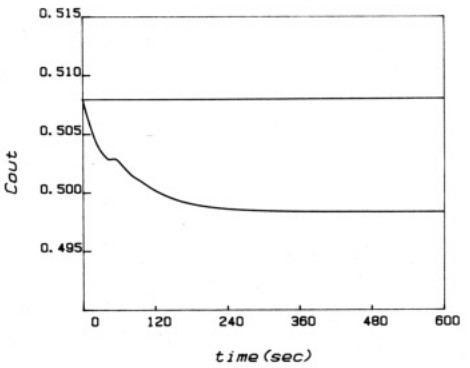

Figure 6. Output response for the case of 2% decrease in the inlet reactant concentration ($\alpha = 0$, $N_o = 5$, $\Delta T_o = 20$ s).

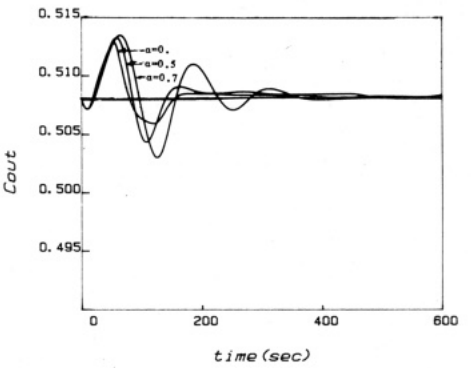

Figure 7. Effects of changing the filter constant with an integration step of 10 s ($N_i = 40$). Response to 2% increase in inert concentration.

Three types of controllers were implemented on the reactor. The first is the conventional PID controller. The second is a self-tuning regular (an adaptive controller) proposed by Astrom and Wittenmark (1973). The third is based on the two-phase approach as described above.

Results

In Figure 5, the response of the three controllers to a 2% step increase in the inlet reactant concentration is compared. The PID controller constants were tuned to yield the best performance using the reaction curve and Ziegler–Nichols tuning method. Two different adaptive controllers were implemented. The first is based on the linear model with parameters $n = 3$, $m = 5$, and $b = 0$ in eq 3. The second controller employs $n = 3$, $m = 2$, and $b = 4$. Obviously, some improvement is possible here with further tuning of the parameters. The two-phase approach was implemented with the following set of parameters: $N_i = 20$, $\Delta T_i = 1$ s, $\Delta T_o = 20$ s, $N_o = 5$, filter constant $\alpha = 0.7$, and Euler's method of integration (with a step size = ΔT_o). Both the identification and optimization problems were solved by using the Davidon–Fletcher–Powell method of optimization. It should be noted that ΔT_o need not be the same as sampling ΔT_i. ΔT_o refers to the interval where the control action remains the same; thus it can be chosen arbitrarily.

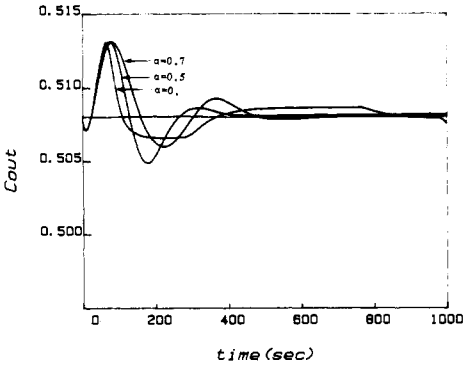

Figure 8. Effects of changing the filter constant with an integration step of 20 s (N_i = 20). Response to 2% increase in inlet concentration.

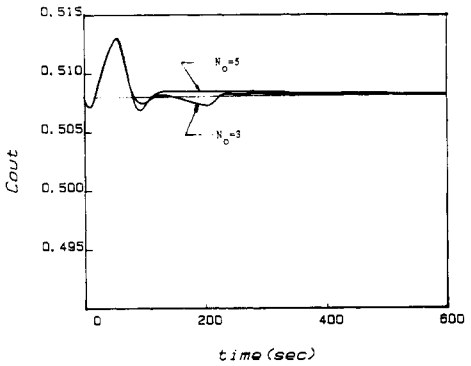

Figure 9. Effects of varying the optimization horizon (ΔT_o = 10 s, α = 0.2).

Figure 6 shows the response of the same set of controllers for a 2% decrease in the inlet concentration of A_i. The PID and STR fail to keep the process stable, mainly because the disturbance has now made it impossible to maintain the outlet concentration at its original set point. The two-phase nonlinear controller recognizes this and brings it as close as possible to the original set point, but yielding a steady-state offset. In fact, this is the maximum possible outlet concentration for the new inlet concentration.

In this case, where the set point is not attainable, integral action clearly should not be used in the PID controller. Indeed, a stable feedback controller can be obtained by using proportional action, but its reaction is very sluggish at best.

Figures 7 and 8 show the system responses for different values of the filter time constant. In the simulations represented in the figures, Euler's method is used to solve the differential equations in the control block with an integration step of ΔT_o. Note that the error in integration may be viewed as a modeling error. Clearly, the filter is not necessary for a small value of integration step ΔT_o as shown in Figure 7 (where ΔT_o = 10 s). But, as a larger value of integration step is used (e.g., ΔT_o = 20 s in Figure 8), higher values of α help slow the feedback and stabilize the control system.

Figure 9 shows the effect of changing the horizon of the controller. As expected, a longer horizon exhibits better control quality in this example.

In Figure 10, the effects are compared of different integration schemes used in the evaluation of the gradient in the optimization scheme. Euler's method for solving differential equations in the optimization phase does not work as well as the method of collocations and the fourth-order Runge–Kutta method. The method of collocation generally works better than Euler's method and

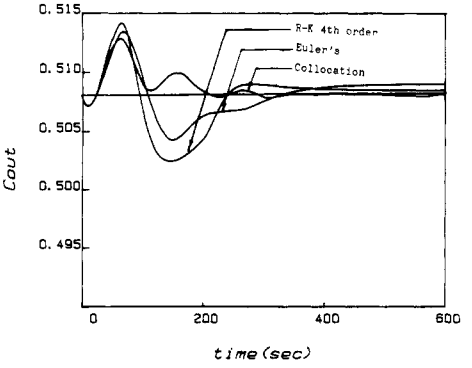

Figure 10. Effects of different integration algorithms on the performance of the two-phase regulatory controller (ΔT_o = 20 s, N_o = 5, α = 0.2, N_i = 40).

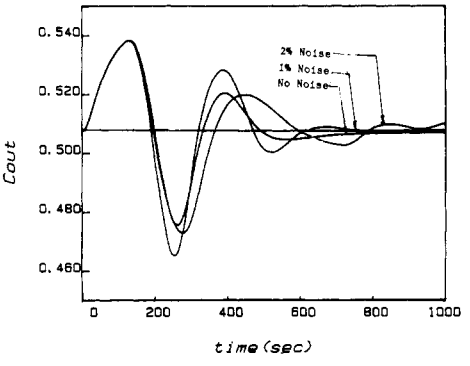

Figure 11. Effects of measurement noise with different values of the noise amplitudes (A_i = 1.07, N_i = 100, α = 0.7, ΔT_o = 20 s, N_o = 6).

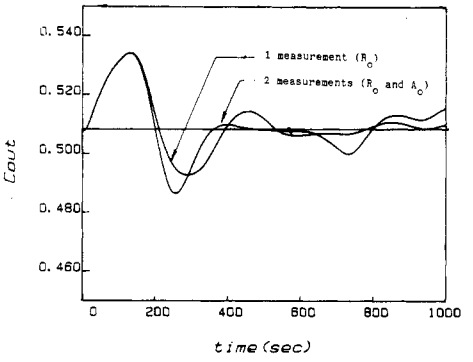

Figure 12. System under high intensity noises (±5%) for measurements A_o and R_o, N_i = 100, ΔT_i = 1 s, N_o = 5, ΔT_o = 20 s, A_i = 1.06, α = 0.7).

the Runge–Kutta fourth-order method in the control phase because of the high accuracy of this method, but it is not suitable in the identification phase because it converges more slowly than Euler's or the fourth-order Runge–Kutta method when fitting equally spaced data to the model.

Figures 11 and 12 show the output behavior when random noise is introduced in measurements. The process remains reasonably stable even in the presence of noise in measurements. Figure 11 shows the effects of the amplitude of the noise. Note that the actual process values (before corruption by noise) are plotted in the figures. It is seen that higher amplitude yields poorer identification results, and hence the overall system becomes less stable. However, this problem can be solved by increasing the number of sampling (N_i). With high intensity noise, online identification can be improved by taking measurement of one more variable. Figure 12 shows the result of control with two simultaneous measurements of A_o and R_o. The two-phase approach works very well even though the ad-

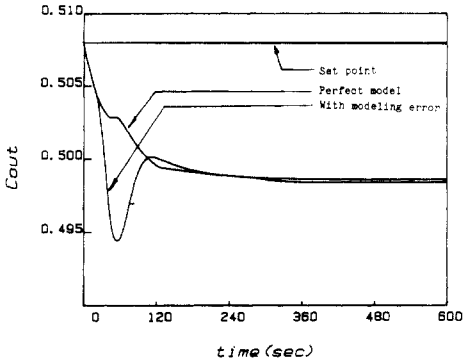

Figure 13. Effect of modeling error (controller setting same as those used in Figure 6).

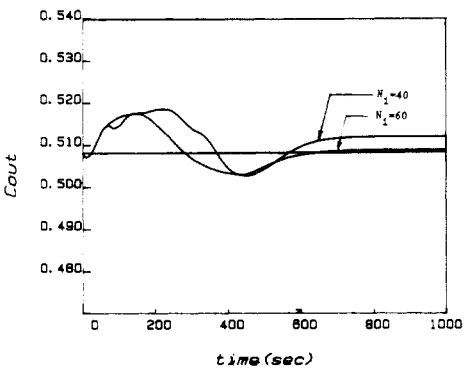

Figure 14. Control with modeling errors on activation energy (+5% error in Q_+ and Q_-). Measurements used, A_o, R_o; identified variables, T_o, A_i, Q_+, Q_-; ΔT_o = 20 s; ΔT_i = 1 s.

ditional measurement of A_0 as well as the original measurement of R_0 is influenced by the white noise of the same strength (±5% of the absolute value of real data).

In an attempt to evaluate the robustness of the proposed nonlinear controller, a 10% error is introduced in the reaction rate expressions to produce a mismatch between the plant and the model used for identification. As seen in Figure 13, the resulting output shows some oscillations due to the error introduced but recovers to attain a steady-state value very close to the optimum one.

If there exists some error in the activation energy in the model, it is possible to identify parameters in exponential terms by using the horizon search. Figure 14 demonstrates the performance of the two-phase approach with four identified variables using two measurements. A single measurement is insufficient with this much error in the model. In the case of N_i = 40, the value of the identified variable (A_i) did not converge closely to its true value in the identification phase. Therefore, it is necessary to increase the number of samplings to 60 in each horizon in order to remove the offset as shown in Figure 14.

Figure 15 shows the effect of adding constraints on process variables. This is also handled very nicely by the two-phase approach. The constrained optimization was implemented by using the GRG method. This was preferred over the SQP method which leads to infeasible intermediate solutions.

There exists an offset in the controlled variable for the constrained case. This is a natural consequence of restricting T_{out} to be less than 435, which implies that the output set point can no longer be attained.

The CPU time required to do the control calculation is about 2 s on a VAX 11/750 computer. The identification phase takes about 4 s. We made no attempt to optimize the efficiency of the calculations although there are numerous ways to reduce the computing times. With the increasing power of on-line computers, computing times will not be a major issue.

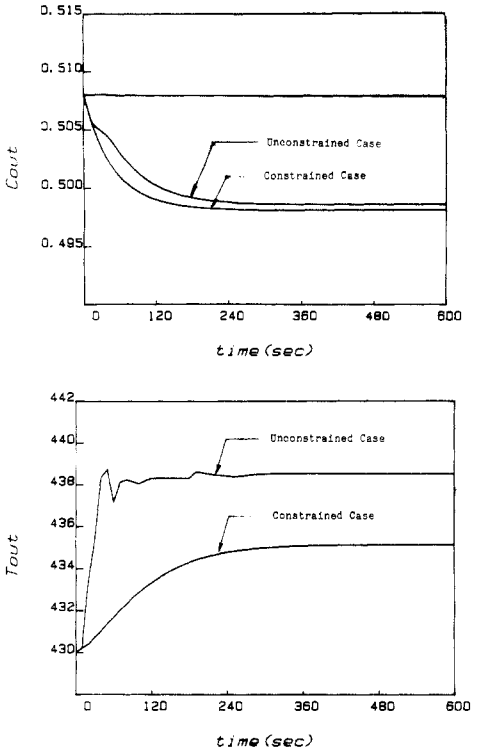

Figure 15. Effect of adding operating constraints on state variable ($T_o \leq 435$ K, A_i = 0.98, α = 0, ΔT_o = 10 s).

Conclusions and Significance

The basic concepts behind model-based computer control algorithms such as Dynamic Matrix Control are extended to deal with nonlinear processes as well. A key feature of these algorithms is the model identification step where one tries to identify the process model based on all available operational information on the process. Following this concept, a new approach is proposed which consists of identification and optimization phases. The proposed two-phase approach relies heavily on the powerful new algorithms available for optimization and increased computing power available on line. Such on-line adaptation enables the use of a low-order approximate process model and the exploitation of all available process measurements. Availability of an identified process model provides the capability of forecasting the future process behavior and the capability of selecting the best control action, which will not violate any constraints.

The algorithm was tested by using a simulated CSTR, in which a reversible first-order reaction is taking place. The nonlinearities introduced by the temperature dependence of the reaction rate term make the process quite difficult to control by conventional techniques. The two-phase approach proved to be superior to an adaptive (self-tuning) controller and a PID controller, which are based on linearized process models. The algorithm is shown to be insensitive to the choice of integration used (whether Euler's, fourth-order R–K, or collocation). Standard optimization packages were used in the algorithm. Any noise in the measurements is automatically filtered out by the identification process. The filter block used in the feedback path provides a convenient tuning parameter for operator to desensitize the system to modeling errors.

The algorithm is also tested from the viewpoint of robustness by deliberately introducing errors in such crucial

parameters as the activation energy. Although more measurements are required, the algorithm handled this situation rather well. The algorithm was also shown to be capable of maintaining good control in the presence of constraints on manipulated and output variables.

The results of the application to the CSTR problem show that this approach has considerable promise in dealing with process nonlinearities, operating constraints, and noisy and insufficient set of measurements, all of which are very important factors when controlling chemical processes. The issues are addressed in a direct manner by the two-phase approach.

We have not addressed theoretically the stability characteristics of the overall system for the nonlinear case. However, in the case of linear processes, this approach reduces to linear inferential model control, for which theoretical work exists.

Acknowledgment

Financial support provided by the National Science Foundation through Grant CPE-82-19701 in gratefully acknowledged.

Nomenclature

A = reactant
A_i = inlet concentration of the reactant
A_o = outlet concentration of the reactant
$C_\pm$ = frequency factor
C_p = heat capacity
C_{out} = output concentration of the product
F = transfer function of the filter
$\mathbf{G}_c$ = transfer function of the controller
$\mathbf{G}_p$ = transfer function of the process
h = constraint function
K = gas constant
l_i = Lagrange interpolation coefficient
m = manipulated variables
n = order of the linear model
N_i = number of observations for identification in the immediate past
N_o = number of intervals for optimization
p = parameters
q = adjoint variables
$Q_\pm$ = activation energy
r = order of the linear model
R = product
R_i = inlet concentration of the product
R_o = outlet concentration of the product
t = time
w = output function
x = state variables
x_0 = initial states
y = measurable outputs
y_s = set point
z = measured variables
$\bar{z}$ = actual measurements

Greek Symbols

α = parameters of a linear input/output model
β = parameters of a linear input/output model
ρ = density
τ = time constant
θ = parameter vector
η = white noise
ΔT_i = measurement sampling interval
ΔT_o = time interval in which control stays constant
Φ = objective function
ϕ = $(y_s - y)^2$
τ = dead time

Superscript

T = transpose of a matrix

Appendix: Application of the Method of Collocation to the Optimization Problems with Ordinary Differential Equations as Its Constraints

Consider the following optimization problem:

$$\min_{m(t)} \Phi[y(t_f),m(t_f),t_f] \tag{A-1}$$

s.t.
$$dy/dt = f(y,m,t) \tag{A-2}$$
$$h(y,m,t) = 0 \tag{A-3}$$
$$g(y,m,t) \le 0 \tag{A-4}$$

using polynomial approximations

$$y_n(t) = \sum_{i=0}^{n} y_i l_i(t)$$

where

$$l_i(i) = \prod_{j=0,j\neq i}^{n} (t - t_j)/(t_i - t_j) \tag{A-5}$$

Here $t_0 = 0$ and t_i, $i = 1, n$ are zeros of an nth-order Legendre polynomial defined from 0 to t_f. The control profile may also be approximated by

$$m_n = \sum_{i=1}^{n} m_i \bar{l}_i(t) \tag{A-6}$$

Then eq 10 can be replaced by

$$\min_{\{y_i,m_i\}} \Phi[y_n(t_f),m_n(t_f),t_f] \tag{A-7}$$

s.t.

$$r_i = dy_n(t_i)/dt - f(y_i,m_i,t_i) = 0 \qquad i = 1,...,n \tag{A-8}$$
$$h(t_p,y_n(t_p,m_n(t_p))) = 0 \tag{A-9}$$
$$g(t_p,y_n(t_p,m_n(t_p))) \le 0 \tag{A-10}$$

where t_p represents the point constraints that are considered in the optimization problem. Hence eq A-7 is in the general form of the nonlinear programming problem without differential equations and can be solved by a general purpose nonlinear programming package.

After determining the optimal $m(t)$, the value of $m(t)$ is implemented at the current time. One disadvantage with this approach is that $m(t)$ is computed assuming it to be continuous in time, whereas it is implemented as a discrete function in time.

The procedure of implementing the above algorithm in the two-phase approach is as follows.

Step 1. Solve eq A-7 by using appropriate nonlinear programming packages (e.g., D–F–P method for unconstrained case, GRG or Powell's method of constrained case).

Step 2. Use Lagrange interpolating polynomial to find the value of $m(t)$ at time $0.5\Delta T_o$.

Step 3. Control the process using the new value of manipulated variables calculated in step 2 during the time period $(0,\Delta T_o)$.

Step 4. Move the zero of the horizon to ΔT_o; go back to step 1.

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Hydraulic Characteristics of Sieve and Valve Trays

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The hydraulic characteristics of sieve and Koch type-T valve trays have been measured in a 0.63-m-diameter absorption column, with air–water system. The parameters measured include dry-tray pressure drop, hydrostatic head of liquid measured at the tray center, and total pressure drop. The operating conditions and equipment employed are representative of those encountered in industrial practice. The measured data compared favorably with few reliable data existing in open literature.

The sieve tray and the valve tray are widely used distillation column internals. Sufficient and reliable data on their hydraulic characteristics are still required for better accurate design purposes.

Eduljee (1958) expressed the dry-plate pressure drop for sieve plate as

$$\Delta P_d = 0.187 \frac{v_h^2}{c^2} \frac{\rho_g}{\rho_l} \tag{1}$$

where v_h = hole velocity, ft/s; ΔP_d = dry-tray pressure drop, in. of liquid; ρ_g, ρ_l = densities of gas and liquid, respectively, lb/ft^3; and c = orifice coefficient, dimensionless, with value of 0.83 for $^1/_4$-in.-diameter hole. Similarly, the total pressure drop was expressed as

$$\Delta P_t = \left(0.187 \frac{v_h^2}{c^2} \frac{\rho_g}{\rho_l} \right) + h_l + \frac{32.1}{\rho_l} \tag{2}$$

where h_l = height of liquid on tray, in. of liquid; and ΔP_t = total pressure drop, in. of liquid.

Bernard and Sargent (1966) measured the density of foam and integrated the vertical profile of foam densities to provide a measure of liquid holdup. Thomas and Campbell (1967) gave useful information on static liquid heads and dynamic heads.

Kupferberg and Jameson (1970) collected data on pressure drop and clear liquid height from sieve tray in laboratory size equipment. These data were later supported by the results of Kharbanda and Chu (1970) on hydraulic studies conducted on sieve tray. Furthermore, on the basis of experimental results, the latter authors derived an equation in the form of additive model for estimating total pressure drop in terms of head of liquid on tray, velocity through the hole, and terms including pressure drop through dry perforation.

However, Eduljee (1972) remarked on the closeness of the two independent data of the two sets of authors mentioned above, especially for a total hydrostatic head of 57.15 mmH_2O measured on sieve trays at minimum vapor velocity.

Thomas and Ogboja (1978) presented a useful review of the previous works on this subject. While Colwell (1981) developed a general correlation from data collected from rectangular columns, Dhulesia (1984) gave a modified version of the Hofhius and Zuiderweg (1979) correlation and also presented data collected from rectangular column.

Bennett et al. (1983) obtained data in a 14-cm-diameter column for trays with small outlet weir heights ranging from 0 to 25 mm and also with tray designs exhibiting large surface tension pressure drop. Furthermore, these investigators, among other things, presented a model for correlating height of liquid on the tray. However, the new corelation for ΔP_T put forward by these authors takes the form

$$\Delta P_T = \Delta P_D + h_L + \Delta P_\sigma \tag{3}$$

where ΔP_T = total pressure drop, of liquid; ΔP_D = dry-hole pressure drop, m of liquid; ΔP_σ = pressure drop due to surface tension, m of liquid; and h_L = height of liquid on tray, m of liquid.

The dry-hole pressure drop, ΔP_D, is defined as

$$\Delta P_D = \frac{a}{c^2} \frac{\rho_G}{\rho_L} \frac{v_H^2}{g} \tag{4}$$

where the value of a, according to Liebson et al. (1957), is given as 0.499.

The term for the pressure drop due to surface tension, ΔP_σ, as given in eq 3 is expressed as

$$\Delta P_\sigma = \frac{6\sigma}{g\rho_l d_{Bmax}} \tag{5}$$

where

$$d_{Bmax} = b \left[\frac{d_H \sigma}{g(\rho_l - \rho_g)} \right]^{1/3} \tag{6}$$

and where b = constant of value 1.27; d_{Bmax} = departure bubble diameter from seive tray, m; d_H = hole diameter, m; and σ = surface tension, N/m.

In the case of the valve tray, Bolles (1976) put forward a model for dry-valve-tray pressure drop for the condition existing when all valves are open, while the total pressure

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