On-line Optimization of Constrained Multivariable Chemical Processes

A two-phase approach to the control and operation of complex chemical processes at their optimum operating conditions is presented. The first phase consists of on-line parameter identification and state estimation of approximate nonlinear dynamic process models using on-line and off-line measurements. In the second phase, the optimum operating strategy is determined by integrating and optimizing this identified process model over a selected time horizon into the future. The method is particularly suited to those processes that exhibit slow dynamic responses and are subject to disturbances that have a significant economic impact. Examples include batch chemical reactors, large distillation towers, and processes with significant holdup times such as large fluidized-bed reactors.

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Introduction

The term on-line optimization is used here to indicate the continuous reevaluation and alteration of operating conditions of a process so that the economic productivity of the process is maximized subject to operational constraints. In the hierarchical view of the overall process management functions, the optimization layer lies between the regulatory control layer and the production scheduling layer. The function of the optimizing layer is to provide the set points for the lower level regulatory control layer.

A comprehensive review of the state of the art in optimizing control is provided in an article by Arkun and Stephanopoulos (1980a). A successful industrial application is noted in a paper by Prett and Gillette (1979), who combined the power of modern day computers and computer-oriented regulatory control algorithms to optimize the operation of a fluid catalytic cracker. Some of the theoretical basis for the hierarchical decomposition and structure of optimizing controllers is set forth in Morari and Stephanopoulos (1980) and in two articles by Arkun and Stephanopoulos (1980b, 1981). Industrial interest in this area appears to be growing with the computerization of plant management functions (Cutler and Perry, 1983; Haggin, 1984.)

The objective of this paper is to provide a framework for the solution of the general on-line optimization problem and to use this framework to develop readily implementable computer algorithms that are applicable to chemical process systems. Particular attention is paid to process nonlinearity, use of imperfect models, presence of operational constraints, insufficient and noisy measurements, ever-changing process disturbances, and time-varying parameters.

Most plants have some type of scheme to optimize operation. Often this is accomplished through ad hoc techniques or through experience over a long period of plant operation. In this article we will be interested in systematic procedures for achieving a well-defined economic optimum, rather than temporary or ad hoc solutions to specific situations. We will focus our attention on achieving this in an on-line fashion since the dynamic nature of the process disturbances, parameters, and other important process variables generally preclude the possibility of achieving an economic optimum through off-line optimization methods (Webb et al. 1980; Prett and Gillette, 1979; Davis et al. 1974; Haggin, 1984.)

The specific function of on-line optimization is best understood through the hierarchical decomposition of plant management set forth by Mesarovic et al. (1970). Figure 1 shows the basic concepts of this decomposition. The lowest level is occupied by regulatory controllers whose function is to regulate the process at given set points in the presence of short-term disturbances that are typically random in nature. The set points for these controllers are provided by the optimizing control layer. In order for the optimization to pay off it is necessary that the regulatory controllers perform efficiently and are able to maintain the process at the set points. Sometimes the distinction between the two layers may be blurred. If the optimization layer tends to

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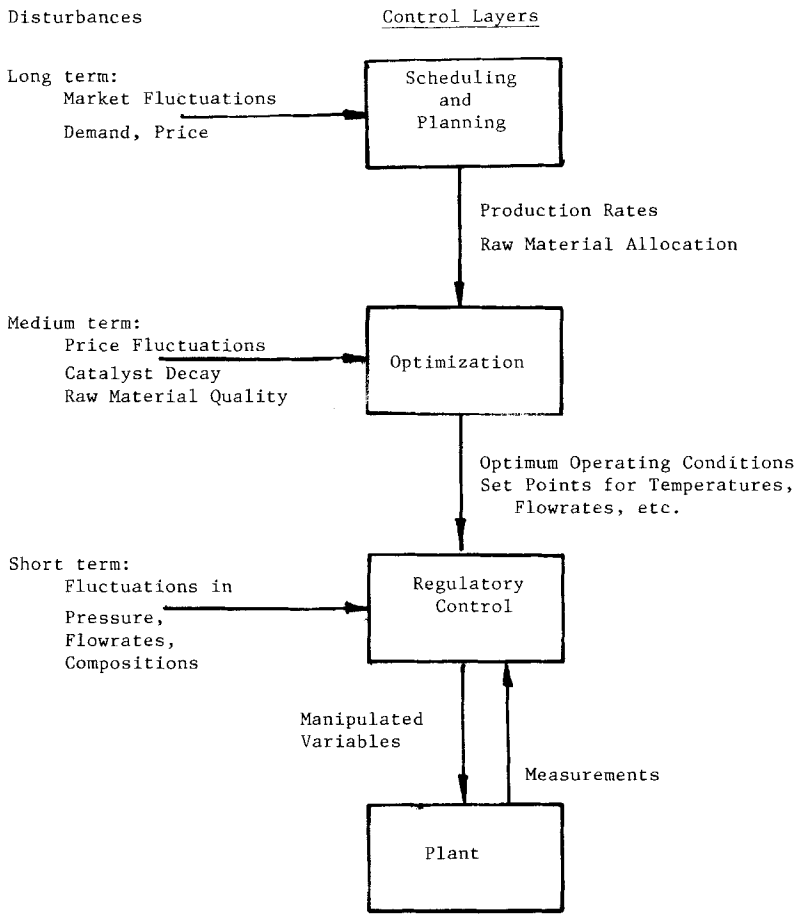

Figure 1. Multilevel decomposition of control tasks.

drive the process to the limits of its operational constraints, two alternatives have been suggested. One is to alter the regulatory control structure (Arkun and Stephanopoulos, 1981), the other is to incorporate the new binding constraints into the regulation itself (Cutler and Ramaker, 1979; Garcia and Morari, 1982) by using a suitable multivariable regulatory control algorithm, such as dynamic matrix control (DMC) or internal model control (IMC).

Problem Formulation

The general problem in plant operation can be stated as follows:

Given an objective function

$$\phi(x, m, d, t) \tag{1}$$

and available measurements $y(t)$, determine the manipulated input variable $m(t)$ such that

$$\Phi = \int_o^T \phi \, dt \tag{2}$$

is maximized subject to operating constraints:

$$h(x, m, p, t) \leq 0 \tag{3}$$

Here x and d respectively denote the state and disturbance.

In order to seek a solution to the problem it is necessary to establish the following:

1. A process model that defines a relationship between the manipulated inputs m and the state x.
2. The characteristics of the stochastic disturbance d.

Since the process itself may change its characteristic over time (e.g., the catalytic efficiency deteriorates over time), it is necessary to continuously revise the process model using the most recent measurements. Also, since the disturbances change their values over time, it is necessary to continuously estimate their values using the most recent measurements. Hence, the optimization must also be continuously performed on-line.

An obvious remedy to the problem of the model/plant mismatch is to use the available measurements and update the process model. Prett and Gillette (1979) employed a steady state model based on fundamental physical and chemical relationships, which are updated using available measurements. They reported a successful application of the procedure to a fluid catalytic cracking operation. Garcia and Morari (1981) suggested the use of linear input/output models because of the wealth of techniques available for identifying such models. In their approach, only steady state optimization was considered so that first-order gradient information available from the linear input/output model was sufficient. When the process parameters change widely, as can happen in optimization moves, methods based on a linear model can fail to converge, as noted by Bhattacharya and Joseph (1982). Also, there is no single way to prop-

erly exploit secondary process measurements with a linear model.

Development of the Two-phase Approach

In this paper, we consider the problem of plant operation based on the idea of a moving time horizon. Given the present time $\bar{t}$, the measurements taken during the past time horizon ending at $\bar{t}$ are available together with partial knowledge of the physical and chemical principles governing the plant and of some parameters crucial in the principles. Then, based on this information, the optimal time plan for the manipulation of input variables (e.g., set points) must be selected for the future time horizon starting at $\bar{t}$. As the present time $\bar{t}$ moves forward so do the past and future time horizons for our problem.

The plant is modeled using differential equations of the form

$$\dot{x} = f(x, m, p, t) \tag{4}$$

with observations $\bar{y}$ of

$$y = g(x, m, p, t), \tag{5}$$

where p represents the parameters and disturbances that are time-varying and hence need to be identified on-line.

Models based on fundamental physical and chemical laws describing the major events in the system are preferred over a general black box model. The former will have a wider range of validity and physically more meaningful variables to identify. The order of the models should be kept to a minimum to avoid unnecessary computational loads. A good compromise should be made between the simplicity of the model and the range of validity.

We would like to emphasize here that if the plant is operating at steady state most of the time then a dynamic model may not be necessary and steady state optimization methods can be utilized. This depends on the frequency of the input disturbances and the time required by the process to settle down.

In our approach, the problem stated above is divided into two phases. The first phase is concerned with the identification of the process model and the estimation of the disturbances entering the process. The second phase deals with finding a suitable path over time for the manipulated input variables that will maximize the objective function. This decomposition of the problem is not new. Similar approaches are suggested by Bamberger and Isermann (1978) and Mukai et al. (1981). The differences lie in the details of the implementation.

Since our approach will be digitally implemented, it is convenient to describe the events in discrete time. Figure 2 depicts the moving time horizons for an on-line implementation. In this figure we want to distinguish between two distinct periods. One period represents the immediate past, consisting of time $\bar{t} - N_i\Delta T_i$ to the present time, $\bar{t}$, where ΔT_i is the interval at which observations are available on the plant. Although it is not necessary to assume that the data are equally spaced in time, it is convenient to do in theory as well as in practice. The other period represents the immediate future, consisting of time $\bar{t}$ to $\bar{t} + N_o\Delta T_o$.

The choice of $N_o\Delta T_o$ and $N_i\Delta T_i$ is made such that the variables p can be determined reasonable accurately from past data and that the resulting model can be used to predict the behavior reasonably well over the future period. Obviously the selection

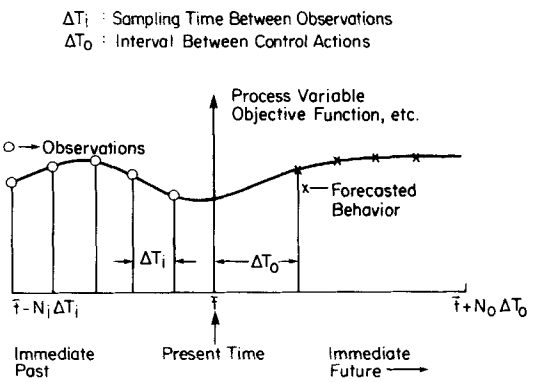

Figure 2. Scenario of on-line optimization scheme.

would have to depend heavily on the process at hand. Later on we shall establish some guidelines for the selection.

Identification problem

The identification problem can be stated as follows:

Given a set of observations $\bar{y}(\bar{t}), \bar{y}(\bar{t} - T_i), \bar{y}(\bar{t} - 2\Delta T_i), \ldots, \bar{y}(\bar{t} - N_i\Delta T_i)$ and the process model, Eqs. 3 and 4, determine p and $x_o = x(\bar{t} - N_i\Delta T_i)$ such that some measure of the model error is minimized.

Prior knowledge about the variables p can greatly simplify this phase and make it solvable on-line. First consider the disturbances. The disturbances of consequence to the objective function are the slowly varying kind. Thus one simplification is to assume that they are constant over the time interval considered. Recall that the time interval of our moving horizon is much shorter than the life span of our scheme. Similarly, if variation in the parameters is sufficiently large even on our short interval, then one could attempt to postulate some model for the variation (e.g., exponential decay or linear variation, etc.), thus avoiding the need to calculate its value at each point in the interval. Lastly, some of the initial states may be known or available from past data. This can also be used to reduce the number of variables p.

System identification is a very rich field with a host of different techniques. The available choices narrow down significantly when dealing with nonlinear systems. A more complete discussion of alternative approaches to the problem is given in a companion paper (Jang et al., 1986). A direct search method is suggested in this paper to determine the parameters so as to minimize a suitable measure of the error in estimation. A least-square formulation is suggested here and has been found to perform well in a number of examples studied (Jang et al.).

The least-square problem is formulated as

$$\underset{p,x_o}{\text{Min}} \sum_{j=0}^{N_i} \|\bar{y}_j - y_j\|^2 \tag{6}$$

Subject to

$$\dot{x} = f(x, m, p, t) \tag{7}$$

$$x(\bar{t} - N_i\Delta T_i) = x_o \tag{8}$$

$$y_j = g(x, m, p, t_j) \tag{9}$$

$$t_j = \bar{t} - j\Delta T_i \tag{10}$$

This is an equality-constrained optimization problem that can be solved by a standard nonlinear programming (NLP) package with some modifications described below.

This optimization problem must be executed whenever one anticipates a change of reasonable magnitude in the variables p. All available measurements, including data from samples analyzed in the laboratory should be used in this phase to guarantee good accuracy.

Most NLP packages do not permit inclusion of ODE constraints. The gradient of the objective function subject to the ODE constraints can be determined as follows:

$$\frac{\partial}{\partial p}\sum_{j=0}^{N_i}\|\bar{y}_j - y_j\|^2 = -2\sum_{j=0}^{N_i}\left(\frac{\partial y_j}{\partial p}\right)^T(\bar{y}_j - y_j) \tag{11}$$

$$\frac{\partial}{\partial x_o}\sum_{j=0}^{N_i}\|\bar{y}_j - y_j\|^2 = -2\sum_{j=0}^{N_i}\left(\frac{\partial y_j}{\partial x_o}\right)^T(\bar{y}_j - y_j) \tag{12}$$

where $\partial y_j/\partial p$ and $\partial y_j/\partial x_o$ are obtained by solving the following simultaneous ordinary differential equations.
For $\partial y_j/\partial p$:

$$\frac{d}{dt}\left(\frac{\partial x}{\partial p}\right) = \frac{\partial}{\partial p}f(x, m, p) \tag{13}$$

with

$$\left.\frac{\partial x}{\partial p}\right|_{t-N_i\Delta T_i} = 0 \tag{14}$$

$$\frac{\partial y}{\partial p} = \frac{\partial g}{\partial p}(x, m, p) + \frac{\partial x}{\partial p}\frac{\partial g}{\partial x}(x, m, p) \tag{15}$$

and for $\partial y_j/\partial x_o$:

$$\frac{d}{dt}\left(\frac{\partial x}{\partial x_o}\right) = \frac{\partial}{\partial x_o}f(x, m, p) \tag{16}$$

with initial condition

$$\left.\frac{\partial x}{\partial x_o}\right|_{t-N_i\Delta T_i} = 1 \tag{17}$$

$$\frac{\partial y}{\partial x_o} = \frac{\partial x}{\partial x_o}\frac{\partial g}{\partial x}(x, m, p) \tag{18}$$

Note that the above calculations are done at given p, m, and x_o values. (m is known from prior control actions; p, x_o are provided by the optimizing routine.)

An alternative, but less accurate and computationally more intensive way to calculate the derivative is through numerical differentiation.

Optimization phase

The discrete form of the on-line optimization problem can then be stated as follows:

Given a process model, Eqs. 4 and 5, together with estimates of p and $x(\bar{t})$ from the identification phase, determine the set of manipulated inputs $m(\bar{t})$, $m(\bar{t} + \Delta T_o)$, $m(\bar{t} + 2\Delta T_o)$, ..., $m[\bar{t} + (N_o - 1)\Delta T_o]$ such that the objective function

$$\Phi = \int_{\bar{t}}^{\bar{t}+N\Delta T_o}\phi(x, m, p, t)dt \tag{19}$$

is maximized subject to the process constraints above, Eq. 3. Here the manipulated input is assumed piece-wise constant: $m(t) = m(\bar{t} + j\Delta T_o)$ $\bar{t} + j\Delta T_o < t < \bar{t} + (j+1)\Delta T_o$. Note that we have retained the continuous form of the model in this discrete formulation since the process is continuous even though the observations and control actions are discrete.

First, note that unlike the identification phase, where the optimization variables p were treated as constant over the time interval, we now have to determine a function $m(t)$ on the interval shown in Figure 2 to minimize the objective function. Thus we must find $m_1, m_2, \ldots, m_{N_o}$ where

$$m = m_j \quad \bar{t} + (j-1)(\Delta T_o) \le t < \bar{t} + j(\Delta T_o) \tag{20}$$

The number, N_o, of subintervals will determine the number of optimization variables. The determination of the gradient of the objective function is slightly more complicated this time and requires the solution of an adjoint set of equations as described in the following steps. Details of its derivation are given in Jang (1986).

Step 1. Using the initial conditions and parameters given by the identification phase, integrate the state equations

$$\dot{x} = f(x, m_i, p, t) \tag{21}$$

over the horizon $[\bar{t}, \bar{t} + N_o\Delta T_o]$

Step 2. Solve the following adjoint differential equations backwards

$$-\frac{dq}{dt} = \left(\frac{\partial f}{\partial x}\right)^T q + \left(\frac{\partial \phi}{\partial x}\right)^T \tag{22}$$

$$q(t + N_o\Delta T_o) = 0 \tag{23}$$

Step 3. Calculate the gradient:

$$\frac{\partial \Phi}{\partial m_i} = \left(\frac{\partial f}{\partial m}\right)_i^T q_i + \left(\frac{\partial \phi}{\partial m}\right)_i^T \tag{24}$$

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

Again, it is necessary to integrate the state equations over the horizon in order to evaluate the gradient.

Implementation

Figure 3 shows a flow chart of the algorithm implementation. Note that the identification phase is executed conditionally.

The identification phase is needed only when there is a substantial difference between the output of the model and that of the process. This is very important. Without a sufficient amount of persistent excitation of the process so that enough process modes are excited, the parameters may become unidentifiable or nearly unidentifiable. In other words, the model using several different sets of parameter values may result in the same or similar outputs, thus making it impossible or difficult to find the

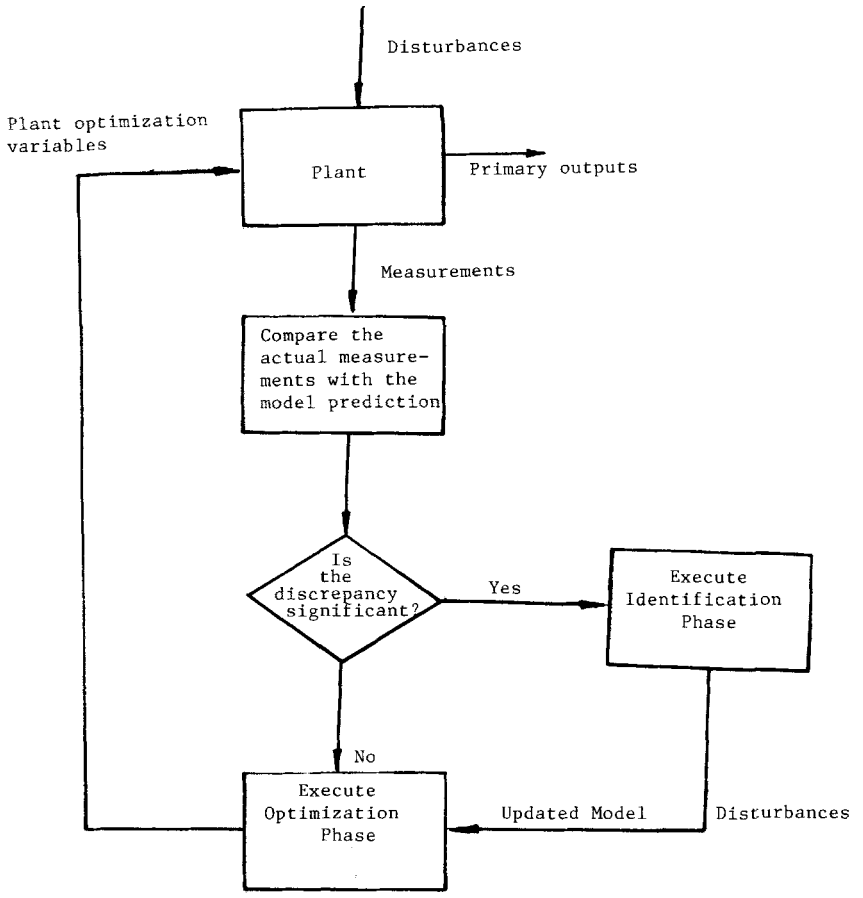

Figure 3. Two-phase approach to on-line optimization.

correct set of parameter values. Unfortunately, if the process is not naturally persistently excited by disturbances, this problem of unidentifiability may occur. When the identification phase is combined with the optimization phase, this problem may be further amplified. Because of its objective, the optimization phase tends to put the process into a calm steady state. This may lead to the problem of near or true unidentifiability and the resulting model may no longer reflect the process accurately. Hence, the optimization phase may yield input commands that are grossly suboptimal, thus inducing a wild behavior of the process. However, such behavior will help the identification phase by exciting enough modes and the resulting model becomes more accurate. Consequently, this accurate model will help the optimization phase and the process may become calm again.

In this fashion, the process under the two-phase method may exhibit a sequence of wild and calm periods. In order to prevent such a behavior, it is very important to employ the identification phase only when it is needed and only when there is a sufficient amount of excitation.

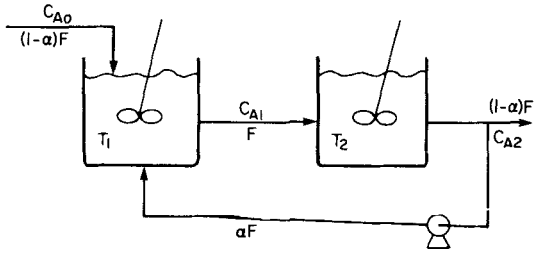

Figure 4. Two-CSTR system used in example (Garcia and Morari, 1981).

Example

To illustrate the concepts presented above, the method is applied to a two-CSTR system originally described in Garcia and Morari (1981). The method was also applied to a problem selected from industry and the results are given in a forthcoming paper by Chen and Joseph (1985a).

Figure 4 shows the schematic of the two-CSTR process. Regulatory controllers are used to maintain constant temperatures in the two reactors. The dynamics associated with these controllers are neglected. The optimizer's task is to adjust the set points of the two temperature controllers to maintain maximum production of substance B. The reactions taking place are:

$$A + B \underset{k_-}{\overset{k_+}{\rightleftharpoons}} 2B$$

with Rate $= k_+ C_A C_B - k_- C_B^2$, and $k_\pm = A_\pm e^{-E_\pm/RT}$.

The plant is described by the equations:

$$\tau_1 \mathring{C}_{A1} = 0.5(C_{A0} + C_{A2}) - C_{A1} - \tau_1(k_+ C_{A1} C_{B1} - k_- C_{B1}^2)$$

$$\tau_1 \mathring{C}_{B1} = 0.5\, C_{B2} - C_{B1} + \tau_1(k_+ C_{A1} C_{B1} - k_- C_{B1}^2)$$

Table 1. Data Used in Simulation of Example CSTR Process

Properties	Symbols	Values
Tank 1 mean residence time	τ_1	30 min
Tank 2 mean residence time	τ_2	25 min
Activation energies divided by Boltzmann's constant	$E+/R$ $E-/R$	17,786 K 23,523 K
Recycle ratio	α	0.5
Frequency factors	A_+ A_-	9.73×10^{22} m^3/kmol · s 3.1×10^{30} m^3/kmol · s

$$\tau_2 \mathring{C}_{A2} = C_{A1} - C_{A2} - \tau_2(k_+ C_{A2} C_{B2} - k_- C_{B2}^2)$$

$$\tau_1 \mathring{C}_{B2} = C_{B1} - C_{B2} + \tau_2(k_+ C_{A2} C_{B2} - k_- C_{B2}^2)$$

The plant is simulated using the parameters shown in Table 1.

The identification problem

The on-line measurements available are concentration of B only (C_{B1}, C_{B2}) in both tanks. These measurements are assumed to be corrupted by Gaussian random noise.

A process model identical in form to the plant equations above is used in the identification phase. The set of variables to be identified is $C_{A1}(\bar{t})$, $C_{A2}(\bar{t})$, A_+, and A_-. The states C_{A1} and C_{A2} are not measured and hence the initial values must be estimated from the measurements of the concentration of B.

Table 2 shows the results of some identification studies with varying amounts of measurement noise and a varying number of measurements. The variables are normalized so that a value of 1.00 implies exact identification. Obviously, greater measurement noise must be compensated by a larger number of measurements. In these studies we have used a sampling time of 6 s (chosen arbitrarily). An alternative approach to reduce the noise is via time series filtering.

Identification requires that the process be perturbed in some way. In many chemical processes, the naturally present disturbances may be sufficient. If there is not enough noise to excite the various modes of the system, then pseudorandom binary perturbations may be imposed on the input variables. In this example an excitation signal was added to C_{A0} to excite the system. The variable metric Davidon-Fletcher-Powell algorithm was used to solve the nonlinear programming problem.

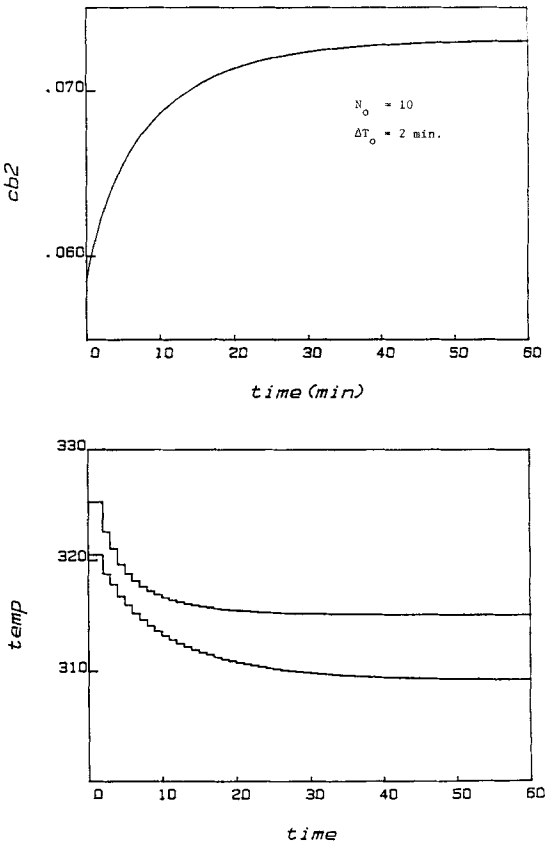

Figure 5. Results of optimization with perfect model.

Optimization phase

The objective function to be maximized is

$$\Phi = \int_{\bar{t}}^{\bar{t}+N_o\Delta T_o} C_{B2}(t)\,dt$$

subject to the equations above. Figure 5 shows the performance of the optimization phase alone (assuming that the model is perfect and all states are measured). The results shown are using $N_o = 10$ and $T_o = 2$ min. The system was started at a nonoptimal point ($T_1 = 307$ K, $T_2 = 302$ K). The on-line optimizer gradually decreases the temperatures to their optimum steady state values.

Table 2. Effect of Measurement Noise and Number of Observations on Accuracy of Identified Variables

No. of Observations	Measurement Noise/Signal Ratio %	Identified Variables				Max. Error in Estimation %
		$\bar{C}_{A1,0}$	$\bar{C}_{A2,0}$	A_+	A_-	
10	10	1.0006	−0.5335	0.9044	0.4593	150
20	10	1.057	0.7243	1.131	0.7511	28
50	10	0.8266	1.228	1.044	0.9626	27
100	10	1.047	0.8726	0.9538	1.052	22
10	5	0.9756	0.4976	0.9637	0.6583	50
20	5	1.030	0.8574	0.9787	0.8922	15
50	5	0.9185	1.128	1.1111	1.038	1.28
100	5	0.9961	1.027	0.9663	1.015	3.3
10	1	1.001	0.9052	0.9802	0.9504	9
20	1	1.032	0.9625	0.9463	1.020	5.3
50	1	0.9892	1.019	1.018	1.037	4
100	1	0.9847	0.9933	1.007	0.9947	1.5

Figure 6 shows the true history of the concentration of B when identification is incorporated into the optimization scheme. In this case, the plant was started at the same point as in Figure 5 but the model parameters A_+ and A_- were initialized to be 20% of the actual value. It takes almost twice as long to reach the steady state optimum because of the need to find the correct model. To aid the identification step the system was excited by adding a 1% random noise to the inflow concentration C_{A0}.

Figures 7a and 7b show the result of adding random noise to the measured signal. The noise is filtered out by the least-square identification step. There is very little difference between the results shown in Figures 6 and 7.

Figure 8 shows a comparison of three different integration algorithms used for integrating the state equations and adjoint equations. The use of a less accurate integration scheme merely slows down the time it takes to reach the optimum, due to the error in the computed gradient. Most optimization schemes generally work well even with approximate gradients in place of the exact gradients. In Euler's scheme a step size of 1 min was used. The Runge-Kutta fourth-order scheme used an adjustable step size. The computation time per horizon for the Runge-Kutta method is 5 s while for Euler's method it is only 0.5 s.

Figure 9 shows the effect of varying N_o on the optimization while keeping the time increment ΔT_o constant. Even using N_o = 2, surprisingly good results are obtained for this example. While this may not be true in general, it does suggest that in these repetitive predictive schemes a fine division of the time horizon may not be needed. Figure 10 confirms this view, where the improvement attained by a tenfold decrease in ΔT_o while keeping the length H_o of the horizon constant is quite small.

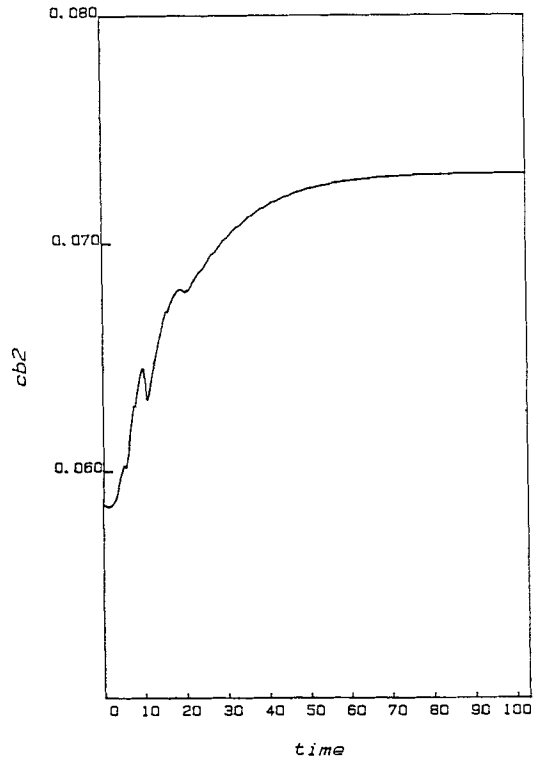

Figure 6. Results of on-line optimization of CSTR system without measurement noise.

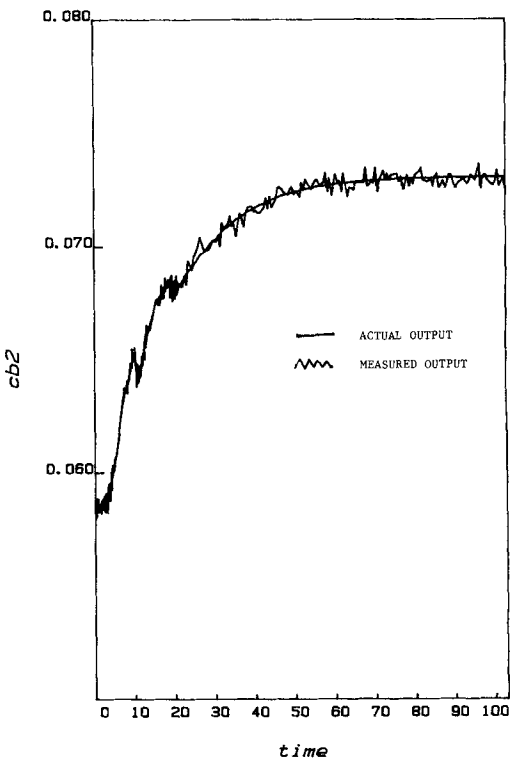

Figure 7a. Results of on-line optimization of CSTR system with 1% measurement noise.

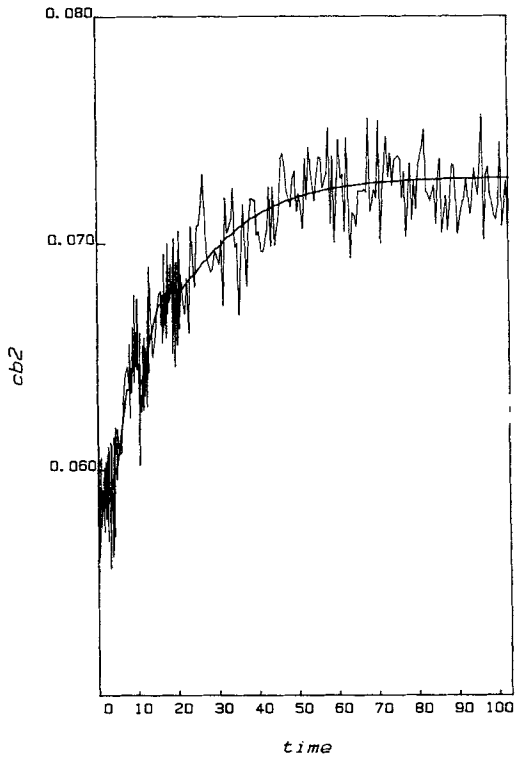

Figure 7b. Results of on-line optimization of CSTR system with 5% measurement noise.

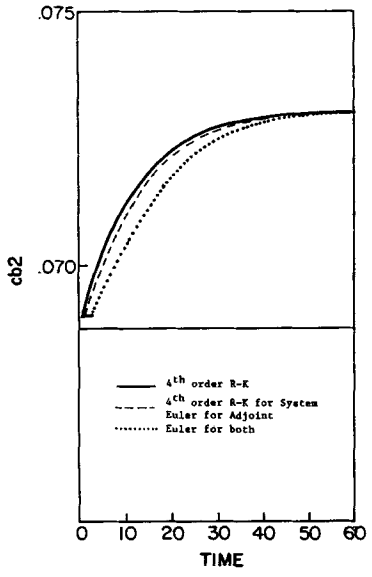

Figure 8. Comparison of different integration algorithms on performance of on-line optimization algorithm.

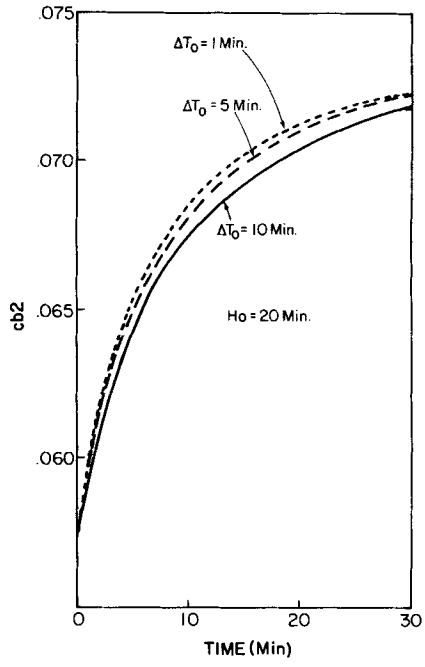

Figure 10. Effect of ΔT_o on performance of algorithm.

Tracking the optimum

In a practical application, the ability of the optimizer to follow variations in the long-term disturbances is important. In other words, the optimum of the process will shift with the disturbances and the on-line optimizer should track this changing target. Such a situation was simulated by changing the input C_{A0} occasionally. The identification step was turned on whenever a predetermined difference between the model and the process (0.1% between measurement and prediction) was detected. This was followed by an implementation of the newly determined optimum conditions. The identification was turned off when the process reached a new plateau, again determined by comparing the model output with the process output.

Table 3 gives the times when disturbances are imposed and the ultimate optimum steady state values for each disturbance. Figure 11 shows the result, showing the points at which the on-line optimizer was turned on and off. A total of five variables (C_{A1}, C_{A2}, C_{B1}, C_{B2}, C_{A0}) were identified in this case.

The identification phase converged quickly to the correct value of the disturbance being identified. Figure 12 shows an example of the convergence of the identification phase.

It is important to recognize that the success of the algorithm depends strongly on the ability to model the process well. If some of the disturbances cannot be modeled, then the performance can be expected to degrade. These and other issues related to modeling errors are discussed in Jang (1986).

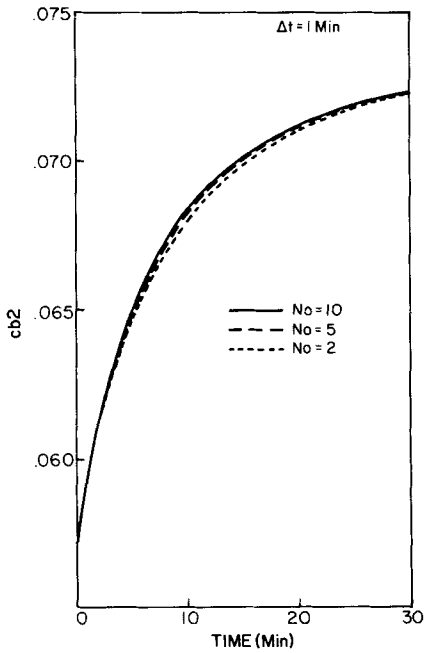

Figure 9. Effect of varying N_o on performance of algorithm.

Constrained optimization

The following constraints were added to the optimization phase: $T_1 \leq 312$ K, $T_2 \leq 312$ K. Since these are constraints on the manipulated variables, they are readily accommodated during the search for the optimum. The successive quadratic programming (SQP) algorithm, more specifically Powell's implementation of this method (Crane et al., 1980), was used.

Table 3. Alternate Optimum Steady State Values of Objective Output for Process Disturbances Imposed at Various Times

Time min	C_{A0} kmol/m^3	C^*_{B2} kmol/m^3
0	0.1	0.0731
300	0.06	0.0420
800	0.2	0.1536
1,500	0.1	0.0731

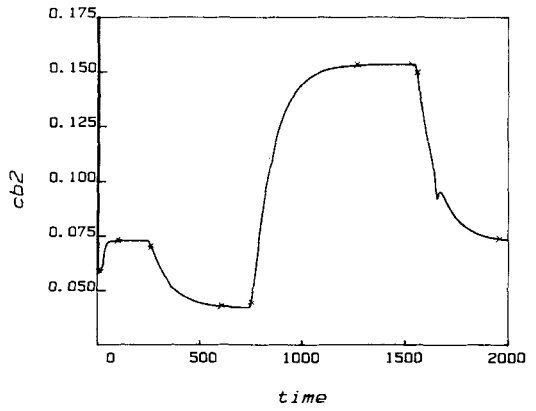

Figure 11. Tracking of optimum in presence of constantly changing input disturbance.
x, points at which on-line optimizer is turned on or off.

The results are shown in Figure 13. Obviously, the optimum profit reached in this case is less than the unconstrained case, but the reponse time is about the same.

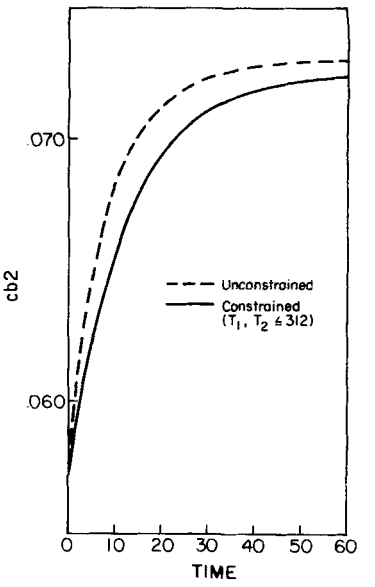

Figure 13. Effect of adding constraints on process.

Discussion

In addition to the results reported above, a number of other studies were also carried out. Based on these, a few guidelines can be given for the selection of some of the parameters such as N_i, N_o, ΔT_i, and ΔT_o used in the two-phase algorithm. These are:

1. The length $N_i \Delta T_i$ of the past horizon should be selected such that the variables p, which are to be identified (model parameters, disturbances), do not vary significantly over the period. Otherwise the assumption of constant p used in the identification phase is violated.

2. Decreasing the integration interval ΔT_i and ΔT_o while keeping the lengths of the horizons increases the computer time required to obtain the gradient of the objective function.

3. The choice of ΔT_i is limited by the intervals at which plant data are available. However, if data are available at smaller intervals, time series filtering should be employed to reduce noise in the measurements used for identification.

4. The size of the problem to be solved in the optimization phase is directly related to the choice of N_o and ΔT_o. Keep N_o as small as possible. This recommendation is supported by results on linear control systems as well (Garcia and Morari, 1982). However, if constraints are present then keeping N_o small may not be feasible.

5. The future horizon should only extend to the point where the process can settle down. Making it longer will emphasize steady state optimization at unnecessarily greater computational expense. If steady state optimization is desired, it is better to exploit that fact and save computation.

6. Allow enough time for regulatory controllers to act between changes in their set points. The regulatory controllers are like a cascade loop inside the optimization loop.

7. In extrapolating too far into the future, there is a danger that the process model may become invalid or inaccurate. Extrapolate only as far as the variables p are expected to remain constant.

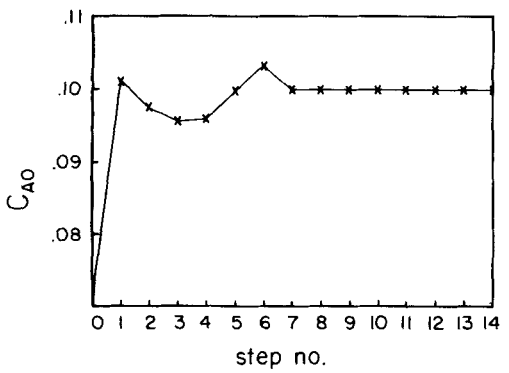

Figure 12. Convergence of estimates for inlet concentration C_{Ao} for first identification period.

The results of the application study indicate that this two-phase approach holds considerable promise as a tool for on-line optimization. The steady state version of this approach has been tested on a more realistic example of the optimization of an ethylene oxide reactor (Chen, 1985; Chen and Joseph, 1985a). The method can also be adapted to regulate nonlinear process systems (Chen and Joseph, 1985b).

Many questions remain unanswered. The important question of stability has not been addressed. Drawing upon the analogy with linear systems, we can say that instability can develop if the modeling error becomes too large, because of the feedback loop formed by the identification phase. The issue of computational efficiency of the approach has not been addressed either. There are ways to enhance the efficiency of these repetitive calculations. Systematic study of the various steps involved is required to identify points where computational efficiency can be enhanced. Lastly, more application studies are required to get a better grasp of the shortcomings as well as to provide guidelines for the selection of process models, parameters used in the design of the optimizer, tolerances used in the optimizer, and parameters used in the identification step.

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Notation

A_+, A_- = frequency factors in reaction rate expressions, $m^3/kmol \cdot s$
C_{Ai} = concentration of A in tank i, $kmol/m^3$
C_{Bi} = concentration of B in tank i, $kmol/m^3$
d = disturbances
$E+/R$ = activation energy used in rate constraints, K
H_o = time length of the horizon for optimization phase
m = manipulated variables
N_i = number of observations used in identification phase
N_o = number of stages used in optimization phase
P = parameters to be identified
q = state variables of adjoint equations
R = gas constant
t = current time
T = final time
ΔT_i = sampling time interval for observations
ΔT_o = time interval within which manipulated variables remain constant
x = state variables
y = measurements
x_o = initial states

Greek letters

α = recycle ratio in reactor
ϕ = operating cost
Φ = objective function
τ_1, τ_2 = time constants of example process, min

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