Optimal Stochastic Control of Nonlinear Systems

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An algorithm is proposed for the feedback control of nonlinear systems, the observations of which are corrupted with noise of unknown statistics. The feedback loop contains a nonlinear Kalman filter, which produces sequential least-square estimates of the state of the system, and a controller designed to minimize an instantaneous performance criterion based on the state estimates. The scheme requires the on-line integration of $n(n + 3)/2$ differential equations, where n is the number of unknown states and parameters. The scheme is applied to the feedback control of a CSTR with a first-order exothermic reaction the temperature measurements of which are corrupted with random noise.

Most of the work in chemical process control has been directed toward deterministic systems, that is, those which can be described precisely by a specified mathematical model. However, in actual systems uncertainties arise because of random fluctuations in inputs, imprecise knowledge of physical parameters such as chemical reaction rate constants, and the corruption of measurements by experimental errors. A dynamic system involving random inputs and measurement errors which also contains variables subject to external control is termed a *stochastic control system*. If these variables are determined so that the system performance, as measured by some criterion, is as good as possible, we have optimal control of the stochastic system.

The theory of optimal control for linear systems with quadratic performance criteria and additive white noise dynamical and measurement errors is well known (*1, 2, 5, 15, 16, 18*). The optimal nonlinear stochastic control problem has been formulated (*11, 12*), but the resulting partial differential equations cannot be solved in general. The objective of this work is to consider practical on-line techniques for the approximate optimal control of nonlinear systems subject to dynamical and measurement disturbances. We will consider specifically nonlinear lumped-parameter systems, the observations of which are corrupted by additive noise. In other words, the actual output from the process has a degree of randomness which can be attributed to a noisy signal superimposed on the true signal. The extension to the case of noisy dynamical inputs is straightforward. In practice, observational errors are usually more severe because they are not damped by the system.

Let us formulate a general nonlinear stochastic optimal control problem. We consider a system described by the n_1 vector $\mathbf{x}(t)$, the output of which is represented by the m vector $\mathbf{y}(t)$. The output $\mathbf{y}(t)$ contains an additive noisy component $\boldsymbol{\eta}(t)$. System parameters are represented by the n_2 vector $\mathbf{k}$ and the control variables by the p vector $\mathbf{u}(t)$. The control problem is

System	$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{k}, t)$	(1)
Observation	$\mathbf{y} = \mathbf{h}(\mathbf{x}, t) + \boldsymbol{\eta}$	(2)
Performance index	$J = E\{\int_0^{t_f} F(\mathbf{x}, \mathbf{u}, t)\,dt\}$	(3)

It is desired to choose $\mathbf{u}(t)$ to minimize J, where $E\{\cdot\}$ represents the expectation operation. In general, it is possible to have $\mathbf{u}(t)$ depend only on the initial state of the system and time, open-loop control, or to give $\mathbf{u}(t)$ associated with starting at each possible state of the system, feedback control. For a specified initial state the optimal open-loop and feedback solutions are equivalent for a deterministic process. It is well known that for a stochastic process the open-loop and feedback solutions in general do not yield the same results. Open-loop control, based only on the initial state and time, is not able to compensate for randomness entering the process and is unacceptable. Thus, $\mathbf{u}(t)$ must be determined as a feedback law when the system involves random variables.

The problem we wish to solve is given by Equations (1) to (3). The solution of even the deterministic nonlinear optimal control problem in terms of a feedback control law is not possible in general. In the deterministic case it is necessary to use approximate methods to determine a feedback control law. Thus, in the stochastic case it will be necessary to consider approximate schemes also. In order to provide a basis for the scheme to be studied, let us consider briefly the linear-quadratic optimal stochastic control problem.

LINEAR-QUADRATIC CASE

The linear-quadratic analogue to Equations (1) to (3) is

System	$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}u$	(4)
Observation	$\mathbf{y} = \mathbf{H}\mathbf{x} + \boldsymbol{\eta}$	(5)
Performance Index	$J = E\{\int_0^{t_f} [\mathbf{x}^T\mathbf{Q}\mathbf{x} + ru^2]dt\}$	(6)

where we have taken a scalar control $u(t)$ for convenience. The initial state of the system is normally distributed with mean $\mathbf{x}_0$ and covariance $\mathbf{P}_0$, and the observation error $\boldsymbol{\eta}$ is Gaussian white noise with $E[\boldsymbol{\eta}(t)] = 0$ and $E[\boldsymbol{\eta}(t)\,\boldsymbol{\eta}(\tau)^T] = \mathbf{N}(t)\delta(t - \tau)$. The system is assumed to have been normalized so that the desired state is the origin.

We define the conditional mean and covariance of the state by

$$\boldsymbol{\mu}(t) = E[\mathbf{x}(t)|\mathbf{y}(\tau), u(\tau), 0 < \tau < t] \quad (7)$$

$$\mathbf{P}(t) = E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T|\mathbf{y}(\tau), u(\tau), 0 < \tau < t] \quad (8)$$

These quantities are governed by the Kalman filter equations (*8*)

$$\dot{\boldsymbol{\mu}} = \mathbf{A}\boldsymbol{\mu} + \mathbf{b}u + \mathbf{P}\mathbf{H}^T\mathbf{N}^{-1}(\mathbf{y} - \mathbf{H}\boldsymbol{\mu}) \quad (9)$$

$$\dot{\mathbf{P}} = \mathbf{A}\mathbf{P} + \mathbf{P}\mathbf{A}^T - \mathbf{P}\mathbf{H}^T\mathbf{N}^{-1}\mathbf{H}\mathbf{P} \quad (10)$$

with initial conditions

$$\boldsymbol{\mu}(0) = \mathbf{x}_0, \mathbf{P}(0) = \mathbf{P}_0 \quad (11)$$

$\boldsymbol{\mu}(t)$ represents the maximum likelihood or minimum vari-

ance estimate of $\mathbf{x}(t)$ conditioned on the observations $\mathbf{y}(\tau)$, $0 < \tau < t$, and $\mathbf{P}(t)$ represents the covariance of the estimate error.

We wish to determine $u(t)$ to minimize J given by Equation (6). The method of solution of this problem can be found elsewhere (*1, 2*). The optimal value of $u(t)$ is given by the feedback proportional law

$$u(t) = -\frac{1}{r}\boldsymbol{\mu}^T\mathbf{B}\mathbf{b} \tag{12}$$

where

$$\dot{\mathbf{B}} + \mathbf{B}\mathbf{A} + \mathbf{A}^T\mathbf{B} - \frac{1}{r}\mathbf{B}\mathbf{b}\mathbf{b}^T\mathbf{B} + \mathbf{Q} = 0 \tag{13}$$

$$\mathbf{B}(t_f) = 0$$

A comparison can be made with the optimal feedback control for the deterministic system. In the deterministic case, $\boldsymbol{\eta} = 0$, $\mathbf{y} = \mathbf{H}\mathbf{x}$, and $\boldsymbol{\mu} = \mathbf{x}$ with $\mathbf{P} = 0$. The optimal return function

$$V(t, \boldsymbol{\mu}) = \min_u E\{\int_t^{t_f} [\mathbf{x}^T\mathbf{Q}\mathbf{x} + ru^2]dt|\boldsymbol{\mu}(t)\} \tag{14}$$

$$-\infty < \boldsymbol{\mu} < \infty$$

$$0 < t < t_f$$

is equal to $\mathbf{x}^T\mathbf{B}\mathbf{x}$ in the deterministic case, with $\mathbf{B}$ governed by the Ricatti equation, Equation (13). In the stochastic case, $V(t, \boldsymbol{\mu}) = \boldsymbol{\mu}^T\mathbf{B}\boldsymbol{\mu} + \lambda(t)$, where

$$\dot{\lambda} + tr(\mathbf{Q}\mathbf{P}) + tr\{(\mathbf{P}\mathbf{H}^T\mathbf{N}^{-1})^T\mathbf{B}\mathbf{P}\mathbf{H}^T\} = 0 \tag{15}$$

$$\lambda(t_f) = 0$$

Thus, $\lambda(t)$ represents the additional cost to the performance index for the stochastic system over that for the deterministic system. This additional cost can be viewed as a result of the incomplete knowledge of the true state of the system. The optimal stochastic control law, Equation (12), is identical to the optimal deterministic law, the only difference being that $\mathbf{x}(t)$ is replaced in the stochastic case by the maximum likelihood estimate $\boldsymbol{\mu}(t)$ from the Kalman filter.

Thus, the stochastic control solution in the linear-quadratic case has the interesting property of being identical to the control obtained by solving the deterministic problem obtained by replacing the random variables in the stochastic problem by their expected values. The general procedure of replacing random variables by their expected values and of solving the resulting deterministic control problem yields what is called *certainty equivalent control* (*1, 5*). In the linear-quadratic case the certainty equivalent control is identical to the optimal stochastic feedback control. In general this is not the case.

The optimal control loop thus consists of a Kalman filter after the observation element, the output of which is sent to the optimal deterministic controller. A signal flow diagram of the situation is shown in Figure 1.

NONLINEAR CASE

Although the structure of the optimal control for the nonlinear system is unknown, a reasonable approximation is to use a configuration as in Figure 1, that is, to separate the filtering and control functions. We desire to produce the expected values of the system state in the element labeled *filter*. The analogue of the Kalman filter for nonlinear system and observation, Equations (1) and (2), is the so-called *nonlinear filter* or *nonlinear Kalman filter* (*3, 4, 7*):

$$\dot{\hat{\mathbf{x}}} = \mathbf{f}(\hat{\mathbf{x}}, \mathbf{u}, \mathbf{k}, t) + \mathbf{P}\mathbf{h}_x^T\mathbf{M}(\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, t)) \tag{16}$$

$$\dot{\mathbf{P}} = \mathbf{f}_x\mathbf{P} + \mathbf{P}\mathbf{f}_x^T + \mathbf{P}[\mathbf{h}_x^T\mathbf{M}(\mathbf{y} - \mathbf{h}(\mathbf{x}, t))]_x\mathbf{P} \tag{17}$$

where $\hat{\mathbf{x}}$ is the minimum least-square estimate of $\mathbf{x}$, corresponding to $\boldsymbol{\mu}$ in Equation (9). $\mathbf{P}$ is no longer precisely the covariance matrix of the estimate error, but it can be roughly interpreted as such. Similarly, the diagonal weighting matrix $\mathbf{M}$ can be associated with $\mathbf{N}^{-1}$. However, the only required property of the measurement error $\boldsymbol{\eta}$ is that it be a zero-mean random process. This is important because the statistical properties of stochastic measurement errors encountered in practice are normally unknown.

In addition to state estimation, filtering can be used to estimate unknown parameters. If we define the $n_1 + n_2$-vector $\mathbf{z}$ by $(x_1, \ldots, x_{n_1}, k_1, \ldots, k_{n_2})$, and $\mathbf{g}$ by $(f_1, \ldots, f_{n_1}, 0, \ldots, 0)$, then affixing

$$\dot{\mathbf{k}} = 0 \tag{18}$$

to Equation (1), we get the new state equation

$$\dot{\mathbf{z}} = \mathbf{g}(\mathbf{z}, \mathbf{u}, \mathbf{t}) \tag{19}$$

$\mathbf{x}$ in Equations (16) and (17) can be replaced by the $n(= n_1 + n_2)$ vector $\mathbf{z}$, and $\hat{\mathbf{z}}$ yields both state and parameter estimates.

Thus, for a nonlinear system and observation, the Kalman filter in Figure 1 is replaced by the nonlinear filter, Equations (16) and (17). The nonlinear filter would be implemented by a process control computer which integrates Equations (16) and (17) in real time. The computer is required to integrate $n(n + 3)/2$ differential equations in real time [n for $\hat{\mathbf{z}}$ and $n(n + 1)/2$ for $\mathbf{P}$, which is symmetric]. This situation is depicted in Figure 2.

One might pose the question why not use a very simple filter, for example, an *R-C* filter, instead of the nonlinear filter? If all that were required were a smoothing of y, then a simple filter would be adequate. However, the key function performed by the nonlinear filter is the estimation of unmeasured states and imprecisely known parameter values, a task which a simple filter cannot perform.

We now devote our attention to the element in Figure 2

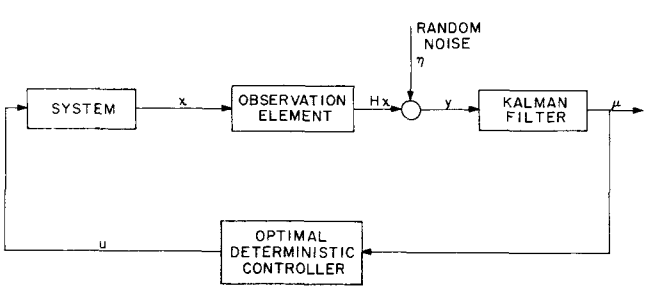

Fig. 1. Optimal stochastic control for linear system with quadratic performance index.

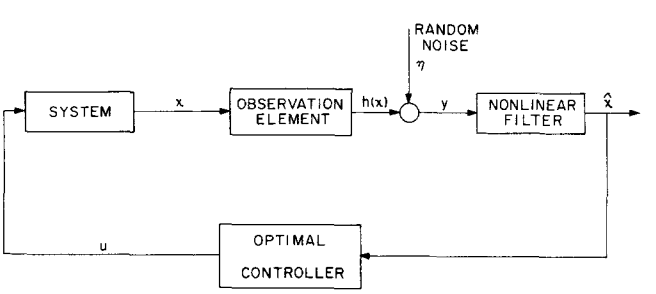

Fig. 2. Proposed configuration for the optimal feedback control of nonlinear stochastic systems.

labeled *controller*. Since the filter is specified, we desire to consider the question of designing the control element in some optimal way. The scheme pictured in Figure 2 has been examined by Seinfeld et al. (*14*) for the case in which the controller function is fixed. The feedback proportional control of a continuous stirred tank reactor (CSTR) was considered with and without the filter in the loop. Significant improvements in performance were obtained when the filter was used, and in some cases the reactor was prevented from entering limit cycle behavior by the filter.

In developing a technique for approximate optimal control in the framework of Figure 2, we must keep several points in mind:

1. Since the computer is required to integrate $n(n + 3)/2$ differential equations in real time for the filter, the control implementation should involve a minimum amount of additional computation.
2. The scheme must be able to incorporate any constraints which may exist on the control variables.
3. The schemes should be independent of the initial disturbance or the type of measurement noise.

It is reasonable to sacrifice some degree of optimality to achieve these objectives. We propose to design the controller to achieve an instantaneous rather than an overall optimum. This general idea has been used for nonlinear deterministic feedback control (*6, 9, 10, 13, 17*). Encouraging results using this concept have been obtained by Lapidus (*6, 10*), Paradis and Perlmutter (*13*), and Wanninger and Stevens (*17*). Sometimes the minimization of an instantaneous measure of the deviation of the system from a desired state is related to the corresponding minimization of a Lyapunov function (*9, 10*), although we will not pursue this point here. We will assume that the desired state of the system is stable.

Let us assume that the objective of the control is to drive the system to a desired state $\mathbf{x}^d$. In general, the control may be constrained between upper and lower bounds $\mathbf{u}^* \geq \mathbf{u} \geq \mathbf{u}_*$. The particular form of Equation (3) that we consider is that in which $F(\mathbf{x}) = (\mathbf{x} - \mathbf{x}^d)^T\mathbf{Q}(\mathbf{x} - \mathbf{x}^d)$, where $\mathbf{Q}$ is a diagonal matrix with elements $q_i \geq 0$, $i = 1, 2, \ldots, n_1$. However, we do not know $\mathbf{x}$, the true system state, rather only the estimated state $\hat{\mathbf{x}}$, so we must reformulate the performance criterion with respect to $\hat{\mathbf{x}}$. The new instantaneous criterion of system deviation from the desired state is

$$F(\hat{\mathbf{x}}) = (\hat{\mathbf{x}} - \mathbf{x}^d)^T\mathbf{Q}(\hat{\mathbf{x}} - \mathbf{x}^d) \tag{20}$$

We now desire to choose $\mathbf{u}$ subject to $\mathbf{u}^* \geq \mathbf{u} \geq \mathbf{u}_*$ such that F will be a minimum. Physically, F is a measure of the estimated distance of the state from the desired state. By minimizing $\dot{F}$ at each instant of time, the rate of movement toward $\mathbf{x}^d$ is a maximum. We have that

$$\dot{F} = 2\,(\hat{\mathbf{x}} - \mathbf{x}^d)^T\mathbf{Q}\dot{\hat{\mathbf{x}}} \tag{21}$$

Substituting Equation (16) into (21), we obtain

$$\dot{F} = 2(\hat{\mathbf{x}} - \mathbf{x}^d)^T\mathbf{Q}[\mathbf{f}(\hat{\mathbf{x}}, \mathbf{u}, \mathbf{k}, t) + \mathbf{P}\mathbf{h}_x^T\mathbf{M}(\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, t))] \tag{22}$$

A minimum instantaneous $\dot{F}$ can be obtained from Equation (22) by differentiation with respect to $\mathbf{u}$. A particularly important case is when the right-hand side is linear in $\mathbf{u}$:

$$\dot{\mathbf{x}} = \mathbf{w}(\mathbf{x}, \mathbf{k}, t) + \mathbf{S}(\mathbf{x}, \mathbf{k}, t)\mathbf{u} \tag{23}$$

in which case Equation (22) becomes

$$\dot{F} = 2(\hat{\mathbf{x}} - \mathbf{x}^d)^T\mathbf{Q}[\mathbf{w}(\hat{\mathbf{x}}, \mathbf{k}, t) + \mathbf{S}(\hat{\mathbf{x}}, \mathbf{k}, t)\mathbf{u} + \mathbf{P}\mathbf{h}_x^T\mathbf{M}(\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, t))] \tag{24}$$

Equation (24) can be written in the form

$$\dot{F} = \boldsymbol{\beta}^T\mathbf{u} + \gamma \tag{25}$$

where $\boldsymbol{\beta} = 2\mathbf{S}(\hat{\mathbf{x}}, \mathbf{k}, t)^T\mathbf{Q}(\hat{\mathbf{x}} - \mathbf{x}^d)$, and $\gamma = 2(\mathbf{x} - \mathbf{x}^d)^T\mathbf{Q}[\mathbf{w}(\hat{\mathbf{x}}, \mathbf{k}, t) + \mathbf{P}\mathbf{h}_x^T\mathbf{M}(\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, t))]$. A minimum $\dot{F}$ is obtained if

$$u_i = \begin{cases} u_i^* & \beta_i < 0 \\ & i = 1, 2, \ldots, p \\ u_{i*} & \beta_i > 0 \end{cases} \tag{26}$$

Since we are not obtaining the true optimal solution, a singular interval on which $\beta_i = 0$ for a finite time is of no real significance. If this occurs, we can set the particular u_i equal to its final desired value until $\beta_i \neq 0$, at which time we resume the switching.

The factors enumerated above are all met by this scheme. The only computation required for the control is the purely algebraic determination of $\mathbf{u}$. Whenever a value of u_i predicted from the minimum $\dot{F}$ exceeds a constraint, it is set equal to the constraint. In the case of Equation (26), the control is always on one of the constraints. Neither the initial state of the system nor the statistics of the noise affects the conceptual application of the algorithm. The only free parameters are the elements of $\mathbf{Q}$ and $\mathbf{M}$, q_i, $i = 1, 2, \ldots, n_1$, and m_i, $i = 1, 2, \ldots, m$. The q_i incorporate the importance of driving the different estimated states to the origin. $\mathbf{M}$ arises in the derivation of Equations (16) and (17) and is a weighting matrix, the elements of which reflect the importance of reducing the residuals $y_i - h_i(\hat{\mathbf{x}}, t)$ to zero.

We will now apply this scheme to the feedback control of a CSTR.

OPTIMAL STOCHASTIC CONTROL OF A CSTR

We consider the problem of optimally controlling a CSTR from noisy temperature measurements. For a CSTR in which a first-order exothermic reaction is occurring with heat removal by a coil or jacket

$$\frac{dc}{dt} = \frac{q}{V}(c_0 - c) - Kc \exp(-E_A/T) \tag{27}$$

$$\frac{dT}{dt} = \frac{q}{V}(T_0 - T) - \frac{\Delta H}{\rho C_p} Kc \exp(-E_A/T) - \frac{UA_R}{\rho C_p V}(T - T_c) \tag{28}$$

The observations of the reactor consist of continuous temperature measurements corrupted with additive random noise

$$y(t) = T(t) + \eta(t) \tag{29}$$

It is desired to keep the reactor at the steady state (c^d, T^d) by manipulation of the heat transfer coefficient U, subject to the constraint $U^* \geq U \geq U_*$. At $t = 0$, the reactor is at some condition other than (c^d, T^d). Only the temperature is measured, according to Equation (29). This is physically realistic, because the compositions in a chemical reactor often cannot be measured continuously.

The following parameter values are used:

$K = 7.86 \times 10^{12}$ sec.$^{-1}$ $C_p = 1.0$ cal./(g.)(°K.)
$E_A = 14090$ °K. $\rho = 0.001$ g./cc.
$A_R = 10$ sq. cm. $T_0 = 350$°K.
$V = 1{,}000$ cc. $T_c = 340$°K.
$c_0 = 6.5 \times 10^{-6}$ g.-moles/cc. $U^* = 8 \times 10^{-4}$ cal./(sq.cm.)(sec.)(°K.)
$\Delta H = -27{,}000$ cal./g.-mole $U_* = 0$
$q = 10$ cc.-sec.

The steady state value of U is $U^d = 5 \times 10^{-4}$ cal./(sq. cm.)(sec.)(°K.). The steady state (and the desired state) is

$$c^d = 1.531 \times 10^{-7} \text{ g.-moles/cc.} \qquad T^d = 460.91°\text{K.}$$

and the initial state is taken as

$$c(0) = 3.531 \times 10^{-7} \text{ g.-moles/cc.} \quad T(0) = 440.91°\text{K.}$$

These values have been chosen to afford a comparison with the work of Paradis and Perlmutter (*13*) and Grethlein and Lapidus (*6*), who considered the analogous deterministic problem with measurement of both T and c. For this particular set of parameter values, there exist three steady states at T values of 350° (stable), 414° (unstable), and 460.91°K. (stable).

If we define

$$x_1 = \frac{c - c^d}{c_0} \qquad \tau = qt/V$$
$$x_2 = \frac{T - T^d}{T_0} \qquad u = U/U^d$$
$$\phi = c^d/c_0 \qquad E_0 = E_A/T_0$$
$$\psi = T^d/T_0 \qquad k = U^d A_R/\rho C_p q$$
$$\theta = \ln(VK/q) \qquad L = \gamma \Delta H/T_0$$

then Equations (27) and (28) become

$$\frac{dx_1}{d\tau} = 1 - x_1 - \phi - (x_1 + \phi)\exp\left(\theta - \frac{E_0}{(x_2 + \psi)}\right) \tag{30}$$

$$\frac{dx_2}{d\tau} = 1 - x_2 - \psi - L(x_1 + \phi)\exp\left(\theta - \frac{E_0}{(x_2 + \psi)}\right) - k(x_2 + \psi - \psi_c)u \tag{31}$$

Sequential Estimation of States and Parameters

The nonlinear filter can be used to estimate sequentially states and parameters in the CSTR model from the output y. Let us first consider the estimation of c and T assuming that all the constant parameters in Equations (30) and (31) are known. It is essential that the properties of the filter be ascertained prior to its use in the control algorithm.

The reactor behavior is simulated as follows. For the sequential estimation study we set $U = U^d$ and integrate Equations (16) and (17) simultaneously with Equations (30), (31), and (29). The noisy measurements are generated by Equation (29). Two forms of Equation (29) were used in the simulation:

$$\text{(I)} \quad y = (x_2 + \psi)\,\text{GAUSS}\ (0, 0.1) + x_2 \tag{32}$$

$$\text{(II)} \quad y = x_2\,[0.1\,\text{GAUSS}\ (0, \sigma) + 1.0] \tag{33}$$

where GAUSS (a, σ) is a normally distributed random variable routine with mean a and standard deviation σ. In error model (I), deviations the order of ±50°K. were generated, whereas in error model (II), deviations of ±3°K. were obtained. The first case was used to test the behavior of the algorithm in the presence of large errors. The true values of c and T are shown in Figures 3 and 4 for the transient decay of the reactor state from $[c(0), T(0)]$ to the steady state (c^d, T^d). The estimated values $\hat{c}$ and $\hat{T}$ are shown in Figures 3 and 4 by the curves labeled 1. The initial conditions used for the integration of Equations (16) and (17) for curves 1 were $\hat{c}(0) = c^d$, $\hat{T}(0) = T^d$, $P_{11}(0) = 2$, $P_{12}(0) = 2$, $P_{22}(0) = 2$. The value of M used was 20. Additional cases were examined with different values of the initial conditions and M, all of which converged more or less the same as curves 1 in Figures 3 and 4.

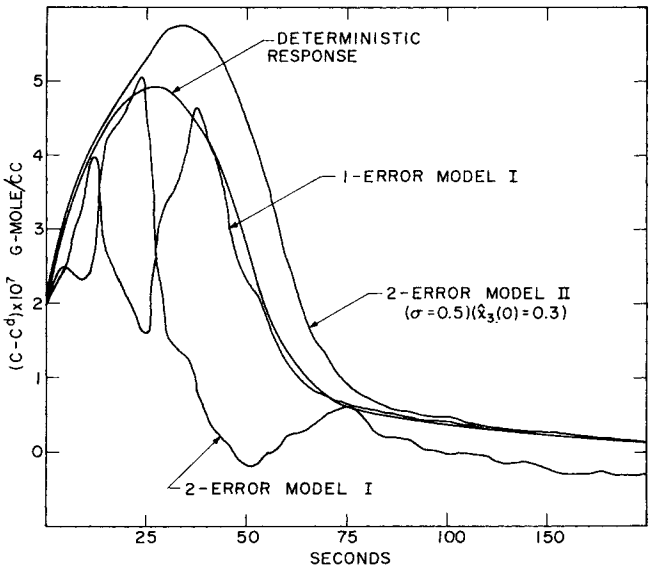

Fig. 3. True (deterministic) and filtered concentrations from noisy temperature measurements of the dynamic response of CSTR.

Next we consider the estimation of c and T and an unknown constant parameter. We assumed that k in Equation (31) was imprecisely known. The measurements were generated by Equations (32) and (33) by using the true value of k to generate the x_1, x_2 trajectories. The estimated values of c and T are shown by the curves labeled 2-error model I and 2-error model II in Figures 3 and 4, corresponding to the error model used to generate y. The estimated values of k are shown in Figure 5. The true value

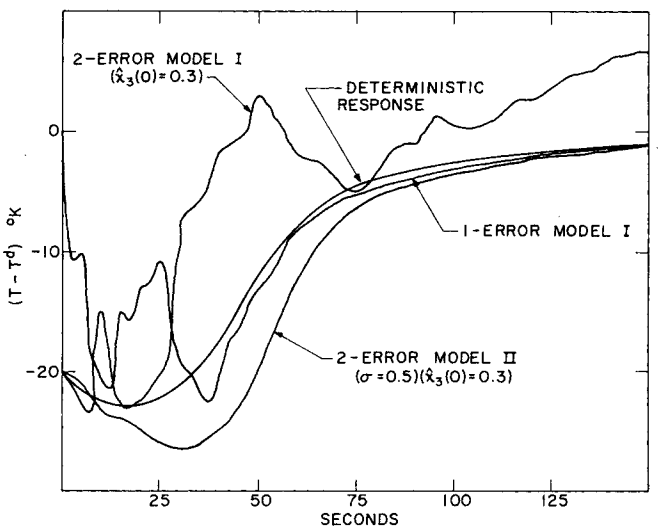

Fig. 4. True (deterministic) and filtered temperatures from noisy temperature measurements of the dynamic response of CSTR.

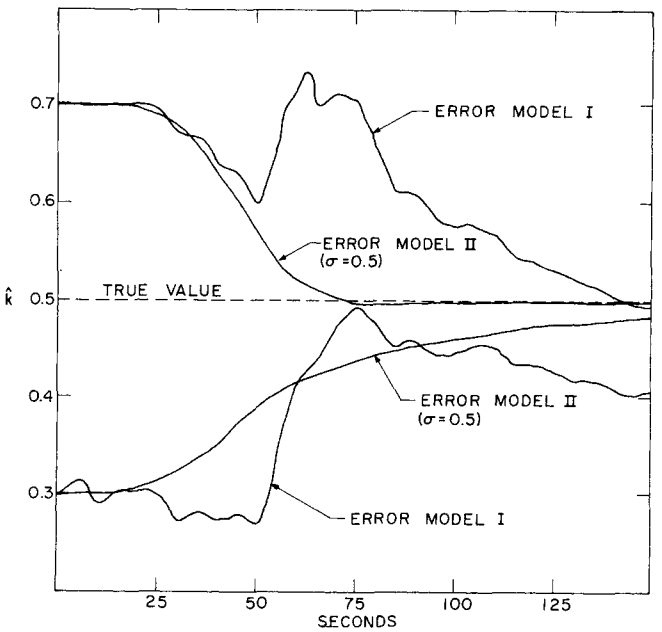

Fig. 5. Sequential estimates of k obtained from noisy temperature measurements of the dynamic response of CSTR.

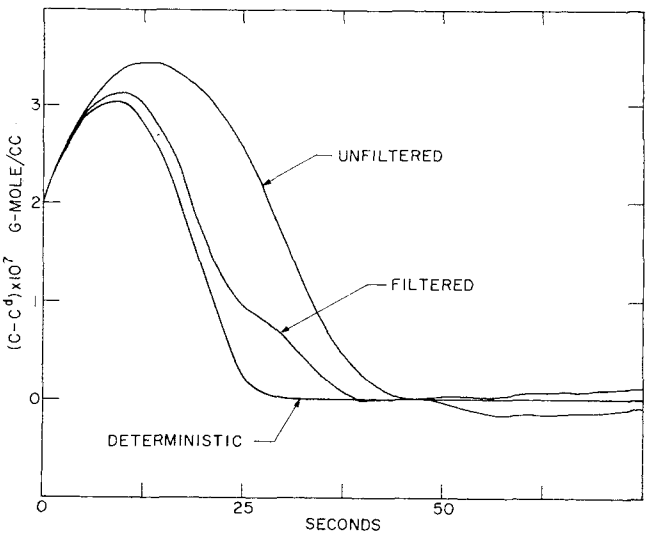

Fig. 6. Comparison of optimal deterministic and stochastic feedback controlled concentration response of CSTR with stochastic unfiltered response.

of k is 0.5. Initial guesses $\hat{k}$ (0) were taken as 0.3 or 0.7. For each initial guess, error models I and II were used. σ in error model II was taken as 0.5. The initial conditions used for the integration of Equations (16) and (17) were $\hat{c}(0) = C(0)$, $\hat{T}(0) = T(0)$, and

$\hat{k}(0)$	$P_{11}(0)$	$P_{12}(0)$	$P_{22}(0)$	$P_{13}(0)$	$P_{23}(0)$	$P_{33}(0)$	$M(I)$	$M(II)$
0.3	1	−1	12	−1	−2	25	5	10
0.7	1	1	12	1	2	25	5	12

These values of $\mathbf{P}(0)$ and M were arrived at after numerical experimentation with other values. These produced the best rates of convergence, although further trials would probably have found better values. The important point to note is the much slower convergence of the filter estimates for unknown parameters. When error model I is used, convergence is not obtained for $\hat{c}$, $\hat{T}$, or $\hat{k}$ as can be seen from the curves labeled 2-error model I in Figures 3 and 4 and the curves labeled error model I in Figure 5. Convergence was obtained for the much less severe error model II but was quite sensitive to the $\mathbf{P}(0)$ and M values used. Convergence is poor for sequential estimation of parameters because the filter equations for constant parameters involve only the forcing term with the residual, $\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}, t)$. This term is multiplied by components of $\mathbf{P}$ which tend to zero at t increases, thus decreasing the effect of poor state estimates on the parameter estimate. Additional numerical experiments were carried out in which it was attempted to estimate θ and E_0 in addition to c and T. Convergence of the estimates was poor, probably because of the sensitivity of the exponential function to small changes in either θ or E_0. The important problem of on-line parameter estimation is still not completely resolved.

Feedback Control

We now consider the simulation of the loop in Figure 2. The optimal deterministic responses computed by Paradis and Perlmutter (*13*) are shown in Figures 6 and 7. By comparison of the deterministic responses in Figures 6 and 7 and 3 and 4 it is seen that significant improvements are obtained by using the bang-bang control law based on the instantaneous minimization of F.

The reactor—filter—controller dynamics are simulated as follows. At $t = 0$ we begin integrating Equations (30), (31), (32), (16), and (17), simultaneously. Since Equations (30) and (31) are of the form of Equation (23) with $\mathbf{u} = u$, the control law is given by Equation (26).

At each step in the integration β is computed by

$$\beta = -2k(\hat{x}_2 + \psi - \psi_c)q_2\hat{x}_2 \tag{34}$$

and u is determined from

$$u = \begin{cases} u^* & \beta < 0 \\ u_* & \beta > 0 \end{cases} \tag{35}$$

where $u^* = U^*/U^d$ and $u_* = U_*/U^d$. The value of u

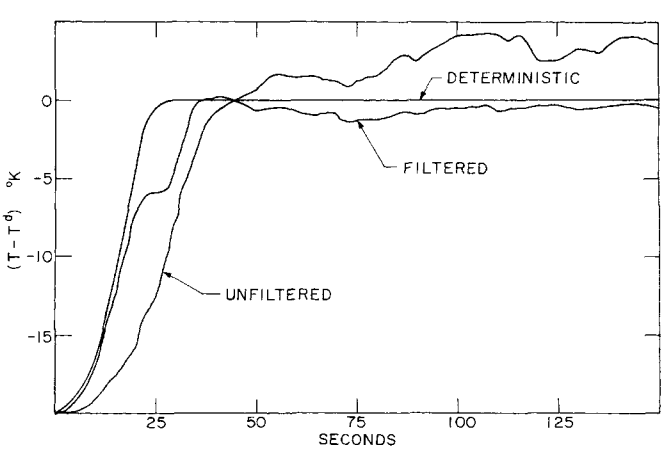

Fig. 7. Comparison of optimal deterministic and stochastic feedback controlled temperature response of CSTR with stochastic unfiltered response.

computed from Equation (35) is used for the next step in the integration. This procedure corresponds to continuous computation of β because the integration step length used is very small when compared with the overall transient time of the system. The estimation of k can also be incorporated into the simulation by the appropriate increase in the dimensionality of Equations (16) and (17). However, since only the sign of $\beta = -2\hat{k}(\hat{x}_2 + \psi - \psi_c)q_2\hat{r}_2$ is important for determining u, a poor estimate of k will not affect the control in this case. For non bang-bang control, a poor parameter estimate could have a significant effect on the control u.

First, it is appropriate to ask what is the effect of the noisy temperature measurements on the optimal scheme if the filter is not included in the loop. With no filter the switching function β is determined by using y in place of $\hat{x}_2$. If temperature measurements are made exactly, the responses are the deterministic curves in Figures 6 and 7. As mentioned, these correspond to curves *a* of Figures 1 and 2 of Paradis and Perlmutter for an unlimited number of switches of u. If the temperature measurements are corrupted according to Equation (32), the switching function computed by using y may no longer be a reliable measure of the deviation of the true state from the desired state. The response in this case, labeled as the *unfiltered responses*, are shown in Figures 6 and 7. We see that the controller based on β is unable to drive the system to the desired state because of the inaccuracy in β determined directly from the measured temperature.

Now let us consider the full configuration of Figure 2. The responses in this case, labeled as the *filtered responses*, are shown in Figures 6 and 7. The same initial conditions as for curves 1 in Figures 3 and 4 were used. The responses closely approximate the deterministic responses, and the effect of the extremely severe output fluctuations generated by Equation (32) are completely eliminated.

The scheme is particularly useful in cases where the feedback control depends on unmeasured states and parameters even if the observed states are measured relatively accurately. The feasibility of employing a filter will depend on the number of states that can be observed, the level of measurement errors, and the desirability of close control of the system. The usual situation in chemical process control involves a multivariable process in which only a few of the states are measured. The algorithm requires the integration of $n(n + 3)/2$ differential equations in real time, for example, twenty for $n = 5$, sixty-five for $n = 10$. As long as the process time constant is the order of minutes or hours (rather than seconds), which is usually the case in chemical processes, a computer can carry out the filter integrations in real time. The calculational problems are purely those involved in the high-speed integration of ordinary differential equations. As the process dimensionality increases, the utility of the scheme actually improves, assuming that a significant number of states are unmeasured.

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NOTATION

$\mathbf{A}$ = $n_1 \times n_1$ matrix
A_R = area for heat transfer, sq.cm.
$\mathbf{b}$ = n_1 vector
$\mathbf{B}$ = $n_1 \times n_1$ matrix satisfying Equation (13)
c = concentration, g.-moles/cc.
C_p = specific heat, cal./(g.) (°K.)
E = expectation operator
E_A = activation energy divided by gas constant, °K.
E_0 = E_A/T_0
$\mathbf{f}$ = n_1 vector function
F = scalar integrand of the performance index
$\mathbf{g}$ = n vector function
$\mathbf{h}$ = m vector function
$\mathbf{H}$ = $m \times n_1$ matrix
J = performance index
$\mathbf{k}$ = n_2 vector of constant parameters
K = frequency factor in reaction rate constant, sec.$^{-1}$
L = $\gamma\Delta H/T_0$
m = dimension of system output vector
$\mathbf{M}$ = $m \times m$ weighting matrix in the nonlinear filter
n_1 = dimension of system state vector
n_2 = dimension of system parameter vector
$\mathbf{N}$ = $m \times m$ covariance matrix
p = dimension of control vector
$\mathbf{P}$ = $n \times n$ covariance matrix
q = flow rate, cc./sec.
$\mathbf{Q}$ = $n_1 \times n_1$ weighting matrix in performance index
r = scalar parameter in performance index
$\mathbf{S}$ = $n_1 \times p$ matrix function
t = time, sec.
T = temperature, °K.
$\mathbf{u}$ = p vector of controls
U = heat transfer coefficient, cal./(sq.cm.) (sec.) (°K.)
V = reactor volume, cc.
$V(t, \boldsymbol{\alpha})$ = optimal return functional
$\mathbf{w}$ = n_1 vector function
$\mathbf{x}$ = n_1 state vector
$\mathbf{y}$ = m output vector
$\mathbf{z}$ = n state vector

Greek Letters

$\boldsymbol{\alpha}$ = least-square state estimate (n_1 vector)
$\boldsymbol{\beta}$ = p vector switching function
γ = function in Equation (25)
$\boldsymbol{\eta}$ = m vector of random errors
θ = ln (VK/q)
$\boldsymbol{\lambda}$ = function governed by Equation (15)
$\boldsymbol{\mu}$ = least-square state estimate (n_1 vector)
ρ = density, g./cc.
σ = standard deviation
τ = time
ϕ = c^d/c_0
ψ = T^d/T_0
ΔH = heat of reaction, cal./g.-mole

Subscripts

0 = initial
* = lower bound

Superscripts

$\hat{}$ = estimated
* = upper bound
d = desired

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Unsteady State Behavior of Multicomponent Distillation Columns:

Part I: Simulation

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A very general form of the basic column equations is presented which allows a wide choice in the form of the specifications of variables required to define the column operation. Variable plate holdups, variable plate efficiencies, heat losses from the column, and finite time liquid flow dynamics are some of the specifications considered. The values of the implicit column variables during the unsteady state period are found by a method which is independent of the numerical procedure chosen to solve the differential equations. Computer runs with the Kutta-Merson method used to solve the differential equations were made for a column approaching steady state at total reflux. The effect of different variable specifications on this computer column are discussed.

The unsteady state behavior of distillation columns has been the subject of much study in the past decade. Complete literature reviews have been made by Archer and Rothfus (*1*), Williams (*23*), and Renfroe (*17*), among others. There is undoubtedly a great deal of industrial work which has not been published. The most complete studies in connection with binary distillation have been carried out by Huckaba and his co-workers (*10, 4*), who obtained good agreement between experimental work and digital computer simulation, and by Gerster and his coworkers (*2, 11*), who obtained good agreement between analogue simulation and experimental work. In both cases the computer work was tailored very closely to the specific system under consideration and involved many simplifying assumptions.

Work in multicomponent systems has been much less detailed and has not been subjected to experimental verification. Rosenbrock (*18, 19*) presented a general model of a distillation column and a numerical method of solving the differential equations. The computer solution was restricted by the assumption of constant molal overflows and holdups. Comparison of computed and experimental results for a complicated transient showed that plate temperature profiles had essentially the same shape. Mah, Michaelson, and Sargent (*12*) proposed a numerical solution method based on finding an exact solution of a linear approximation of the basic column differential equations. Meadows (*13*) simulated a multicomponent batch distillation on a digital computer. His program allowed him to test the effect of various assumptions by providing for the inclusion or exclusion of heat balances on each tray and a choice of constant volume or constant molal holdup on each tray. Peiser and Grover (*16*) reported the use of a very complete column model which included the effects of tray hydraulics and condenser and reboiler heat exchange dynamics. The model was applied to an actual column which was experiencing operating difficulty. The controlled response of the column to a step change in feed concentration of the light key component was computed. The various aspects of this response were used to design a control system for the column. The physical dimensions of the model were varied so as to give the desired controlled response. These changes were then made on the actual