Application of Modern Estimation and Identification Techniques to Chemical Processes

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This paper describes a new application of modern estimation theory to nonlinear chemical processes. A particularly convenient form of the extended Kalman estimator is presented and its applications are discussed. The method described may be used to compute nonmeasureable process states and system parameters in real time with an on-line process control computer. An application of the extended Kalman filter to a six-dimensional nonlinear well-stirred reactor is discussed in detail. The results clearly indicate the feasibility of on-line application of this technique. In some cases these computations could eliminate the requirement for an on-line analysis.

Estimation theory plays an important role in the application of modern control theory to industrial systems. In many industrial processing systems, the state variables are not measurable; in other cases the state variables are measurable but the accuracy is not sufficient for control purposes. Delays inherent in the measurement procedures used for some state variables often produce unwanted time delays within the control loops.

A chemical reactor is an example of an industrial process that contains all three of these measurement problems. Temperature signals which represent certain state variables often contain a great deal of noise, for example, drop-in thermocouples in the BOF process. The concentrations in intermediate chemical reactions that occur within the reactor are nonmeasurable. Measurements are often delayed in applications which use on-line chemical analyzers.

In modern control applications, a description of the physical processes is required. Often in the chemical processing industries, lack of an appropriate mathematical model of the process prevents effective control. Some of the difficulties associated with model building and parameter identification in multivariable systems may be overcome through the use of extended Kalman estimation (*1*). Since the complete nonlinear structure of the model is retained in this technique and a measure of the accuracy of the models is directly obtainable, estimation theory lends itself readily to development of models.

The extended Kalman estimation technique is well established and has been applied to many defense and aerospace systems (*2* to *4*). Recent applications in the electric power industry (*5*) and in supercritical shipboard boilers (*6*) and tubular reactors (*7*) indicate a trend toward process industry applications.

Section I presents a summary of the linear and extended Kalman equations. Section II develops sets of normalized estimation and identification equations for use with the extended Kalman filter. A characteristic set of reactor parameters and typical instrumentation system accuracy is selected. Reactor responses and simulated observations are also computed. The application and results are presented in Section III. A summary which includes the conclusions and recommendations for future study is presented in Section IV.

I. THE EXTENDED KALMAN FILTER

Linear Kalman Filter

The problem of finite-time optimal filtering and prediction for linear systems with nonstationary random noise was first solved by Kalman (*8*). Additional results for application of this technique to discrete time systems (*9, 10*) led to easy implementation on a digital computer.

The discrete Kalman filter equations specify an optimal estimate of the state of a linear, time-varying, dynamic system observed sequentially in the presence of additive white Gaussian noise. The estimate obtained at each time is the maximum likelihood estimate conditioned on all observations up to that time. This is equivalent to the least-squares estimate of the state, since disturbance noises are Gaussian. The vector difference equation

$$\mathbf{x}_{k+1} = \Phi_k \mathbf{x}_k + \Gamma_k \mathbf{w}_k \tag{1}$$

describes such a system where k denotes a particular in-

stant of time, Φ_k is the state transition matrix at $t = k\Delta t$, and Δt is the sampling interval. The components of $\mathbf{x}_k$ are the states of the system, and $\mathbf{w}_k$ is a zero-mean, white Gaussian noise process that may represent either actual input disturbances or inaccuracies in the system model. At each instant in time, observations represented by the vector $\mathbf{z}_k$ are obtained from the relation

$$\mathbf{z}_k = H_k \mathbf{x}_k + \mathbf{v}_k \tag{2}$$

where $\mathbf{v}_k$ is a zero-mean, white Gaussian noise process assumed to be independent of $\mathbf{w}_k$. The respective covariances of $\mathbf{w}_k$ and $\mathbf{v}_k$ are Q_k and R_k, and it is assumed that an a priori estimate $\hat{\mathbf{x}}_{0/-1}$ has been made with error covariance $P_{0/-1}$. Throughout this paper $\hat{\mathbf{x}}_{j/i}$ will denote the estimate of the state $\mathbf{x}$ at time j, given observations through time i. $P_{j/i}$ will denote the covariance of the error in this estimate. The linear Kalman filter determines the estimate of the state that minimizes the quantity J, as follows:

$$J = \frac{1}{2}(\mathbf{x}_k - \hat{\mathbf{x}}_{k/k})^T P_{k/k}^{-1}(\mathbf{x}_k - \hat{\mathbf{x}}_{k/k}) + \frac{1}{2}\sum_{j=0}^{k-1} \times \{(\mathbf{z}_{j+1} - H_{j+1}\hat{\mathbf{x}}_{j+1/j})^T R_{j+1}^{-1}(\mathbf{z}_{j+1} - H_{j+1}\hat{\mathbf{x}}_{j+1/j})\} \tag{3}$$

where $\mathbf{x}_k$ is the true state of the system at $t = k\Delta t$ obtained from Equation (1) with $\mathbf{w}_k = 0$, superscript T denotes transpose, and superscript -1 denotes matrix inversion.

The estimation equations may be written as a set of prediction and correction equations, as follows:

Prediction:

$$\hat{\mathbf{x}}_{k/k-1} = \Phi_{k-1}\hat{\mathbf{x}}_{k-1/k-1} \tag{4}$$

$$P_{k/k-1} = \Phi_{k-1} P_{k-1/k-1} \Phi_{k-1}^T + \Gamma_{k-1} Q_{k-1} \Gamma_{k-1}^T \tag{5}$$

These equations describe the behavior of the estimate and its covariance at time k based on observations through time $k-1$.

Correction:

$$\hat{\mathbf{x}}_{k/k} = \hat{\mathbf{x}}_{k/k-1} + W_k[\mathbf{z}_k - H_k\hat{\mathbf{x}}_{k/k-1}] \tag{6}$$

$$W_k = P_{k/k-1} H_k^T [H_k P_{k/k-1} H_k^T + R_k]^{-1} \tag{7}$$

$$P_{k/k} = [I - W_k H_k] P_{k/k-1} \tag{8}$$

which account for the observation z_k. The a priori estimate and error covariance are used as initial conditions for these recursive equations.

The Extended Kalman Filter

Suppose the system can be represented by the nonlinear difference equation

$$\mathbf{x}_{k+1} = \mathbf{f}_k(\mathbf{x}_k, \mathbf{u}_k) + \mathbf{w}_k \tag{9}$$

where $\mathbf{f}_k$ is a vector function of the state $\mathbf{x}_k$ and the controls $\mathbf{u}_k$. The observation equations are represented by the relation

$$\mathbf{z}_k = \mathbf{h}_k(\mathbf{x}_k) + \mathbf{v}_k \tag{10}$$

where $\mathbf{h}_k$ is also a vector function of the state variables. The noise vectors $\mathbf{w}_k$ and $\mathbf{v}_k$ have statistical properties similar to those in the linear system. The estimate of $\mathbf{x}_k$, given observations through time k, is denoted by $\hat{\mathbf{x}}_{k/k}$. The extended Kalman filter is represented by the following recursive equations:

Prediction:

$$\hat{\mathbf{x}}_{k/k-1} = \mathbf{f}_{k-1}(\hat{\mathbf{x}}_{k-1/k-1}, \mathbf{u}_{k-1}) \tag{11}$$

$$\hat{\mathbf{z}}_{k/k-1} = \mathbf{h}_k(\hat{\mathbf{x}}_{k/k-1}) \tag{12}$$

$$P_{k/k-1} = \Phi_{k-1} P_{k-1/k-1} \Phi_{k-1}^T + Q_{k-1} \tag{13}$$

Correction:

$$\hat{\mathbf{x}}_{k/k} = \hat{\mathbf{x}}_{k/k-1} + W_k(\mathbf{z}_k - \hat{\mathbf{z}}_{k/k-1}) \tag{14}$$

$$P_{k/k} = (I - W_k H_k) P_{k/k-1} \tag{15}$$

where

$$\Phi_{k-1} = (\mathbf{f}_{k-1})_{x_{k-1}} = \partial \mathbf{f}_{k-1}/\partial \mathbf{x}_{k-1} \,|\, _{\hat{\mathbf{x}}_{k-1/k-1}} \tag{16}$$

$$H_k = (\mathbf{h}_k)_{\hat{x}_{k/k}} = \partial \mathbf{h}_k/\partial \mathbf{x}_k |\, \hat{\mathbf{x}}_{k/k} \tag{17}$$

The a priori initial values for the recursive equations are

$$\hat{\mathbf{x}}_{0/-1} = E[\mathbf{x}_0] = \bar{\mathbf{x}}_0 \tag{18}$$

$$P_{0/-1} = E[(\mathbf{x}_0 - \bar{\mathbf{x}}_0)(\mathbf{x}_0 - \bar{\mathbf{x}}_0)^T] \tag{19}$$

where E denotes expected value operator and the overbar denotes the mean value.

In Equations (14) and (15) the value of the estimator gain W_k is determined by the filter performance criterion. For the performance criterion of Equation (3), an approximate estimator gain can be obtained from the set of equations linearized about the present estimate of the state (*1*). Under these conditions the approximate optimum* gain is

$$W_k = P_{k/k-1} H_k^T (H_k P_{k/k-1} H_k^T + R_k)^{-1} \tag{20}$$

Bias Problems

In the case where f_k and h_k are linear functions, it can be shown that $(\mathbf{x}_k - \hat{\mathbf{x}}_{k/k}) = \tilde{\mathbf{x}}_{k/k}$ is a Gaussian variable. Its expected value and covariance are therefore sufficient to describe its probability distribution. In fact

$$\bar{\tilde{\mathbf{x}}}_{k/k} = E[\tilde{\mathbf{x}}_{k/k}] = 0 \tag{21}$$

$$E[\tilde{\mathbf{x}}_{k/k} - \bar{\tilde{\mathbf{x}}}_{k/k})(\tilde{\mathbf{x}}_{k/k} - \bar{\tilde{\mathbf{x}}}_{k/k})^T] = P_{k/k} \tag{22}$$

where $P_{k/k}$ is as given in Equation (15).

When $\mathbf{f}_k$ and $\mathbf{h}_k$ are nonlinear functions, $\tilde{\mathbf{x}}_{k/k}$ is no longer Gaussian. In such cases it may be difficult to obtain a complete description of its probability distribution. However, the first two moments $E[\tilde{\mathbf{x}}_{k/k}]$ and $E[(\tilde{\mathbf{x}}_{k/k} - \bar{\tilde{\mathbf{x}}}_{k/k}) \times (\tilde{\mathbf{x}}_{k/k} - \bar{\tilde{\mathbf{x}}}_{k/k})^T]$ give a good representation of the distribution. These moments are easily approximated. Derivations of the first and second moments are found in the work of Athans (*1*). It was shown that the error covariance equations in the nonlinear case are identical to those in the linear system, but that the expected values are not zero. If these nonzero bias terms are subtracted from Equation (14), the result is a zero-bias nonlinear estimator of second order.

Significance of Filter Parameters

In the specification of the complete extended Kalman estimator, the designer has many options for control of its dynamic response. The initial state estimate and the initial covariance, $\hat{\mathbf{x}}_{0/-1}$ and $P_{0/-1}$, respectively, determine the basic speed of response of the filter. The magnitude of the initial state error $(\mathbf{x}_0 - \hat{\mathbf{x}}_{0/-1})$, will cause an initial error in the covariance matrices which results in an initial error in the weighting gain W_k. The initial error increases the time required for the filter to reach its steady state. Similarly, if $P_{0/-1}$ is large, the weighting gain W_k will initially be large. This also increases the time to reach steady state, since the filter will initially rely on current noisy observations.

*The gain in Equation (20) yields a minimum variance estimator, or a maximum likelihood estimator for the linearized version of Equations (9) and (10) under the stated assumptions on the noises v and w.

From Equation (20) it can be seen that the weighting matrix determines the response characteristics of the filter. For large weighting gains, the filter relies on current observations. The filter tends to use past information to determine the state estimate when the weighting is small. This observation can be used to adjust the filter response for systems that contain uncertainty, w_k. The Q_k matrix, for example, is large for systems that have dynamics that are not well understood. This has the effect of "loosening" the filter, that is, the steady state error is increased. The observation noise covariance R_k has an opposite effect. Consequently, the filter tends to disregard measurements that contain large errors since the weighting gain W_k is reduced for an increase in R_k.

Many practical methods for tuning the Kalman filter have been suggested; however, no analytical method for selecting these parameters has yet been obtained. The work of Mehra (*11*) on the adaptive Kalman filter introduces concepts which may lead to analytical tuning methods.

II. MODERN ESTIMATION APPLIED TO THE NONLINEAR WELL-STIRRED REACTOR

The well-stirred reactor has been studied extensively by many authors. The work of Kalman (*12*) on the application of dynamic programming is probably the first application of modern control theory to a chemical reactor. Subsequently, many authors have studied control of reactors of this type, most notably the work of Aris (*13*). However, in both Kalman and Aris, the system was assumed to be measurable and the dynamics known with zero error.

Limitations of the Extended Kalman Theory

The application of the extended Kalman technique is limited to processes described by relations of the form

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{p}, \mathbf{u}, t) \tag{23}$$

where $\mathbf{x}$, $\mathbf{p}$, $\mathbf{u}$, and t represent the state, parameters, controls, and time, respectively. Most transport phenomena (heat, mass, and momentum) can be represented by lumped-parameter equations of this type. Consequently, the extended Kalman technique has important application in industrial chemical processes.

Derivation of Equations

Consider the adiabatic stirred-reactor problem. A schematic diagram of a physical model of the system is in Figure 1. Suppose that two substances A and B enter the reactor at a flow rate F and temperature T_i. Suppose also that an irreversible exothermic reaction

$$2A \xrightarrow{K} B \tag{24}$$

occurs in the reactor. Assume that the reactor wall has sufficient mass to influence the dynamics of the system. Also assume that the reactor cooler behaves as a perfectly mixed heat sink. Three energy balances and one mass balance define a mathematical model of this system:

Energy balance on reactor contents:

$$\rho V C_p \frac{dT}{dt} = \rho F C_p (T_i - T) + \Delta H \cdot K \cdot V e^{-E/RT} C_A^2 - hA (T - T_w) \tag{25}$$

Energy balance on wall:

$$\rho_w V_w C_{pw} \frac{dT_w}{dt} = hA (T - T_w) - h_w A_w (T_w - T_c) \tag{26}$$

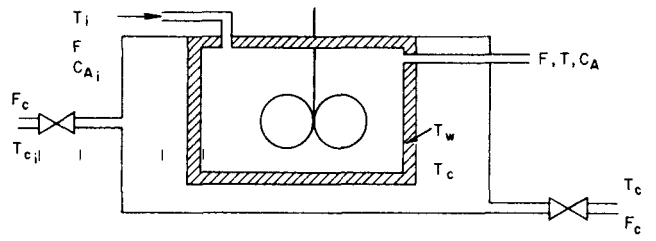

Fig. 1. Physical model of stirred reactor.

Energy balance on cooler:

$$\rho_c V_c C_{pc} \frac{dT_c}{dt} = \rho_c F_c C_{pc} (T_{c_i} - T_c) + h_w A_w (T_w - T_c) \tag{27}$$

Mass balance on reactor contents:

$$V \frac{dC_A}{dt} = F (C_{A_i} - C_A) - K V e^{-E/RT} C_A^2 \tag{28}$$

1. Normalized Estimation Equations. It is convenient to normalize Equations (25) to (28) about an operating point in the temperature-concentration plane T_s, C_s. Note that this operating point is not necessarily an equilibrium point. Let the normalized state variables be defined by the relations

$$x_1 = \frac{T - T_s}{T_s}, \quad x_2 = \frac{T_w - T_s}{T_s}, \quad x_3 = \frac{T_c - T_s}{T_s}$$

$$x_4 = \frac{C_A - C_s}{C_s}, \quad u_1 = \frac{T_i - T_s}{T_s}, \quad u_2 = \frac{T_{c_i} - T_s}{T_s}$$

$$u_3 = \frac{C_{A_i} - C_s}{C_s} \tag{29}$$

The normalized equations may be determined by substitution of Equation (29) into Equations (25) to (28). The resulting equations are

$$\dot{x}_1 = -(c_1 + c_4) x_1 + c_3 (1 + x_4)^2 \exp [K_1 x_1/(1 + x_1)] + c_4 x_2 + c_1 u_1 \tag{30}$$

$$\dot{x}_2 = -(c_9 + c_6) x_2 + c_5 x_1 + c_6 x_3 \tag{31}$$

$$\dot{x}_3 = -(c_7 + c_8) x_3 + c_8 x_2 + c_7 u_2 \tag{32}$$

$$\dot{x}_4 = -c_1 x_4 - c_2 (1 + x_4)^2 \exp [K_1 x_1/(1 + x_1)] + c_1 u_3 \tag{33}$$

where $\dot{x}_i$, $i = 1, \ldots, 4$ represents the derivative with respect to $\tau (\beta t = \tau)$.

Normalized Identification Equations. In the development of identification equations for chemical processes, the implicit functional relations between parameters must be considered. This functional dependence is best shown by example. Consider the energy balance on the reactor contents, Equation (25), in the form

$$\frac{dT}{dt} = \frac{F}{V} (T_i - T) + \frac{\Delta H K e^{-E/RT}}{\rho C_p} C_A^2 - \frac{hA}{\rho V C_p} (T - T_w) \tag{34}$$

Let

$$x_5 = \frac{\Delta H K e^{-E/RT}}{\rho C_p} \tag{35}$$

then

$$\frac{dx_5}{dT} = \frac{E\ \Delta H\ K\ e^{-E/RT}}{RT^2\ \rho C_p} \tag{36}$$

By the chain rule

$$\frac{dx_5}{dt} = \frac{E\ \Delta H\ K\ e^{-E/RT}}{RT^2\ \rho C_p}\ \frac{dT}{dt} = \frac{E}{RT^2}\ x_5\ \frac{dT}{dt} \tag{37}$$

Similarly for the reactor mass balance, let

$$x_6 = K\ e^{-E/RT} \tag{38}$$

then

$$\frac{dx_6}{dt} = \frac{E}{RT^2}\ x_6\ \frac{dT}{dt} \tag{39}$$

Notice that the states x_5 and x_6 contain several quantities which are usually not known accurately. The Arrhenius constant K and the activation energy E are least known in reactor design. Also, the heat of reaction ΔH is often not known precisely. For these reasons the additional state variables x_5 and x_6 may be used to determine K and ΔH directly.

The relations defined in Equations (29) may be used to renormalize the set of Equations (25) to (28), (37), and (39), which form the augmented state space. The resulting normalized equations are

$$\frac{dx_1}{d\tau} = c_1(u_1 - x_1) + x_5\ \frac{C_s^2}{\beta T_s}\ (1 + x_4)^2 - c_4(x_1 - x_2) \tag{40}$$

$$\frac{dx_2}{d\tau} = c_5\ (x_1 - x_2) - c_6\ (x_2 - x_3) \tag{41}$$

$$\frac{dx_3}{d\tau} = c_7\ (u_2 - x_3) + c_8\ (x_2 - x_3) \tag{42}$$

$$\frac{dx_4}{d\tau} = c_1\ (u_3 - x_4) - \frac{C_s}{\beta}\ x_6\ (1 + x_4)^2 \tag{43}$$

$$\frac{dx_5}{d\tau} = \frac{K_1\ x_5}{(1 + x_1)^2}\ \frac{dx_1}{d\tau} \tag{44}$$

$$\frac{dx_6}{d\tau} = \frac{K_1\ x_6}{(1 + x_1)^2}\ \frac{dx_1}{d\tau} \tag{45}$$

The above six equations describe the state of the normalized chemical reactor if the variables x_5 and x_6 are to be estimated by the extended Kalman filter.

These equations may be written in vector notation in the form

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \tag{46}$$

In regulatory systems the objective is to maintain the state at a specified value. In this example the desired state is (T_s, C_s). The controls required to maintain this condition at steady state may be found by setting to zero the left-hand sides of Equations (30) to (33) and Equations (40) to (45). The resulting controls for both the estimation and the identification equations are

$$\begin{aligned} u_1 &= -c_3/c_1 \\ u_2 &= 0 \\ u_3 &= c_2/c_1 \end{aligned} \tag{47}$$

Substituting these values into the two sets of equations yields

Estimation:

$$\begin{aligned} \dot{x}_1 &= -(c_1 + c_4)\,x_1 + c_3(1 + x_4)^2 \exp\left[\frac{K_1 x_1}{1 + x_1}\right] + c_4 x_2 - c_3 \\ \dot{x}_2 &= -(c_5 + c_6)\,x_2 + c_5 x_1 + c_6 x_3 \\ \dot{x}_3 &= -(c_7 + c_8)\,x_3 + c_8 x_2 \\ \dot{x}_4 &= -c_1 x_4 - c_2\,(1 + x_4)^2 \exp\left[\frac{K_1 x_1}{1 + x_1}\right] + c_2 \end{aligned} \tag{48}$$

Identification:

$$\begin{aligned} \dot{x}_1 &= -c_1 x_1 + x_5\ \frac{C_s^2}{\beta T_s}\ (1 + x_4)^2 - c_4(x_1 - x_2) - c_3 \\ \dot{x}_2 &= c_5\ (x_1 - x_2) - c_6(x_2 - x_3) \\ \dot{x}_3 &= -(c_7 + c_8)\,x_3 + c_8 x_2 \\ \dot{x}_4 &= -c_1 x_4 - \frac{C_s}{\beta}\ x_6(1 + x_4)^2 + c_2 \\ \dot{x}_5 &= K_1\ \frac{x_5}{(1 + x_1)^2}\ \dot{x}_1 \\ \dot{x}_6 &= K_1\ \frac{x_6}{(1 + x_1)^2}\ \dot{x}_1 \end{aligned} \tag{49}$$

Measurement Equations. In this example only temperature signals are assumed to be measurable, and the measurements are assumed to contain random noise. The measurement equations can be written as

$$z_i(\tau) = x_i(\tau) + v_i(\tau) \quad i = 1, 2, 3 \tag{50}$$

where the v_i are independent, zero-mean, white Gaussian random processes and are uncorrelated in the τ domain.

In vector matrix form these equations are given by

$$z = Hx + v \tag{51}$$

where, in the case of identification equations,

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \tag{52}$$

Calculation of the Jacobian Matrix

Estimation Equations. The Jacobian matrix for Equations (47) and (48) may be obtained by computing the partial derivatives of the state equations. The resulting φ matrix is summarized below

$$\varphi = \begin{bmatrix} f_{11} & f_{12} & 0 & f_{14} \\ f_{21} & f_{22} & f_{23} & 0 \\ 0 & f_{32} & f_{33} & 0 \\ f_{41} & 0 & 0 & f_{44} \end{bmatrix}$$

where

$$\begin{aligned} f_{11} &= -(c_1 + c_4) + c_3\ B^2\ K_1 DE \\ f_{12} &= c_4;\quad f_{14} = 2c_3\ BE;\quad f_{21} = c_5 \\ f_{22} &= -(c_5 + c_6);\quad f_{23} = c_6;\quad f_{32} = c_8 \\ f_{33} &= -(c_7 + c_8);\quad f_{41} = -c_2 B^2 K_1 DE \\ f_{44} &= -c_1 - 2c_2\ EB \end{aligned} \tag{54}$$

and

$$\begin{aligned} B &= (1 + x_4);\quad E = \exp\,(K_1 x_1/1 + x_1) \\ D &= (1 + x_1)^{-2} \end{aligned} \tag{55}$$

Identification Equations. The Jacobian matrix for the identification equations, Equation (49), is obtained in a manner similar to that above. The results are

$$\varphi = \begin{bmatrix} f_{11} & f_{12} & 0 & f_{14} & f_{15} & 0 \\ f_{21} & f_{22} & f_{23} & 0 & 0 & 0 \\ 0 & f_{32} & f_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & f_{44} & 0 & f_{46} \\ f_{51} & f_{52} & 0 & f_{54} & f_{55} & 0 \\ f_{61} & f_{62} & 0 & f_{64} & f_{65} & f_{66} \end{bmatrix} \tag{56}$$

where

$$c_9 = \frac{C_S^2}{\beta T_S}$$

$$f_{11} = -(c_1 + c_4);\quad f_{12} = c_4;\quad f_{14} = 2x_5\, c_9(1 + x_4)$$

$$f_{15} = c_9(1 + x_4)^2$$

$$f_{21} = c_5;\quad f_{22} = -(c_5 + c_6);\quad f_{23} = c_6$$

$$f_{32} = c_8;\quad f_{33} = -(c_7 + c_8);$$

$$f_{44} = -c_1 - 2\frac{C_S}{\beta} x_6(1 + x_4)$$

$$f_{46} = -\frac{C_S}{\beta}(1 + x_4)^2;\quad f_{51} = K_1 x_5 \left\{ \frac{f_{11}}{(1 + x_1)^2} - \frac{2\dot{x}_1}{(1 + x_1)^3} \right\}$$

$$f_{52} = \frac{K_1 x_5}{(1 + x_4)^2} f_{12};\quad f_{54} = \frac{K_1 x_5}{(1 + x_1)^2} f_{14}; \tag{57}$$

$$f_{55} = \frac{K_1}{(1 + x_1)^2}\dot{x}_1 + f_{15};$$

$$f_{61} = \frac{K_1 x_6}{(1 + x_1)^2} \left\{ f_{11} - \frac{2\dot{x}_1}{(1 + x_1)} \right\}$$

$$f_{62} = \frac{K_1 x_6}{(1 + x_1)^2} f_{12};\quad f_{64} = \frac{K_1 x_6}{(1 + x_1)^2} f_{14}$$

$$f_{65} = \frac{K_1 x_6}{(1 + x_1)^2} f_{15};\quad f_{66} = \frac{K_1 \dot{x}_1}{(1 + x_1)^2}$$

These relations can be used directly in the covariance equations for the estimation and identification of the states of the chemical reactor.

Process Parameters

Reactor System. In order to evaluate the performance of the extended Kalman estimator applied to chemical processes, parameters c_1 to c_8 must be selected to match the response of typical reactors. Assume that the reactor holdup time is 20 min. Then with $\beta = 1/240$, the resulting normalized time constant is 5 sec., and $c_1 = 0.2$. Selection of $c_2 = 0.2$ and $c_3 = 1.0$ implies that the rate of mass reduction of A is approximately one-fifth the rate of heat generation. Let $c_4 = c_5 = c_6 = c_8 = 0.5$, which implies that all heat transfer rates are equal. If the dynamic response of the cooling jacket is four times slower than the reactor holdup time, c_7 must be 0.05. Use of these constants in Equations (47) and (48) produces typical responses found in chemical reactors.

Instrumentation System. For this model the standard deviation of the instruments is assumed to be 10% of the nominal values. For an unnormalized thermocouple range of ±10°F., the normalized standard deviation is 2°F.

Reactor Response

Assume that the reactor is initially at a controlled steady state. Suppose a plant disturbance of 10% in the feed concentration occurs at the initial time. Figure 2 shows the simulated response without instrument noise. The details of how these curves were obtained are discussed in the following sections.

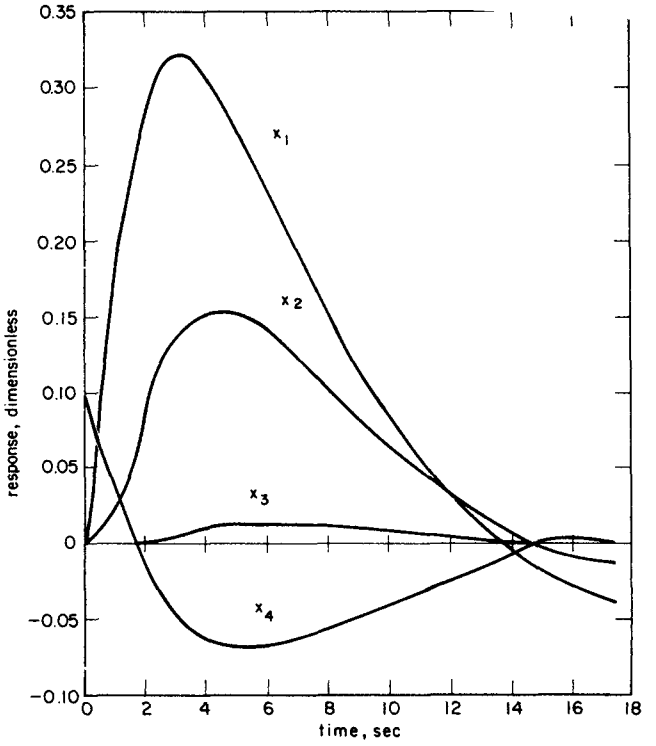

Fig. 2. Rypical reactor response.

Notice that the peak temperature response is nearly four times that of the concentration upset. The wall and cooler responses are not as sensitive to upsets in concentration due to their relatively slow dynamic response. This response will be used as a basis of comparison for the evaluation of the performance of the filter.

Observations

Typical observations of this system are shown in Figure 3. Note that the standard deviations of all temperature

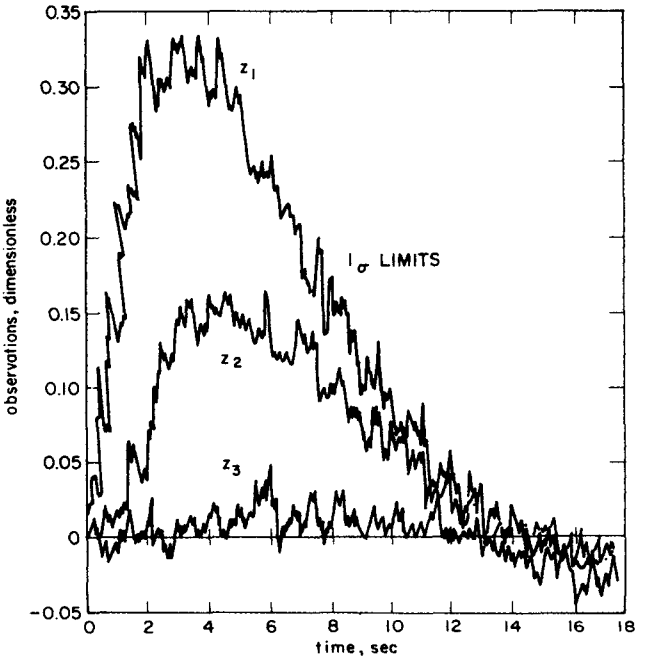

Fig. 3. Simulated observations.

variables is 0.10 in the normalized space. The responses shown in Figure 3 simulate the behavior of observed variables in typical chemical processing systems.

III. APPLICATION AND RESULTS

Computational Method

The information flow in a computer-controlled system is represented in Figure 4. The dashed line represents the interface between the computer and the process. The state estimator receives process observations $\mathbf{z}$, and produces optimal estimates of the state variables $\hat{\mathbf{x}}$ and their error covariance. These estimates are then used to compute the control $\hat{\mathbf{u}}$ required to maximize the performance, J, of the overall control system. Note that this criterion differs from that of Equation (3).

In order to simulate the behavior of the extended Kalman estimator applied to a real process, the model developed in Section II was used to represent a chemical processing system. The process equations given by Equation (48) for concentration estimation, and Equation (49) for process identification, may be written in the form

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{w} \tag{58}$$

where $\mathbf{w}$ is a fictitious, zero-mean, Gaussian white-noise vector. The vector $\mathbf{w}$ is used to account for uncertainty in the process model. To obtain a discrete version of the process equations for use in the estimator, the Euler integration method is utilized:

$$\frac{\mathbf{x}_{k+1} - \mathbf{x}_k}{\Delta} = \mathbf{f}(\mathbf{x}_k) + \mathbf{w}_k \tag{59}$$

or

$$\mathbf{x}_{k+1} = \mathbf{f}'(\mathbf{x}_k) + \mathbf{w}_k \tag{60}$$

where

$$\mathbf{f}'(\mathbf{x}_k) = \mathbf{x}_k + \Delta\mathbf{f}(\mathbf{x}_k) \tag{61}$$

and Δ denotes the sampling interval. The Jacobian of $\mathbf{f}'(\mathbf{x}_k)$ becomes $I + \Delta\varphi$. Note that for large Δ, the above integration method will generate significant error. In this case, the vector $\mathbf{w}_k$ represents the integration error.

The discrete observation equations to be used in the filter are given by

$$\mathbf{z}_k = H\,\mathbf{x}_k + \mathbf{v}_k \tag{62}$$

with H defined by Equation (52).

The discrete system and measurement equations corresponding to Equations (9) and (10) in Section I are given by Equations (60) and (61). The extended Kalman estimator is then completely specified by Equations (11) to (20) in Section I.

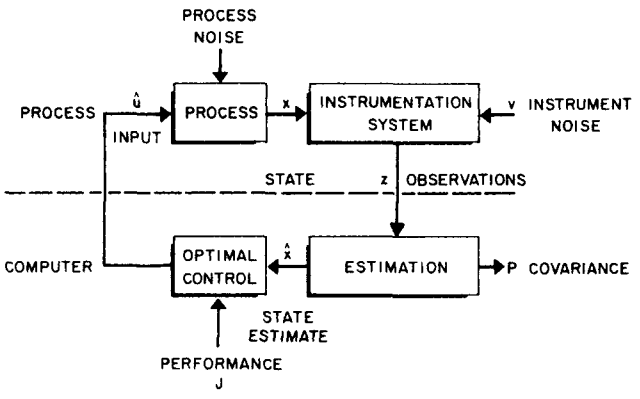

Fig. 4. Information flow in a physical system.

Implementation

Generation of True Trajectory. The Euler integration method was used to obtain typical responses shown in Figure 2. In order to obtain a suitable basis for comparing results, the discrete process equations (60) were integrated without additive noise and with small sampling intervals ($\Delta = 0.001$ sec.) for increased precision. These results were then used as the "true" solution of the reactor equations.

Computer-generated random noise was subsequently added to the observable states of the "true solution." This trajectory then simulated the "real process," and typical observations are shown in Figure 3.

Computation of Extended Kalman Estimate. The extended Kalman filter was operated at a rate of once every 0.5 sec.; in real time this corresponds to once every 30 sec. The input data in the estimator consisted of the simulated process data and the initial conditions on the estimator. The process equations used in the estimator are given by Equation (60) with $\Delta = 0.5$. Note that these are not the same equations as those used to simulate the "real process." Clearly the system equations used in the Kalman filter are *not* the same as those used in the simulation. The model does not have to be exact. This important fact is often overlooked in the use of the extended Kalman filter. An exact description of the dynamics of the process is not required to achieve good results, since the uncertainty in the process model can be included in the filter by the judicious choice of the Q_k matrix.

Typical computer run times were 1.8 msec. per iteration on a Univac 1108 coded in Fortran V. Approximate storage requirement for real-time application is 800 floating-point words. Since no attempt was made to streamline the computer code, refinement is possible.

Tuning of Estimator

To operate the Kalman estimator, the values of Q_k, R_k, $\hat{\mathbf{x}}_{0/-1}$, and $P_{0/-1}$ must be selected. R_k may be accurately represented by a diagonal matrix with the variances of the advertised or measured instrument error on the diagonal. This is generally found to be a good approximation to the true value of R_k, since errors in different sensors are usually not correlated. For this study, R_k was assumed constant, given by

$$R_k = \begin{bmatrix} 0.01 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.01 \end{bmatrix} \tag{63}$$

Note that a varying R_k presents no difficulty in implementation of this method. An example of a time-varying measurement covariance is the bomb thermocouple in the BOF.

The initial estimated error in the state estimate was arbitrarily set at zero for all runs, that is, $\hat{\mathbf{x}}_{0/-1} = \underline{0}$. The values for $P_{0/-1}$ and Q_k are more difficult to determine. The value of $P_{0/-1}$ determines the basic response time for the filter, and the value of Q_k determines the steady state estimation error. It is not difficult, however, to determine these parameters for most systems.

Results

Estimation Without Identification. In the estimation example, the principal requirement of the estimator is to compute the optimal estimate of the concentration of component A in the reactor.

The initial covariance is given by

$$P_{0/-1} = \begin{bmatrix} 1\times10^{-2} & 0 & 0 & 0 \\ 0 & 1\times10^{-2} & 0 & 0 \\ 0 & 0 & 1\times10^{-2} & 0 \\ 0 & 0 & 0 & 1\times10^{-2} \end{bmatrix} \quad (64)$$

with plant noise covariance of

$$Q_k = \begin{bmatrix} 1\times10^{-4} & 0 & 0 & 0 \\ 0 & 1\times10^{-4} & 0 & 0 \\ 0 & 0 & 1\times10^{-4} & 0 \\ 0 & 0 & 0 & 1\times10^{-4} \end{bmatrix} \quad (65)$$

A typical result is shown in Figure 5.

Note that the estimates $\hat{x}_1$, $\hat{x}_2$, and $\hat{x}_3$ approximate the true states almost immediately; however, the estimate $\hat{x}_4$ requires several samples to track the true state. This is simply because the actual error between the initial state and the estimated initial state is zero for x_1, x_2, and x_3 and 0.1 for x_4. Thus there is no transient for the first three states and a large transient for the x_4 state variable. The overshoot at the peaks of each of the states is due to integration error. Overshoot would be reduced by more sophisticated integration routines.

The oscillation error toward the end of the trajectories is due to the instrument noise **v**.

Estimation and Identification. The identification equations, Equation (49), and their Jacobian matrix, Equation (56), could be programmed and executed in a manner similar to that above. Note, however, that the computer program used for estimation can also be used for identification with very little modification. This can be accomplished by reformulating the identification problem with deviations from nominal values of the unknown parameters as the additional state variable. These deviations can be written as

$$c_3 = c_3^\circ + \delta c_3 \quad (66)$$

and

$$c_2 = c_2^\circ + \delta c_2 \quad (67)$$

where c_1° and c_2° are the prior estimates of these constants.

The additional state equations become

$$\dot{x}_5 = \delta\dot{c}_3 = \frac{d}{d\tau}(\delta c_3) = 0 \quad (68)$$

$$\dot{x}_6 = \delta\dot{c}_2 = \frac{d}{d\tau}(\delta c_2) = 0 \quad (69)$$

A 5% change in c_2 and c_3 was introduced in the filter equations to simulate parameter identification. The "true" system remained the same as in Figure 2, so that $\hat{x}_5$ and $\hat{x}_6$ should be zero with perfect identifications.

For the example run

$$P_{0/-1} = \begin{bmatrix} 0.1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0025 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0025 \end{bmatrix} \quad (70)$$

and

$$Q = \begin{bmatrix} 1\times10^{-3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1\times10^{-3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1\times10^{-3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.5\times10^{-3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.5\times10^{-3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.5\times10^{-3} \end{bmatrix} \quad (71)$$

The results for this example are shown in Figure 6. Notice the increase in sensitivity to integration error

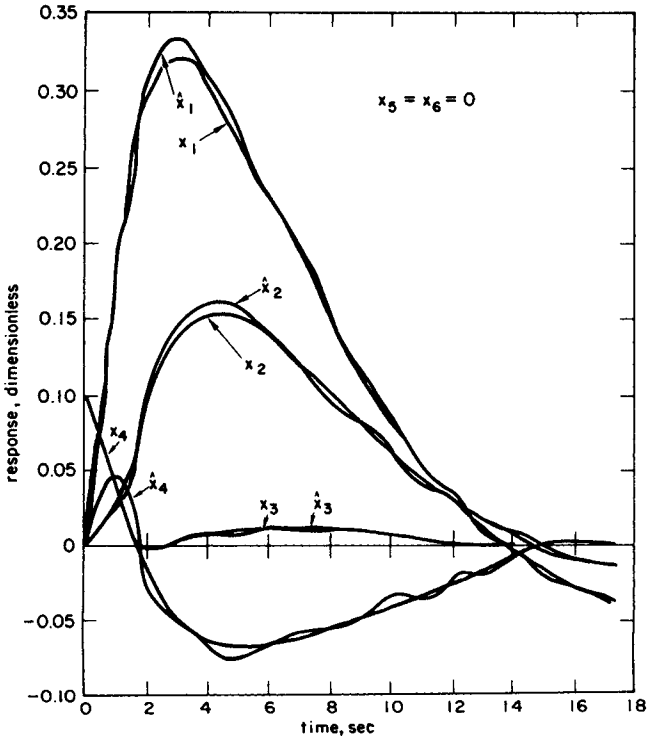

Fig. 5. Estimation without identification.

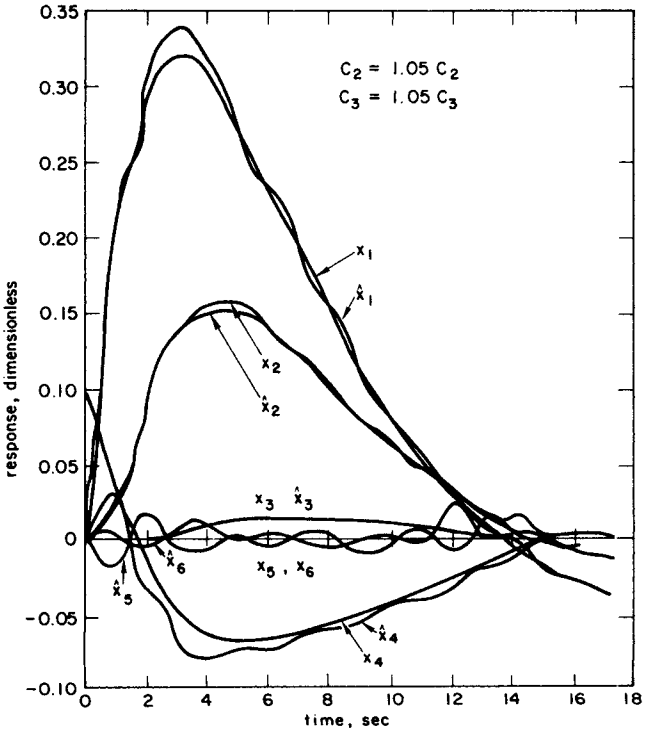

Fig. 6. Estimation with identification.

(larger reactor-temperature overshoot). This is due to the fact that the filter is much more sensitive to plant noise or uncertainty when estimating so many states with so few observables. The estimates for x_5 and x_6 are, however, very good, considering the fact that the filter equations contain a programmed 5% parameter variation.

SUMMARY

Conclusions

The results of the above examples clearly indicate the feasibility of applying the extended Kalman filter to industrial processes. The computer program for the six-dimensional filter requires approximately 800 words. With only three observables, the inversion was performed using Cramer's rule. Since sample times of industrial processes are often on the order of 0.5 to 5 min. and since approximately 1.8 msec. is required to process each observation, computer processing speed is more than adequate even with present-day control computers.

Other Applications

The following two additional applications are prime candidates for immediate application in the processing industry.

Model Development. Often in the development of a process model, complexity is added incrementally. The major problem is how to determine when the model fits observed data. The Kalman method provides a convenient framework for comparing models of varying complexity with observed plant data.

Prediction of Equilibrium State. Extended Kalman estimation can be derived with the estimator output as the predicted steady state. This prediction can then be used as input to steady state optimization techniques which determine optimum process set points.

Recommendations for Future Study

Precomputation of W_k. In certain applications the process disturbances may be similar enough to warrant precomputation of the weighting matrix W_k. This would eliminate computation of the covariance equations and hence considerably reduce processing requirements.

Better Integration Methods. In the estimator, Euler integration is used to represent the process equations. Clearly more complex integration routines could be used in certain regions of the state space.

Bias Elimination. Further work should be performed to predict the effects of the bias term, and when it should be included in the filter.

Better Tuning Techniques. The work of Mehra (*11*) is only an initial attempt to compute tuning parameters analytically. Further work in developing methods for tuning the extended Kalman filter should be performed.

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NOTATION

A = reactor wall surface area, sq. ft.
A_w = wall cooler surface area, sq. ft.
C_A = weight concentration A in reactor, lb./cu. ft.
C_{A_i} = inlet concentration of A, lb./cu. ft.
C_p = average heat capacity of reactor contents, B.t.u./(lb.)(°R.)
C_{pc} = average coolant heat capacity, B.t.u./(lb.)(°R.)
C_{pw} = average heat capacity of wall, B.t.u./(lb.)(°R.)
c_1 = constant = $F/V\beta$
c_2 = constant = $K/\beta\, C_s \exp(-E/RT_s)$
c_3 = constant = $(\Delta H\, K\, e^{-K_1} C_s^2)/\rho\, C_p\, \beta\, T_s)$
c_4 = constant = $hA/(\rho V\, C_p\, \beta)$
c_5 = constant = $hA/(\rho_w\, V_w\, C_{pw}\, \beta)$
c_6 = constant = $(h_w A_w)/(C_{pw}\, \rho_w V_w\, \beta)$
c_7 = constant = $F_c/(V_c\, \beta)$
c_8 = constant = $(h_w A_w)/(\rho_c V_c\, C_{pc}\, \beta)$
c_9 = constant = $C_s^2/(\beta\, T_s)$
E = activation energy, atm./cu. ft.
F = volumetric flow rate through reactor, cu. ft./sec.
F_c = volumetric flow rate through cooler, cu. ft./sec.
ΔH = heat of reaction, B.t.u./lb.
h = film coefficient in reactor, B.t.u./(sq. ft.)(°F.)(sec.)
h_w = film coefficient between wall and cooler, B.t.u./(sq. ft.) (°F.) (sec.)
K = Arrhenius rate constant, lb./sec.
K_1 = constant = E/RT_s
R = gas constant, (atm.) (cu. ft.)/°R.
T = reactor temperature, °R.
T_c = cooler temperature, °R.
T_i = inlet stream temperature, °R.
T_w = wall temperature, °R.
t = time, min.
V = volume of reactor, cu. ft.
V_c = volume of cooler, cu. ft.
V_w = volume of wall, cut. ft.

Greek Letters

β = time scale factor ($\beta t = \tau$)
ρ = average density of reactor contents, lb./cu. ft.
ρ_w = average density of wall, lb. cu. ft.
ρ_c = average density of coolant, lb./cu. ft.

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