NOTATION

a_p = particle surface area, m^2
C_D = drag coefficient
d_o = nozzle diameter, m
d_p = particle diameter, m
h = heat transfer coefficient, $W/cm^2 \cdot K$
m = particle mass, kg
Nu = Nusselt number, $hd_p/\bar{k}$
Q = net heat flow to the particle, Eq. 7, W
r = distance in the radial direction, mm
Re = Reynolds number $[\bar{\rho}_f|U_{Pz} - U_f|d_p/\bar{\mu}_f]$
t = time, s
T_a = ambient temperature, K
T_f = field temperature
T_p = particle temperature, K
U_f = axial fluid velocity, m/s
U_{Pz} = axial particle velocity, m/s
v_{Pl} = radial particle injection velocity, m/s
x = mass fraction of the particle in the liquid state
z = distance in the axial direction, mm
σ_g = geometric standard deviation of the powder size
ρ_f = fluid density, kg/m^3
ρ_p = particle density, kg/m^3
μ_f = fluid viscosity, kg/m·s
ϵ = particle emissivity
σ = Stefan-Boltzman constant
λ_m = laten heat of fusion, J/kg
λ_v = laten heat of vaporization, J/kg

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Fault Diagnosis in Nonlinear Chemical Processes

Part I. Theory

We propose a two-level identification strategy to detect and diagnose process faults and their causes. The strategy can be applied to processes represented by process models nonlinear in the states but linear in the coefficients. Relations to calculate both the observer for the states and the least squares estimator for the coefficients are specified in detail.

K. WATANABE and D. M. HIMMELBLAU

Department of Chemical Engineering, The University of Texas, Austin, TX 78712

SCOPE

A two-level strategy for the detection and diagnosis of faults in industrial processes is presented. By fault is meant degradation in process performance; by diagnosis is meant identification of the cause(s) of the fault. Faults can be related quantitatively to elements in process models including both the states and the parameters. Detection of a change and the isolation of the reasons for the change in the process parameters are problems of both theoretical and practical interest in the process industries.

Previous work has focused on the use of simultaneous estimation of the model states and parameters or hierarchical

K. Watanabe is on leave from Hosei University at Koganei, Tokyo, Japan.

identification. Another branch of work has made use of the extended Kalman filter. All of these strategies have been accompanied by evidence via simulation that they are satisfactory. Yet, *convergence to correct estimates* of both states and parameters is not guaranteed, and both biased and imprecise estimates have been demonstrated to occur rendering the strategies useless for fault detection (although perhaps adequate for process control purposes).

The proposed strategy involves state estimation by a Luenberger observer in the presence of faults followed by parameter identification via a least squares procedure. We do not use linearized models because a nonlinearity in a process influences the value of the estimated states and parameters, and can lead to confusion as to whether the values calculated really represent faults or simply represent the effect of excursions in states beyond the valid region for linearization. We do make use of the ordinary time record of the process responses rather than introduce an external disturbance into one or more of the process inputs.

CONCLUSIONS AND SIGNIFICANCE

For fault detection and diagnosis, the state estimation and parameter identification must have the capability of: (a) retrieving the proper states and parameters in a process model in the presence of faults as well as noise; (b) being applicable to nonlinear processes; and (c) being executed on-line with digital computers so that the code to implement the strategy must facilitate fast computation times and minimum core memory. We have developed a straightforward design procedure for a two-level strategy to meet these three criteria.

The strategy represents an improvement over existing work in so far as it is less likely to lead to biased estimates of process model parameters, and hence less likely to mislead the analyst in diagnosing the causes of faults. It does have the characteristic of having a higher variance than an extended Kalman filter. The two-level strategy can be applied to the ordinary time record of a wide variety of processes including those with general reactions.

1. INTRODUCTION

From the standpoint of safety, energy conservation, and efficiency in the operation of processes, the diagnosis of process faults has great significance and has been investigated from many aspects. Process faults, i.e., changes in process characteristics that degrade process performance, can be detected by three mechanisms (Willsky, 1976): *alarm* (the binary decision either that something has gone wrong or that everything is satisfactory); *isolation* (determination of the source of the faulty performance); and *estimation* (determination of the extent of the fault).

An alarm decision can be made, for example, by examining the residual values between the outputs measured by instruments and the output generated by a state estimation filter designed for normal operation. If the residuals are zero or close to zero, the process is normal; otherwise, it is abnormal. In line with this idea, Beard (1971) and Jones (1973) applied a state estimation filter to make alarm decisions. Subsequently, using a Kalman filter, Willsky et al. (1975) and Willsky and Jones (1976) dealt with the detection of a jump in the states. Gai and Curry (1976) and Chien and Adams (1976) described how to detect step and ramp changes in the process states.

Isolation and estimation of process faults are possible under some circumstances by solely estimating the process states under conditions in which process performance degrades. Such faults can be identified by noting those states that exceed some prespecified threshold; if the states are estimated correctly under faulty conditions, the values of the state vector may assist in detecting the cause of the faults.

For more general applications of fault detection and diagnosis, both the states and parameters should be estimated (not necessarily simultaneously). In general, simultaneous estimation of both the states and the parameters involves the solution of difficult nonlinear problems (Rajbman and Shinha, 1977). Formulation of the problem of simultaneous estimation as a direct nonlinear optimization problem is one of the most common approaches (Seinfeld and Gavalas, 1970; Gavalas et al., 1972; Chandler et al., 1972; Emig and Hosten, 1973; Laurgeau et al., 1974; Watanabe and Shimizu, 1975; Markham and Srayder, 1976; Kalogerkis and Luus, 1980). Such a formulation is relatively simple, but the solution procedure requires long computation times, exhibits numerical instability, and may yield nonoptimal solutions.

A second approach to state and parameter estimation is to use a hierarchical identification scheme (Bar-Shalom, 1972; Arafeh and Sage, 1974; Sastry and Gauvrit, 1978). These investigators reported their strategies to be effective in estimating and identifying large-scale processes, but this second approach is only an alternative to a nonlinear optimization strategy, hence it can also lead to nonoptimal estimates.

Many authors have selected the extended Kalman filter (Jazwinski, 1970; Athans, 1971; Soeda and Yoshimura, 1973) as an attractive approach to estimation. Johnson (1976) applied the filter to a freely spinning rigid spacecraft, Himmelblau (1978) applied it to identify the faulty parameters in a nonlinear chemical process, and Yoshimura et al. (1979) and Ishii et al. (1980) applied it to a linear discrete model with abrupt and/or trend changes in the parameters. All these investigators demonstrated satisfactory results via simulation. Nevertheless, in general the use of the extended Kalman filter does not guarantee convergence of the estimates of both states and parameters to their proper values (Yoshimura et al., 1980), and the accuracy of the estimates is poor (Sastry and Gauvrit, 1978). Furthermore, the computation load is not negligible.

Our proposed strategy is more closely akin to hierarchical identification than the other techniques mentioned above. The lower two boxes on the righthand side of Figure 1 show the basic information flow of the strategy in contrast to that used for an extended Kalman filter. We are concerned with the detection of faults in a class of deteriorating processes nonlinear in the states but linear in the parameters. We describe an estimator and identifier that: (1) yields unbiased estimation of the process states from measurements containing noise with zero mean; and (2) provides unique estimates of the parameters in the sense of least squares error. Calculations executed using the algorithm are rapid and simple, and need relatively little storage in memory so that the method can be implemented by a microprocessor.

Here is the basic idea as applied to the class of processes in which the model is known but the coefficients in the model are unknown. For the first stage of the overall estimation, we employ a linear reduced-order state estimation filter to reconstruct unbiased estimates of all the state variables for a nonlinear process model with unknown coefficients having a particular form (Eq. 1). In general, a linear Luenberger observer and/or a linear Kalman filter will not be able to yield unbiased estimates of the state variables of a nonlinear model. However, we have chosen a special form for the process model and for the filter so that even if the model is nonlinear, a linear Luenberger observer can reconstruct the state variables even if faults develop that change the values of the coefficients in the model. (The output of the observer itself can be used to make alarm decisions as well as isolate faults that can be

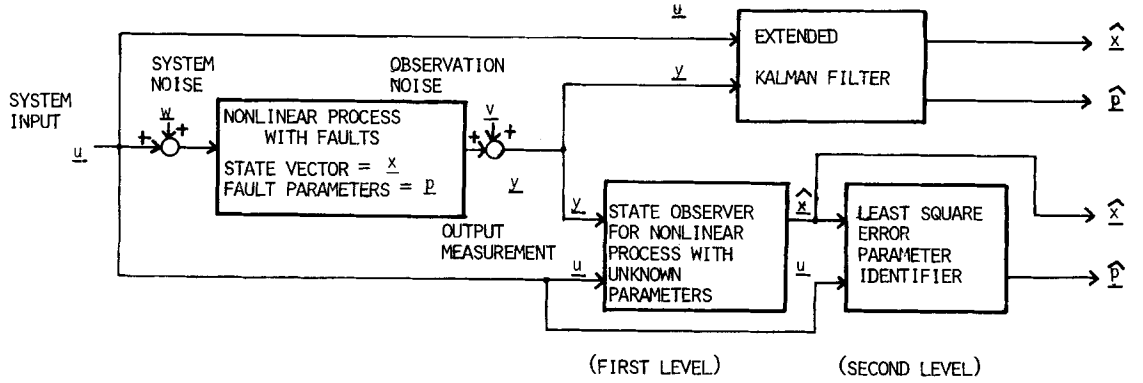

Figure 1. Strategy of state estimation and fault diagnosis.

detected by state variable estimation alone.)

Once all the state variables of the model are known, the second stage of the overall estimation involves parameter identification of the process, a step that is relatively simple. To design an on-line identifier, we choose a linear least squares error function as the cost function, one that provides good parameter estimates if the noise level is low, but that may yield biased estimates if the noise level is excessively high. If on-line identification is not necessary or very high speed computers are available, we could choose a likelihood function as the cost function and get better estimates in the presence of high levels of noise. In either case, since the calculations for the estimation of the states and the parameters are separated, in principle the computation speed to resolve a given problem should be faster than any of the other methods mentioned above.

The class of processes congruent with the proposed strategy is described in more detail in Section 2. The estimator and the identifier are discussed in Sections 3 and 4, respectively. An accompanying article illustrates the procedure, the estimator and the identifier as applied to detecting and diagnosing faults in a chemical reactor.

2. PROCESS DESCRIPTION

Our strategy is applicable to processes that can be represented by the following nonlinear model containing unknown parameters caused by faults

$$\dot{\underline{x}}(t) = A\underline{x}(t) + B\underline{u}(t) + Q\underline{f}(t,\underline{p}) + E\underline{w}(t), \qquad \underline{x}(0) = \underline{x}_0 \quad (1a)$$

$$\underline{y}(t) = [I_m \vdots 0]\underline{x}(t) + \underline{v}(t) \quad (1b)$$

where

- $\underline{x}(t)$ = n-dimensional state vector
- $\underline{u}(t)$ = d-dimensional input vector
- $\underline{w}(t)$ = d-dimensional system noise vector with zero mean
- $\underline{y}(t)$ = m-dimensional output vector
- $\underline{v}(t)$ = m-dimensional observation noise vector with zero mean
- $\underline{f}(t,\underline{p})$ = l-dimensional vector with elements split into: (a) a set of nonlinear functions and (b) another set of linear or nonlinear functions; both sets contain unknown coefficients
- $\underline{p}$ = s-dimensional unknown fault vector
- A,B,E = constant coefficient matrices in the linear part of the process model with appropriate dimensions
- Q = coefficient matrix of the vector $\underline{f}(t,\underline{p})$
- I_m = $m \times m$ dimensional identity matrix

In Eq. 1b we show the state variables being measured directly. However, without any loss of generality, one can linearly transform the process equations so that Eq. 1b is equivalent to a linear combination of independent measurements of state variables (Luenberger, 1971).

The vector function $\underline{f}(t,\underline{p})$ is specified by

$$\underline{f}(t,\underline{p}) = [p_1 f_1(t)\, p_2 f_2(t) \ldots p_s f_s(t) \vdots f_{s+1}(t) \ldots f_l(t)]^T \quad (1c)$$

where $\{p_i$ for $i = 1,2,\ldots,s\}$, the coefficients of the vector, $\underline{p}$, are parameters that might change due to prespecified faults. We shall subsequently refer to the parameters p_i as fault parameters. Note that $\{f_i(t)$ for $i = 1,2,\ldots,s\}$ may be linear and/or nonlinear functions of $\underline{x}(t)$ and $\underline{u}(t)$ but that $\{f_i(t)$ for $i = s+1,\ldots,l\}$ are strictly nonlinear functions of $\underline{x}(t)$ and $\underline{u}(t)$. The formulation of the process model in the form of Eq. 1a in which the nonlinear terms and the terms with unknown parameters are encorporated in the term $Q\underline{f}(t,\underline{p})$ has been selected from many possible model formats to estimate the correct state vector. In Section 3 containing the theoretical development for designing the state estimator, the full import of this term will become clear.

Let us decompose the matrices A and Q as:

$$A \triangleq \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right] \begin{matrix} m \\ n-m \end{matrix}, \qquad \begin{matrix} \leftarrow m \rightarrow & \leftarrow n-m \rightarrow \end{matrix}$$

$$Q \triangleq \left[\begin{array}{c} Q_1 \\ \hline Q_2 \end{array}\right] \triangleq \left[\begin{array}{c|c} Q_{11} & Q_{12} \\ \hline Q_{21} & Q_{22} \end{array}\right] \begin{matrix} s \\ n-s \end{matrix} \quad (1d)$$

$$\begin{matrix} \leftarrow l \rightarrow & \leftarrow s \rightarrow & \leftarrow l-s \rightarrow \end{matrix}$$

and define

$$S(t) \triangleq \begin{bmatrix} Q_{11} \\ \\ Q_{21} \end{bmatrix} \begin{bmatrix} f_1 f_2(t) & & 0 \\ & \ddots & \\ 0 & & f_s(t) \end{bmatrix}, \qquad \underline{q}(t) \triangleq \begin{bmatrix} Q_{12} \\ \\ Q_{22} \end{bmatrix} \begin{bmatrix} f_{s+1}(t) \\ f_{s+2}(t) \\ \vdots \\ f_l(t) \end{bmatrix} \quad (1e)$$

Then the term $Q\underline{f}(t,\underline{p})$ can be written as:

$$Q\underline{f}(t,\underline{p}) \triangleq S(t)\underline{p} + \underline{q}(t) \quad (1f)$$

In Section 4 relation 1f will be used in identifying the unknown parameters uniquely and in developing the identifier.

Process model Eqs. 1, which includes nonlinear functions of $\underline{x}(t)$ and $\underline{x}(t)$ as well as unknown parameters represented by the vector $\underline{p}$, is referred to as a process model nonlinear in the states and linear in the parameters. Although this model superficially may seem to be of restricted scope, it can represent a wide variety of actual nonlinear processes, especially those involving a chemical reactor in which general reactions are taking place.

The problem considered here is how to develop an on-line state estimator and parameter identifier that estimate the correct state variables and subsequently accurately identify the parameters of process Eqs. 1. In the following section, we describe the state estimator (the first level of identification) of the nonlinear process model Eq. 1.

3. STATE ESTIMATION OF NONLINEAR PROCESS WITH UNKNOWN PARAMETERS

Consider the following linear time-invariant state estimation

filter for the linear process Eqs. 1

$$\dot{\underline{z}}(t) = F\underline{z}(t) + K\underline{y}(t) + MB\underline{u}(t), \qquad \underline{z}(0) = \underline{z}_0 \tag{2a}$$

$$\hat{\underline{x}}(t) = D\underline{z}(t) + H\underline{y}(t) \tag{2b}$$

where

$\underline{z}(t)$ = $(n - m)$ dimensional state vector of the filter
$\hat{\underline{x}}(t)$ = n-dimensional estimated state vector of Eqs. 1
F,K,M,D,H = constant filter coefficient matrices with appropriate dimensions
$\underline{u}(t),\underline{y}(t)$ = input and output vector from the process (Eqs. 1), respectively

The filter has the same structure as a linear Luenberger observer.

As shown in most textbooks in modern control theory, the Kalman filter is a very special use of the Luenberger observer. Both can be applied to stochastic models, but the Kalman filter has zero degrees of flexibility in its design because it is given uniquely and automatically from the system coefficient matrices and the covariance matrices of the system and observation noise (Mita and Kogo, 1979). On the other hand, the Luenberger observer (a) has a high degree of freedom in its design, and (b) has been shown to work in the presence of noise for real applications. We make use of this design flexibility in developing our linear state estimation filter.

By analogy with the Luenberger observer, we have a state estimation filter (Eqs. 2) that provides an estimate $\hat{\underline{x}}(t)$ which tends to $\underline{x}(t)$ as $t \to \infty$ if $\underline{v}(t) = 0$ and $\underline{w}(t) = 0$ in the nonlinear process (Eqs. 1). It also provides $\hat{\underline{x}}(t) \cong \underline{x}(t)$ for $t \geq t_s$ (t_s is the settling time for the transient of the filter), if $\underline{v}(t) \neq 0$ and $\underline{w}(t) \neq 0$. We shall consider both the deterministic ($\underline{v}(t) = 0$ and $\underline{w}(t) = 0$) and stochastic ($\underline{v}(t) \neq 0$ and $\underline{w}(t) \neq 0$) cases.

Deterministic Case

We first consider the sufficient conditions on process (Eqs. 1) (with $\underline{v}(t) = 0$ and $\underline{w}(t) = 0$), assuming that filter (Eqs. 2) is used, so that the linear time-invariant filter can be designed, and then present a method to evaluate the elements in the filter coefficient matrices. The sufficient conditions are

(i) rank $[Q_1] = l \leq m$
(ii) The matrix F given by (3a)

$$F = \{A_{22} - Q_2(Q_1)^{\#}A_{12}\} - K_o\{I_m - Q_1(Q_1)^{\#}\}A_{12} \tag{3b}$$

can be stabilized by a proper choice of K_o where

$$(Q_1)^{\#} \triangleq [Q_1^TQ_1]^{-1}Q_1^T \tag{4a}$$

K_o is an $(n - m) \times m$ dimensional arbitrary matrix. If process (Eqs. 1) satisfies the above conditions, the coefficient matrices of the filter are determined as follows

$$L \triangleq Q_2(Q_1)^{\#} + K_o\{I_m - Q_1(Q_1)^{\#}\} \tag{4b}$$

$$M \triangleq [-L \vdots I_{n-m}] \tag{4c}$$

$$H \triangleq \begin{bmatrix} I_m \\ \cdots \\ L \end{bmatrix} \tag{4d}$$

$$K \triangleq -LA_{11} + A_{22}L - LA_{12} + A_{21} \tag{4e}$$

$$F \triangleq A_{22} - Q_2(Q_1)^{\#}A_{12} - K_o\{I_m - Q_1(Q_1)^{\#}\}A_{12} \tag{4f}$$

$$D \triangleq \begin{bmatrix} 0 \\ \cdots \\ I_{n-m} \end{bmatrix} \tag{4g}$$

The proof that Eqs. 3a and 3b are sufficient and the determination of the matrices in Eqs. 4 are in Appendix A.

Note that if $l = m$, the conditions

(i) rank $[Q_1] = l = m$ (5a)

(ii) $F = A_{22} - Q_2(Q_1)^{\#}A_{12}$ is a stable matrix (5b)

yield the state estimator (Eqs. 2) for the process (Eqs. 1) with ($\underline{v}(t) = 0$ and $\underline{w}(t) = 0$) as can be demonstrated directly by analogy with the explanation in Appendix A. For this special case, because Q_1 is a square matrix with full rank, Eq. 4a can be given

$$L = Q_2Q_1^{-1} \tag{6}$$

and we do not have any freedom to choose K_o.

Also, if process (Eqs. 1) with ($\underline{v}(t) = 0$ and $\underline{w}(t) = 0$) satisfies the conditions

(i) rank$[Q_1] = l \leq m$ (7a)

(ii) $A_{12} = 0$ (7b)

(iii) $F = A_{22}$ is a stable matrix, (7c)

a state estimation filter (Eqs. 2) does exist and can be designed. In this case, the matrix F is given by $F = A_{22}$ so that the filter dynamics will be the same as those of subsystem A_{22}. Suppose $m > l$ and $\{I_m - Q_1(Q_1)^{\#}\}A_{12} \neq 0$. Then we have freedom to choose K_o. We can assign all the eigenvalues of F arbitrarily by the proper choice of K_o, if and only if the pair $[\{A_{22} - Q_2(Q_1)^{\#}A_{12}\}, \{I_m - Q_1(Q_1)^{\#}\}A_{12}]$ is completely observable. This condition has been demonstrated by Luenberger (1964, 1966, 1971). Detailed discussion of eigenvalue assignment can be found in the literature (Wonham, 1967; Kimura, 1975; Mita and Kogo, 1979).

Some question may exist as to whether the state estimation scheme ignores the nonlinear terms and hence loses information. This is not correct. In deriving the sufficient conditions for the design of the filter in Section 2 and in designing the filter itself in this Section, we made use of the information in Q_1 in the decomposition of $Q\underline{f}(\underline{x},\underline{p}) = [Q_1^T \vdots Q_2^T]^T\underline{f}(\underline{x},\underline{p})$. We further used the property that the term $f(\underline{x},\underline{p})$ in one or more equations of Eq. 1a is linearly related to the same term in other equations of Eq. 1a. As a simple example of the key idea consider the following two steady state equations

$$x_1 + f(x_1,x_2,\underline{p}) = 0$$

$$x_2 + af(x_1,x_2,\underline{p}) = 0$$

If x_1 is measure as $y_1 = x_1$, we can estimate x_2 as $\hat{\underline{x}}_2 - ay_1$ by substitution. Note we do not use the nonlinear term itself in the estimation but make use of the dependency of the term in the other equation. The state estimation strategy described here is a generalization of the above concept for the process described by Eqs. 1.

Stochastic Case

Next we consider the case when $\underline{v}(t) \neq 0$ and $\underline{w}(t) \neq 0$ in process (Eqs. 1). In this case, if process (Eqs. 1) satisfies the conditions in Eqs. 3a and 3b, the filter error and the estimated state are

$$\dot{\underline{e}}(t) = F\underline{e}(t) + K\underline{v}(t) - ME\underline{w}(t), \qquad \underline{e}(0) = \underline{e}_0 \tag{8a}$$

$$D\underline{e}(t) = \hat{\underline{x}}(t) - \underline{x}(t) \tag{8b}$$

Equations 8a and 8b are derived by rearrangements similar to those used to obtain Eq. A5 in Appendix A. The matrix K is the function of K_o given by Eq. 4e with Eq. 4b. The solution of Eq. 8a is given by

$$\underline{e}(t) = e^{Ft}\underline{e}_0 + \int_0^t e^{-F(t-\eta)}\{K\underline{v}(\eta) - Me\underline{w}(\eta)\}d\eta \tag{8c}$$

Since F is stable, the term $e^{Ft}\underline{e}_o$ converges to zero for $t \geq t_s$.

The integral in Eq. 8c contains the noises $\underline{v}(t)$ and $\underline{w}(t)$ with zero means. Nevertheless, proper choice of K minimizes the noise in $\underline{e}(t)$. The transfer function from $\underline{v}(t)$ and $\underline{w}(t)$ to the error $D\underline{e}(t)$, Eq. 8b, in the steady state is given by:

$$D\underline{e}(i2\pi f) = D[i2\pi fI_{n-m} - F]^{-1}\{K\underline{v}(i2\pi f) - Me\underline{w}(i2\pi f)\} \tag{8d}$$

where

i = $\sqrt{-1}$ and f is the frequency
$D\underline{e}(i2\pi f)$ = Fourier transform of the error in $\underline{\hat{x}}(t)$
$\underline{v}(i2\pi f), \underline{w}(i2\pi f)$ = Fourier transforms of $\underline{v}(t)$ and $\underline{w}(t)$

If we have the freedom to choose K_o after stabilizing F, we can choose an optimal K_o. It is worthwhile to select, for example, a matrix K_o that minimizes the following cost function:

$$J(K_o) = \int_{f_l}^{f_h} \left\{ \max_{\underline{v}} \left(\|D[i2\pi f I_{n-m} - F]^{-1} K \underline{v}\| / \|\underline{v}\| \right) + \max_{\underline{w}} \left(\|[i2\pi f I_{n-m} - F]^{-1} M E \underline{w}\| / \|\underline{w}\| \right) \right\} df \quad (9a)$$

where

$\| \|$ = norm of a vector
f_l, f_h = lowest and highest frequencies of observation noise

By definition of a matrix norm (Wiberg, 1971), the cost function can be rewritten as:

$$J(K_o) = \int_{f_l}^{f_h} \{ \|D[i2\pi f I_{n-m} - F]^{-1} K\| + \|D[i2\pi f I_{n-m} - F]^{-1} M E\| \} df \quad (9b)$$

and the optimal K_o can be determined by a nonlinear optimization scheme. Once K_o is determined, the matrices M, H, K, F and D in the filter (Eqs. 2) can be obtained from Eqs. 4c, 4d, 4e, 4f and 4g, respectively with Eqs. 4b and 1a.

So far, we have demonstrated that a state estimation filter for a nonlinear process with unknown parameters can be developed. Such a filter by itself can be effectively applied to fault detection decisions via alarm as well as to the isolation of faults, if the faults are defined in terms of the state variables (Section 1).

4. IDENTIFICATION OF UNKNOWN FAULT PARAMETERS

To find the specific source of process faults, identification of the unknown process parameters is needed because the deterioration of process performance is usually expressed in terms of parameter changes rather than changes of model structure or states.

From the previous section it is known that if process (Eqs. 1) satisfies the conditions 3a–3b, or 5a–5b, or 7a–7c, we can obtain good estimates of all the state variables. The problem to be considered next is how to identify the unknown parameters associated with faults using the estimated state vector from filter (Eqs. 2). This step comprises the second-level of identification.

We first rewrite the model (Eq. 1a) for the process in a form suitable for parameter identification. By definition 1f, Eq. 1a can be rewritten as

$$\dot{\underline{x}}(t) = A\underline{x}(t) + B\underline{u}(t) + \underline{q}(t) + S(t)\underline{p} \quad (10)$$

We approximate the derivative in Eq. 10 as

$$\dot{\underline{x}}(t) \cong \{\underline{x}(t + \tau) - \underline{x}(t)\}/\tau \quad (11a)$$

where τ is a time interval that is brief in comparison with the shortest time constant of the process and the highest frequency of the observation noise. [The approximation is not needed for a steady state process with $\underline{v}(t) = 0$ and $\underline{w}(t) = 0$.] Now let $t = k\tau$, Eq. 10 can be written as

$$\{\underline{x}(k + 1) - \underline{x}(k)\}/\tau = A\underline{x}(k) + B\underline{u}(k) + \underline{q}(k) + S(k)\underline{p} \quad (11b)$$

Equation 11b can be written as

$$S(k)\underline{p} = \underline{b}(k) \quad (11c)$$

where

$$\underline{b}(k) = [\{\underline{x}(k + 1) - \underline{x}(k)\}/\tau] - A\underline{x}(k) - B\underline{u}(k) - \underline{q}(k) \quad (11d)$$

Utilizing the relation 11c with Eq. 11d, we consider an identifier to obtain $\underline{p}$ for both the deterministic and stochastic cases.

Deterministic Case

Because model (Eq. 10) of the process has no observation noise, $\underline{\hat{x}}(t) = \underline{x}(t)$ for $t \geq t_s$, and Eq. 11c is satisfied by the deterministically estimated state vector. Let the values of $\underline{x}(k)$, $\underline{u}(k)$, $\underline{q}(k)$, $f_i(k)$, $\underline{b}(k)$ and $S(k)$ obtained from the estimated state $\underline{\hat{x}}(k)$ be designated by $\underline{\hat{x}}(k)$, $\underline{u}(k)$, $\hat{\underline{q}}(k)$, $\hat{f}_i(k)$, $\hat{\underline{b}}(k)$ and $\hat{S}(k)$, respectively. Then the unknown parameters are uniquely and exactly identified if the process (Eqs. 1) with $\underline{v}(t) = 0$ and $\underline{w}(t) = 0$ satisfies

(i) rank$[Q_1] = l$ (one of the conditions 3) (12a)

(ii) $f_i(k) \not\equiv 0$ for $i = 1,2, \ldots, s$ (12b)

The proof of these conditions is in Appendix B. The estimate is then given by

$$\hat{\underline{p}} = [\hat{S}(k)^T \hat{S}(k)]^{-1} \hat{S}(k)^T \hat{\underline{b}}(k) \quad (12c)$$

Stochastic Case

Next we consider the case when $v(t) \not\equiv 0$ and $\underline{w}(t) \not\equiv 0$. Again let $\underline{\hat{x}}(k)$, $\underline{u}(k)$, $\hat{\underline{q}}(k)$, $\hat{\underline{b}}(k)$, $\hat{f}_i(k)$ and $\hat{S}(k)$ be the values obtained from $\underline{\hat{x}}(k)$. We obtain an equation corresponding to Eq. 11c as follows

$$\hat{S}(k)\hat{\underline{p}}(k) = \hat{\underline{b}}(k) + \underline{\epsilon}(k) \quad (13a)$$

where $\underline{\epsilon}(k)$ is an unknown error vector due to the observation noise and system noise. Since $\underline{\epsilon}(k)$ is unknown, we can not find $\underline{p}(k)$ which satisfies Eq. 13a exactly. Consequently we try to find $\underline{p}(k)$ which minimizes the following cost function

$$J(\underline{p}(k)) + \sum_{i=k-N}^{k} \lambda^{2(k-i)} \|\underline{\epsilon}(k)\|^2, \quad \text{with } 0 \leq \lambda \leq 1 \quad (13b)$$

where $N \leq k$ and λ is a weighting factor. The choice of a large weighting factor λ leads to slower convergence but smaller variance of the estimates. The estimation which minimizes Eq. 13b is a linear least squares error estimation. If the process (Eqs. 1) satisfies

(i) rank$[Q_1] = l$ (one of the conditions of 3) (14a)

(ii) $f_i(k) \not\equiv 0$ for $i = 1,2, \ldots s$ at least at one time during $(k - N)$ and k, (14b)

the unknown parameters can be obtained uniquely in the sense of the least squares error identification of Eq. 13b. The proof of the conditions is in Appendix C.

We define

$$R(k) \triangleq [\hat{S}(k)^T \hat{S}(k-1)^T \hat{S}(k-2)^T \ldots \hat{S}(k-N)^T]^T \quad (15a)$$

$$W(k) \triangleq [\hat{\underline{b}}(k)^T \hat{\underline{b}}(k-1)^T \hat{\underline{b}}(k-2)^T \ldots \hat{\underline{b}}(k-N)^T]^T \quad (15b)$$

then we have the least squares estimation

$$\hat{\underline{p}}(k) = [R(k)^T R(k)]^{-1} R(k)^T W(k) \quad (15c)$$

If we let

$$U(k) \triangleq \frac{1}{\lambda^2} [R(k)^T R(k)]^{-1} \hat{S}(k + 1)^T \quad (16a)$$

$$V(k) \triangleq [I_n + \hat{S}(k + 1)U(k)]^{-1} \quad (16b)$$

we have an on-line updating algorithm as follows

$$\hat{\underline{p}}(k + 1) = [I_s - U(k)V(k)\hat{S}(k + 1)]\{\hat{\underline{p}}(k) + U(k)\hat{\underline{b}}(k + 1)\} \quad (16c)$$

$$[R(k + 1)^T R(k + 1)]^{-1} = \frac{1}{\lambda^2} [R(k)^T R(k)]^{-1} - U(k)V(k)U(k)^T \quad (16d)$$

where

$U(k) = s \times n$ dimensional matrix
$V(k) = n \times s$ dimensional matrix
$[R(k + i)^T R(k + i)]^{-1} = s \times s$ dimensional matrix

Among the two conditions 12a–12b or 14a–14b, the rank condition, i.e., rank $[Q_1] = l$ which is also one of the conditions 3a–3b,

is more restrictive than Eq. 14b, because Eq. 14b can be satisfied by a proper choice of operating conditions of the process. Then we can roughly say that the unknown fault parameters of the process which satisfies the condition 3a–3b are uniquely identifiable in the sense of the least squares estimation.

APPENDIX A

From Eq. 3a is a generalized inverse of Q_1 is obtained as Eq. 4a. Then the coefficient matrices L, M, H, F, K and D can be obtained as Eqs. 4b–4g by using $Q_1^{\#}$. These matrices satisfy

$$DM + H[I_m \vdots 0] = I_n \tag{A1}$$

$$FM = MA - K[I_m \vdots 0]. \tag{A2}$$

Define an error vector of the filter

$$\underline{e}(t) = \underline{z}(t) - M\underline{x}(t) \tag{A3}$$

which yields

$$\dot{\underline{e}}(t) = \dot{\underline{z}}(t) - M\dot{\underline{x}}(t) \tag{A4}$$

Substitution of Eqs. 1a and 2a into Eq. A4 and rearrangement using the relations Eqs. A1 and A2 leads to

$$\dot{\underline{e}}(t) = F\underline{e}(t) - M\begin{bmatrix}Q_1\\Q_2\end{bmatrix}\underline{f}(t,\underline{p}), \quad \underline{e}(0) = \underline{e}_0 \tag{A5}$$

where $\underline{e}_0$ is nonzero vector. Further from Eqs. 4b and 4c

$$M\begin{bmatrix}Q_1\\Q_2\end{bmatrix} = -LQ_1 + Q_2 = -Q_2 + K_0(Q_1 - Q_1) + Q_2 = 0 \tag{A6}$$

Then we can rewrite Eq. A5 as

$$\dot{\underline{e}}(t) = F\underline{e}(t), \quad \underline{e}(0) = \underline{e}_0 \tag{A7}$$

From Eq. 3b, F is a stable matrix, then

$$\underline{e}(t) = \underline{z}(t) - M\underline{x}(t) \to 0 \text{ as } t \to \infty. \tag{A8}$$

Therefore from Eqs. A7 and 2b, we obtain

$$\hat{\underline{x}}(t) \to D\underline{z}(t) + H\underline{y}(t) = \underline{x}(t) \text{ as } t \to \infty. \tag{A9}$$

APPENDIX B

From the assumption that rank$[Q_1] = l$, the rank of the partitioned matrix is full as follows

$$\underset{\leftarrow s \rightarrow}{\text{rank}\begin{bmatrix}Q_{11}\\Q_{21}\end{bmatrix}} = S \tag{B1}$$

Further, from the assumption

$$f_i(k) \neq 0 \text{ for } i = 1,2,\ldots,s \tag{B2}$$

from Eq. 1e

$$\text{rank}[S(k)] = s \tag{B3}$$

Since $\hat{\underline{x}}(t) = \underline{x}(t)$ for $t \geq t_s$, Eq. 11c must be satisfied by $\hat{\underline{x}}(t)$ for $t \geq t_s$; then

$$\text{rank}[\hat{S}(k) \vdots \hat{\underline{b}}(k)] = s \tag{B4}$$

Therefore, the linear equation

$$\hat{S}(k)\hat{\underline{p}}(k) = \hat{\underline{b}}(k) \tag{B5}$$

has an unique and exact solution

$$\hat{\underline{p}}(k) = [\hat{S}(k)^T\hat{S}(k)]^{-1}\hat{S}(k)^T\hat{\underline{b}}(k) \tag{B6}$$

APPENDIX C

Since $f_i(k) \neq 0$ for $i = 1,2,\ldots,s$, at least at one time point during $(k - N)$ and k,

$$\text{rank}[R(k)] = s \tag{C1}$$

Then $R(k)^TR(k)$ is invertible. Therefore, we have an unique least squares estimate

$$\hat{\underline{p}}(k) = [R(k)^TR(k)]^{-1}R(k)^TW(k) \tag{C2}$$

NOTATION

A	= process coefficient matrix for linear term
$A_{11}, A_{12}, A_{21}, A_{22}$	= partitioned matrix of A
B	= process input matrix
$\underline{b}(k)$	= vector used in identification
$\hat{\underline{b}}(k)$	= estimate of $\underline{b}(k)$
D	= filter coefficient matrix
d	= dimension of vectors $\underline{u}(t)$ and $\underline{w}(t)$
E	= process noise matrix
$\underline{e}(t)$	= filter error vector
$\underline{e}_0$	= initial value of $\underline{e}(t)$
F	= filter coefficient matrix
f	= frequency
$\underline{f}(t,\underline{p})$	= vector of nonlinear functions or linear and/or nonlinear functions with unknown coefficients
$f_i(i = 1,2,\ldots,s)$	= linear or nonlinear functions with unknown coefficient
$f_i(i = s,\ldots,l)$	= nonlinear function
f_l	= lowest frequency of noises
f_h	= highest frequency of noises
$\hat{f}_i(k)$	= estimate of $f_i(k)$
$\underline{f}^*(t)$	= nonlinear vector function of the process under normal condition
H	= filter coefficient matrix
I_m	= m-dimensional identity matrix
i	= $\sqrt{-1}$
$J(\ )$	= cost function
K	= filter coefficient matrix
K_0	= arbitrary matrix used to stabilize F
k	= discrete time
L	= filter coefficient matrix
l	= dimension of vector function $\underline{f}(t,\underline{p})$
M	= filter coefficient matrix
m	= dimension of vector $\underline{y}(t)$ and $\underline{v}(t)$
N	= number of sampled data
n	= dimension of vector $\underline{x}(t)$
$\underline{p}$	= unknown fault parameter vector
$p_i(i = 1,2,\ldots,s)$	= element of vector $\underline{p}$
Q	= process coefficient matrix for nonlinear and/or linear terms with unknown parameters
$Q_1, Q_2, Q_{11}, Q_{12}, Q_{21}, Q_{22}$	= partitioned matrix of Q
$\underline{q}$	= nonlinear vector function
$\hat{\underline{q}}$	= estimate of $\underline{q}$
$R(k)$	= matrix used in parameter identification
r^*	= prespecified ratio of inlet and outlet concentrations
$S(t)$	= matrix used in parameter identification
$\hat{S}(t)$	= estimate of $S(t)$
s	= dimension of vector $\underline{p}$
t	= continuous time
t_s	= settling time for filter transient
$U(k)$	= matrix used in parameter identification
$\underline{u}$	= input vector of process
$u_i(i = 1,2,3)$	= inputs of the process
$V(k)$	= matrix used for parameter identification

$\underline{v}(t)$ = observation noise vector
$W(k)$ = matrix used in parameter identification
$\underline{w}(t)$ = system noise vector
$\underline{x}(t)$ = state vector of process
$\underline{x}_0$ = initial value of $\underline{x}(t)$
$\dot{\underline{x}}(t)$ = derivative of $\underline{x}(t)$
$\hat{\underline{x}}(t)$ = estimate of $\underline{x}(t)$
$\underline{y}(t)$ = output vector of process
$\underline{z}(t)$ = state vector of state estimation filters
$\underline{z}_0$ = initial value of $\underline{z}(t)$
$\hat{\underline{z}}(t)$ = estimated state vector for the extended Kalman filter
z_i = state variables of the filter

Greek Letters

$\underline{\epsilon}(k)$ = error vector in identification
η = continuous time
λ = weighting factor in identifier
τ = sampling interval

Mathematical Symbols

$( )^{\#}$ = generalized inverse of matrix
$( )^T$ = transpose of matrix and vector
$( )^{-1}$ = inverse of square matrix
rank[ ] = rank of matrix
$\| \|$ = norm of vector and matrix
$E[ ]$ = expectation

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