NOTATION

$A(s)$, $B(s)$, $C(s)$, $P(s)$ = process transfer function matrices
$P(s)$, $Q(s)$ = process transfer function matrices (see Figures 1 and 2)
$a_i(s)$ = i^{th} column of $A(s)$
$b_i(s)$ = i^{th} column of $B(s)$
$d(s)$ = effect of the disturbances on the product qualities
$F(s)$ = $\{I + \alpha^T(s)\,[P(s) - \hat{P}(s))]\}^{-1}$
$G_I(s)$ = matrix of controller transfer functions for the inferential control loop
$G_c(s)$ = matrix of controller transfer functions for the feedback control loop
$G_m(s)$ = matrix of measurement lags
$G_L(s)$ = matrix of compensators to match set point changes
$m(s)$ = control effort vector
$m_1(s)$ = reflux ratio
$m_2(s)$ = vapor boilup rate
$R(s)$ = $A(s)\alpha(s) - B(s)$
$r_j(s)$ = $b(s) - a_j^T(s)\alpha(s)$, vector of residuals associated with the j^{th} temperature measurement
s = Laplace transform variable
$u(o)$ = steady state value of disturbance
$u(s)$ = unmeasured disturbance vector
$u_i(s)$ = flow rate of i^{th} component in feed
$v(s)$ = measured disturbance vector
$y(s)$ = product quality vector
$y_1(s)$ = overhead butane composition
$y_2(s)$ = bottoms propane composition
$\alpha(s)$ = matrix of estimator transfer functions
$\theta(s)$ = measured output vector

Superscripts

$\wedge$ = estimated value
-1 = inverse
T = transpose

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Part III. Construction of Optimal and Suboptimal Dynamic Estimators

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Methods are presented for the construction of optimal and suboptimal estimators for inferential control systems. Optimal estimators are constructed with the aid of Kalman filtering techniques applied to linear systems driven by integrated white noise disturbances. The description of the disturbances as integrated white noise leads to optimal dynamic estimators which reduce to optimal static estimators for sustained disturbances. Suboptimal estimators are constructed by prespecifying the structure of the estimator and choosing estimator parameters so as to minimize the mean square error in estimation.

Optimal and suboptimal estimators are compared by using them in an inferential control system which attempts to control the product composition of a simulated multicomponent distillation column. There is little difference in performance between optimal and suboptimal estimators which use temperature and flow measurements to estimate product composition. However, the inferential control system using a simple suboptimal estimator is significantly superior to the policy of maintaining a selected tray temperature constant through a standard feedback control system. The inferential control system is also superior to composition feedback control systems where the measurement delay is greater than 5 min.

Part I discusses the problem of measurement selection and estimator design to achieve optimal steady state behavior. Part II discusses the dynamic behavior of inferential control systems based on ad hoc methods for adding dynamic compensation to the estimator. This work is concerned with the design of optimal and nearly optimal dynamic compensation for the estimator.

An important feature of the design methods is that they yield linear dynamic estimators which reduce to optimal static estimators in the steady state. This is achieved by using a statistical description of the input disturbances which admits the possibility of the process

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remaining near a steady state condition for significant periods of time.

Two different approaches are presented for the design of optimal estimators. The first, and conceptually simpler method, adapts Wiener filtering theory for the class of disturbances under consideration. The second approach is an adaptation of Kalman filtering, and it is presented because of the computational advantages it offers. In either case, the optimal filters are quite complex, even for relatively simple problems. For this reason, we also present methods for designing suboptimal estimators which can have any desired structure.

Estimators designed by the various methods presented are tested on a simulated multicomponent distillation column. Temperature measurements, corrupted by measurement noise, are used to estimate overhead and bottoms product compositions. Disturbances to the column are feed flow and composition changes.

THE PROCESS AND DISTURBANCE MODELS

For the purpose of the estimator design, the measured disturbances and control efforts can be omitted and the input-output model of the process written as

$$y(s) = b^T(s)u(s) \tag{1}$$

$$\theta(s) = A^T(s)u(s) \tag{2}$$

where $y(s)$, $u(s)$ and $\theta(s)$ are the process outputs, disturbances, and measurements, respectively.

The above model can be generated by step tests or impulse tests on the process or process simulation. Luyben (1973) discusses the problem of process modeling in detail. Generally, process transfer functions can be approximated by second-order lag and delay types of functions. The specific form of the transfer functions is not important for the discussion that follows, but it is assumed that neither $A(s)$ nor $b(s)$ exhibit any unstable poles and that the order of the denominator of the transfer functions is at least 1 degree higher than the numerator. This is true in most physical systems.

In the process industries, the input disturbances can be of a sustained nature; that is, the time between disturbances can be long with respect to the response time of the process. Any statistical model of the disturbances must therefore admit the possibility of sustained disturbances. One such model is obtained by summing random step inputs which occur at random time intervals (Figure 1). Mathematically

$$u(t) = \sum_{k=-\infty}^{\infty} a_k u_o(t - t_k) \tag{3}$$

The amplitudes a_k of the step functions u_o are assumed to be completely independent of each other with mean zero and covariance ξ^2, and the successive arrival times t_k are Poisson distributed with average frequencies of arrival ν.

The spectral density of $u(t)$ [that is, the Laplace transform of the autocorrelation matrix of $u(t)$] is given by Chang (1961) and by Laning and Batten (1956):

$$\Phi_{uu}(s) = \frac{\nu\xi^2}{-s^2} \tag{4}$$

Notice that $u(t)$ has the same spectral density as that obtained by passing a white noise (that is, a noise whose spectral density is constant) through an integrator. This characteristic will be seen to force the optimal dynamic estimator to reduce to the optimal static estimator for sustained disturbances. When u is a vector, the spectral density can be written as

$$\Phi_{uu}(s) = \frac{\phi_{\eta\eta}}{-s^2} \tag{5}$$

For simplicity, $\phi_{\eta\eta}$ is assumed to be the identity matrix. If this is not so, the input disturbances can be suitably redefined such that $\phi_{\eta\eta} = I$.

OPTIMAL ESTIMATION

Wiener Formulation

The estimation problem can be stated as follows. Find a transfer function $\alpha(s)$ such that $E\{e^2(t)\}$ is minimized, where

$$\hat{y}(s) = \alpha^T(s)\theta(s) \tag{6}$$

and

$$e(t) = y(t) - \hat{y}(t) \tag{7}$$

and $\hat{y}(t)$ is the estimate of $y(t)$.

When $u(t)$ is a random process, the mean-squared error in estimation [that is, $E\{e^2(t)\}$] is given by (Newton, Gould and Kaiser, 1957; Chang 1961)

$$E\{e^2(t)\} = \frac{1}{2\pi j}\int_{-j\infty}^{+j\infty} \Phi_{ee}(s)ds \tag{8}$$

where $\Phi_{ee}(s)$ is the spectral density of $e(t)$.

But, from Equations (1), (2), (6), and (7)

$$e(s) = b^T(s)u(s) - \alpha^T(s)A^T(s)u(s) \equiv r^T(s)u(s) \tag{9}$$

where $r(s) \equiv b(s) - A(s)\alpha(s)$. Therefore

$$E\{e^2(t)\} = \frac{1}{2\pi j}\int_{-j\infty}^{+j\infty} r^T(-s)\Phi_{uu}(s)r(s)ds \tag{10}$$

where $\Phi_{uu}(s)$ is the spectral density of the input disturbances [Equation (5)]. Substituting (5) into (10),

$$E\{e^2(t)\} = \frac{1}{2\pi j}\int_{-j\infty}^{+j\infty} r(-s)\,\frac{\Phi_{\eta\eta}}{-s^2}\,r(s)ds \tag{11}$$

The integrand has two poles at the origin. In order for the integral to converge, these poles must be cancelled out by zeroes in the numerator. Hence, we require

$$r(0) = 0 \tag{12}$$

From (9), the above condition implies that

$$A(0)\,\alpha(0) = b(0)$$

or

$$\alpha^*(0) = [A^T(0)A(0)]^{-1}A^T(0)b(0) \tag{13}$$

Both (12) and (13) imply perfect estimation for sustained disturbances. This is, they imply perfect estimation in the steady state. To show this, we note that a sustained disturbance can be written as

$$u(s) = \frac{1}{s}u(0)$$

The steady state error in estimation is then given by

$$\lim_{t\to\infty} e(t) = \lim_{s\to 0} se(s) = r^T(0)u(0)$$
$$= 0 \quad \text{when} \quad r(0) = 0$$

The requirement of perfect steady state estimation is somewhat stronger than we would like. Frequently one is satisfied with steady state errors on the order of 25% and more. In such cases, an optimal estimator can be constructed if one first subtracts the unobservable portion of the output from the estimate as follows. Let

$$y(s) \equiv y_1(s) + y_2(s) \tag{14}$$

where

$$y_1(s) \equiv [b^T(s) - r_1^T(0)]u(s) \tag{15}$$

$$y_2(s) \equiv r_1^T(0)u(s) \tag{16}$$

In (16), $r_1(0)$ is the residual remaining from the least-squares solution of

$$A(0)\alpha^*(0) \simeq b(0) \tag{17}$$

where

$$A^T(0)r_1(0) = 0 \tag{18}$$

The best linear estimate of $y(s)$ is the sum of the best linear estimates of $y_1(s)$ and $y_2(s)$. The best linear estimate of $y_1(s)$ can be obtained from the minimization of (11), where $r(s)$ is now given by

$$r(s) = b(s) - r_1(0) - A(s)\alpha^*(s) \tag{19}$$

and

$$r(0) = b(0) - A(0)\alpha^*(0) - r_1(0) = 0 \tag{20}$$

The best linear estimate of $y_2(s)$ given $\theta(s)$ is zero (Joseph, 1975). Hence

$$\hat{y}^*(s) = \hat{y}_1^*(s)$$

The optimal estimator $\alpha^*(s)$ which minimizes (11) and satisfies (13) is given by the solution of

$$\left\{ \frac{A^T(-s)A(s)}{-s^2}\alpha^*(s) \right\}^+ = \left\{ \frac{A^T(-s)}{-s^2} b(s) \right\}^+ \tag{21}$$

where the operator $\{\cdot\}^+$ takes only that portion of the bilateral Laplace transform which relates to positive time (Davis, 1963).

The solution of (21) requires the spectral factorization of the matrices inside the brackets. Although there are several algorithms for carrying out the required factorization (Davis, 1963; Wong, 1961), none are computationally attractive. For this reason, we next consider an adaptation of the Kalman filter to form the operator $\alpha^*(t)$ in the time domain.

KALMAN FORMULATION

The standard Kalman formulation of the estimation problem is as follows.

Given the following linear dynamical system

$$\dot{x}(t) = Fx(t) + G\eta(t) \tag{22a}$$

where $\eta(t)$ is a white noise with

$$E\{\eta(t)\} = 0$$

$$E\{\eta(t)\eta^T(t+\tau)\} = I\delta(\tau)$$

and a set of observations $\theta(t)$, where

$$\theta(t) = Cx(t) + \nu(t) \tag{22b}$$

with

$$E\{\nu(t)\} = 0$$

$$E\{\nu(t)\nu^T(t+\tau)\} = I\delta(\tau)$$

estimate $y(t)$, where

$$y(t) = Dx(t) \tag{22c}$$

The solution of the above problem is to form the optimal estimate of $y^*(t)$ as follows:

$$y^*(t) = D\hat{x}^*(t) \tag{23a}$$

$$\frac{d}{dt}\hat{x}^*(t) = F\hat{x}^*(t) + P(t)C^T[\theta(t) - C\hat{x}^*(t)] \tag{23b}$$

$$\hat{x}^*(0) = E\{x(0)\}$$

$$\dot{P}(t) = FP(t) + P(t)F^T - P(t)C^TCP(t) + GG^T \tag{23c}$$

$$P(0) = E\{x(0)x^T(0)\}$$

The estimator given by the solution of (23) is the same as that given by the solution of (21) when $P(t)$ in (23c) is replaced by the constant matrix P which is the steady state solution of (23c). Thus, the solution of (21) is

$$\alpha^*(s) = D(sI - F + PC^TC)^{-1}PC^T \tag{24}$$

A sufficient condition for the solution of (23) to converge to a steady state value, P, is that the system (C, F) be detectable and that the system (F, G) be controllable (Wonham, 1968).

We now wish to reduce our estimation problem to the form given by (22), with the matrices C, F, and G satisfying the controllability and detectability conditions. The straightforward approach is to first obtain a minimum realization of (1) and (2) of the form

$$\dot{x}(t) = Fx(t) + Gu(t) \tag{25a}$$

$$\theta(t) = Cx(t) + \nu(t) \tag{25b}$$

$$y(t) = Dx(t) \tag{25c}$$

Measurement noise $\nu(t)$ is added to θ to simplify the computation of the Kalman filter. We assume that $\nu(t)$ satisfies

$$E\{\nu(t)\} = 0$$

$$E\{\nu(t)\nu^T(t+\tau)\} = Q\delta(\tau)$$

Now (25) differs from (22) only in that $u(t)$ is not a white noise. However, the autocorrelation function of $u(t)$ is the same as that of integrated white noise, so, neglecting higher moments, we have

$$\dot{u}(t) = \eta(t) \tag{26}$$

The standard approach is to add $u(t)$ to the state of the system $x(t)$ to form a new state vector $z(t)$ where

$$z(t) = \begin{pmatrix} x(t) \\ \cdots\cdots \\ u(t) \end{pmatrix}$$

and

$$z(t) = \begin{pmatrix} F & : & G \\ \cdots & & \cdots \\ 0 & : & 0 \end{pmatrix} z(t) + \begin{pmatrix} 0 \\ \cdots \\ I \end{pmatrix} \eta \tag{27a}$$

$$\theta(t) = (C:0)z(t) + Q\nu(t) \tag{27b}$$

$$y(t) = (D:0)z(t) \tag{27c}$$

The system (27) is now in the desired form [that is, the same as (23c)] but, unfortunately, the matrix pair

$$\left\{ (C:0),\ \begin{pmatrix} F & : & G \\ \cdots & & \cdots \\ 0 & : & 0 \end{pmatrix} \right\}$$

is generally not detectable, and (23c) does not have a finite steady state solution. This result follows immediately from the fact that autocorrelation matrix of $z(t)$ contains the autocorrellation matrix of $u(t)$. This latter matrix has elements which approach infinity as time increases [Recall that the spectral density of $u(t)$ is $1/s^2$, and the inverse transform of this term is t. Therefore, the variance of $u(t)$ increases as t.]

One way around the above difficulty is to construct a system which does not involve the input disturbance as a part of the state vector. Such a construction follows and is parallel to that given in the previous section.

1. Subtract the steady state error of estimation from the output $y(s)$ [see Equation (15)]:

$$y_1(s) = y(s) - r_1^T(0)u(s)$$
$$= (b^T(s) - r_1^T(0))u(s) \qquad (28)$$
$$\equiv b_1^T(s)u(s)$$

2. Define the dynamic error in estimation as

$$v(s) \equiv y_1(s) - \alpha^{T*}(0)\theta(s) \qquad (29)$$

where $\alpha^*(0)$ is the optimal steady state estimator. From (28) and (2)

$$v(s) = [b_1(s) - A(s)\alpha^*(0)]^T u(s)$$
$$= [b_1(s) - A(s)\alpha^*(0)] \frac{\eta(s)}{s} \qquad (30a)$$
$$\equiv E(s)\eta(s)$$

Since $A(0)\alpha^*(0) = b_1(0)$ by construction, the matrix $E(s)$ will not contain a pole at the origin. The observations can be written as

$$\theta(s) = \frac{z(s)}{s} + \nu(s) \qquad (30b)$$

where

$$z(s) = A(s)\eta(s) \qquad (30c)$$

3. Construct a minimal realization of (30) of the form

$$\dot{x}(t) = \tilde{F}x(t) + \tilde{G}\eta(t) \qquad (31a)$$

$$v(t) = \tilde{D}x(t) \qquad (31b)$$

$$\theta(t) = \tilde{C}x(t) \qquad (31c)$$

By construction, $(\tilde{F}, \tilde{G})$ is controllable. Further, since the only unstable modes of the system are associated with the observations θ, the system $(\tilde{C}, \tilde{F})$ will be detectable. Thus, the steady state solution of (23c) will exist, and the desired estimator can be obtained by solving (23). The entire procedure is carried out later in this paper.

SUBOPTIMAL ESTIMATION

The class of suboptimal estimators we are concerned with are those of fixed dimension. The design problem then reduces to choosing the estimator parameters so as to minimize the mean square error in estimator performance. The minimization procedure we suggest follows the methods given by Newton, Gould, and Kaiser (1957).

Given an estimator of the form

$$\alpha = \alpha(s, p_1, p_2, \ldots, p_l) \qquad (32)$$

we wish to minimize

$$E\{e^2(t)\} \quad \text{over} \quad p_1, p_2, \ldots, p_l \qquad (35)$$

where $e(s)$ is the error in estimation given by

$$e(s) = y(s) - \alpha^T(s)\theta(s) \qquad (33)$$

From Equation (10), the mean squared error can be written as

$$\overline{e^2(t)} = \frac{1}{2\pi j}\int_{-j\infty}^{+j\infty} \frac{r^T(-s)r(s)}{-s^2} ds \qquad (34)$$
$$r(s) \equiv b(s) - A(s)\alpha(s)$$

For reasons discussed earlier, we assume that the steady state error has been subtracted from $y(s)$ so that the above integral converges. (This implies that the poles at $s = 0$ will cancel with zeroes in the numerator.)

Consider the evaluation of $\overline{e^2(t)}$ given $p_1, p_2, \ldots, p_l$. If the integrand can be expressed as a ratio of polynomials of order <10, the integral can be evaluated using the tables given in Newton, Gould, and Kaiser (1957). Another approach is to evaluate the integral by the residue theorem. The integral of Equation (34) can be written in expanded form as

$$\overline{e^2(t)} = \frac{1}{2\pi j}\int_{-j\infty}^{+j\infty} \frac{g(s)}{-s^2} ds \qquad (35)$$

where

$$g(s) = \sum_{i=1}^{n}\sum_{k=1}^{m+1}\sum_{q=1}^{m+1} a_{ik}(-s)\alpha_k(-s)a_{iq}(s)\alpha_q(s)$$

where

$$a_{im+1}(s) = b_i(s) \quad \text{and} \quad \alpha_{m+1}(s) = -1$$

Joseph (1975) shows that the summation can be taken outside the integral if the poles at $s = 0$ are not included in the calculation of residues of the individual integrals in the sum. The integral above can be converted into a closed contour integral in the complex plane by closing the contour either to the right or to the left in an infinite semicircle. Since the integral along the infinite semicircle vanishes [recall that both $A(s)$ and $b(s)$ have the denominator at least one order higher than the numerator], the mean squared error is simply the sum of the residues at each of the poles of the integrand enclosed by the contour.

Using the procedure above, the mean square error can be evaluated given the parameters $p_1, p_2, \ldots, p_l$. The constrained optimal estimator can be constructed by using any standard nonlinear programming package to minimize the mean squared error over the parameters $p_1, p_2, \ldots, p_l$. (See, for example, Lasdon et al., 1973).

The above ideas of suboptimal estimation can be extended to include systems containing time delays in their transfer functions. The evaluation of integrals containing time delay terms is discussed by Brosilow and Naphtali (1965). Joseph (1975) describes how the techniques can be adapted to integrals of the form given in Equation (35). (Owing to poles at the origin, the method of Brosilow and Naphtali must be modified slightly.)

INFERENTIAL CONTROL USING OPTIMAL AND SUBOPTIMAL ESTIMATORS

We now consider a process described by

$$y(s) = b^T(s)u(s) + c(s)m(s) \qquad (36)$$

$$\theta(s) = A^T(s)u(s) + P(s)m(s) \qquad (37)$$

The control problem is to determine $m(s)$ from measurements $\theta(s)$ such that $E\{y^2(t)\}$ is minimized. Since $m(s)$ is a measured quality, the problem can be simplified by defining a variable $\theta'(s) = \theta(s) - P(s)m(s) = A^T(s)u(s)$ and determining a transfer function relating $\theta'(s)$ and $m(s)$. Let this transfer function be denoted by $W(s)$. The proposed configuration is shown in Figure 2.

The problem is similar to the compensator design for semifree configurations discussed in Newton, Gould, and Kaiser (1957). Extending their results to the vector case, we can write the function $W(s)$ which minimizes $E\{y^2(t)\}$ as

$$W(s) = -\frac{1}{c(s)\alpha} c^{T*}(s) \qquad (38)$$

provided $c(s)$ is a minimum phase transfer function. Here, $\alpha^*(s)$ is the optimum estimator for $b^T(s)u(s)$ from $A^T(s)u(s)$. Let

$$d(s) = b^T(s)u(s) \qquad (39)$$

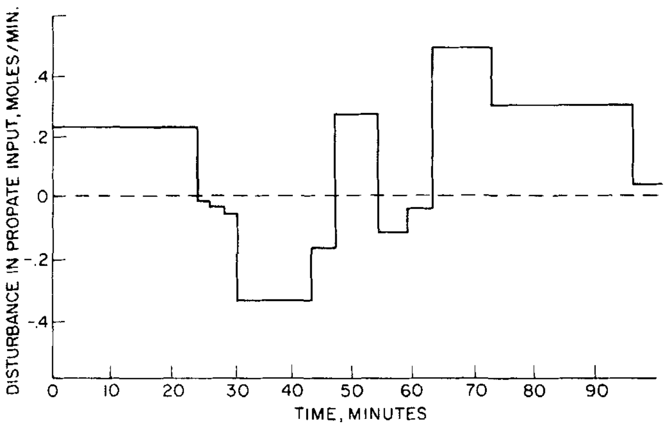

Fig. 1. Typical input disturbance.

If measurements of u were available, then $d(s)$ would be known, and in order to minimize

$$y(s) = d(s) + c(s)m(s) \tag{40}$$

one would choose

$$c(s)m(s) = -d(s) \tag{41}$$

or

$$m(s) = -\frac{d(s)}{c(s)} \tag{42}$$

provided $c(s)$ is minimum phase. Now, $\alpha^{T*}(s)\theta'(s)$ is an optimal estimate of $d(s)$. Equation (38) implies that the control problem and estimation problem can be treated independently (see the separation theorem of optimal control theory).

If $c(s)$ is not minimum phase or a suboptimal estimator is used to estimate $d(s)$, then the design of controller and estimator should be carried out simultaneously. The techniques of the previous sections can be applied to such design problems by changing the objective function to $E\{y^2(t)\}$, where

$$y(s) = b^T(s)u(s) + c(s)G(s)\alpha^T(s)A^T(s)u(s) \tag{43}$$

A simpler approach is to carry out the design of the estimator and controller separately even for suboptimal control systems. Here, the controller transfer function is chosen such that

$$G(s)c(s) \cong -1$$

over a desired frequency range. Then

$$y(s) = d(s) + c(s)G(s)\hat{d}(s) = d(s) - \hat{d}(s) \tag{44}$$

The better the approximation of $d(s)$ to $\hat{d}(s)$ and $c(s)G(s)$ to -1, the smaller the deviation of $y(t)$ from zero.

APPLICATION TO MULTICOMPONENT DISTILLATION

The techniques of output estimation and inferential control are tested on the dynamic model of a multicomponent distillation column selected from the literature (Amundson, 1958). The objective of the study is to compare the effectiveness of optimal and suboptimal estimation to track the output composition and to compare conventional feedback controllers with inferential control systems. Optimal and suboptimal estimators using single and multiple temperature measurements are constructed using linear input-output models of the process to estimate the bottom product composition. The column is subject to random step input changes in the input flow rates of various components, and the actual and estimated compositions are monitored. Inferential control systems using suboptimal estimators are compared against single temperature feedback control. Finally, the effect of time delays in the measurements on the estimation and control systems are investigated. All studies were conducted on a nonlinear simulation model of the column using a digital computer (UNIVAC 1108).

Description of the Column

The dynamic model of the column is the same as that used in Part II and was obtained by writing a mass balance on each of the stages. The resulting set of differential equations were integrated using a modification of Euler's implicit method. Details of the computational method are given in a thesis by Jawaid (1970).

The mole fraction of propane in the bottoms was selected as the controlled variable. Control was accomplished by manipulating the vapor boil up from the reboiler. The input disturbances were taken as the changes in the flow rates of individual components in the feed. A linear input-output model of the process, constructed by step input tests, is given in Part II. For reference purposes, part of the model is reproduced below:

$$\theta_3 = \frac{-15.91}{12s+1}u_2 + \frac{-4.23}{5s+1}u_3 \tag{45}$$

$$\theta_8 = \frac{-16.43}{10s+1}u_2 + \frac{-0.47}{5s+1}u_3 \tag{46}$$

$$y = \frac{0.0253}{13s+1}u_2 + \frac{0.0045}{4s+1}u_3 \tag{47}$$

The input disturbances were modeled as a sequence of random amplitude step inputs arriving at random intervals of time. The samples of the input disturbances used in the estimation and control study were generated to obey specified statistics using pseudo random number tables. The time interval between arrivals of successive inputs were modeled to obey the Poisson distribution, and the amplitudes of the steps were modeled as Gaussian random variables with mean zero. Figure 1 shows a typical input disturbance function.

Suboptimal Estimators

Suboptimal estimator used in this study are of the form

$$\alpha(s) = \left[\alpha_{10}\frac{\tau_{a1}s+1}{\tau_{b1}s+1}, \alpha_{20}\frac{\tau_{a2}s+1}{\tau_{b2}s+1}, \ldots\right] \tag{48}$$

The constants α_{10}, α_{20} . . . are those associated with the optimal steady state estimator. The time constants τ_{a1}, τ_{b2} . ., etc., were determined such that the expected error in estimation was minimized. The minimization was carried out using a generalized reduced gradient algorithm (Lasdon et al., 1973). The largest optimization problem solved had five measurements and five inputs yielding a total of ten optimization variables and took approximately 20 s of CPU time on a UNIVAC 1108 computer. The function being minimized was not very sensitive to changes in the optimizing variables near the optimum.

Optimal Estimators

Optimal estimators for estimating the bottoms propane were constructed using the methods described earlier. Attention was restricted to only two input disturbances (u_2 and u_3) to reduce computational complexity. The problem of estimating y from θ_3 and θ_8 [see Equations (45), (46), and (47)] is considered in detail to illustrate the procedures. First, the dynamic error in estimation is calculated from Equation (29):

$$v(s) = y(s) - \alpha^{T*}(o)\theta(s) = \left(\frac{0.01591}{12s+1} + \frac{0.00945}{10s+1} - \frac{0.0253}{13s+1}\right)u_2 + \left(\frac{0.0045}{5s+1} - \frac{0.0045}{4s+1}\right)u_3 \quad (49)$$

The statistics of the input disturbances were computed as follows. Input disturbance u_2 was assumed to consist of step inputs whose amplitudes were Gaussian distributed with mean zero and standard deviation 0.34 mole/min. This represents 10% of the steady state feed flow rate of propane; u_3 was modeled similarly but with a standard deviation of 0.68. The step disturbances were assumed to arrive at the rate of 6 inputs/hr; that is

$$\nu = \frac{1}{10}\,\text{min}$$

With these parameters, the spectral density of the input disturbances becomes

$$\Phi_{uu}(s) = \begin{bmatrix} \dfrac{.0116}{-s^2} & 0 \\ 0 & \dfrac{0.0464}{-s^2} \end{bmatrix}; \quad u = \begin{pmatrix} u_2 \\ u_3 \end{pmatrix}$$

These disturbances can be modeled as

$$u(s) = \frac{I\eta(s)}{s} \qquad \eta = \begin{pmatrix} \eta_2 \\ \eta_3 \end{pmatrix}$$

where

$$E\{\eta\} = 0 \quad \text{and} \quad E\{\eta(t)\eta(t+\tau)\} = \text{diag}[0.0116, 0.0464]\cdot\delta(\tau)$$

The dynamic error becomes

$$v(s) = \left(\frac{0.0159}{s(12s+1)} + \frac{0.00945}{s(10s+1)} - \frac{0.0253}{s(13s+1)}\right)\eta_2 + \left(\frac{0.0045}{s(5s+1)} - \frac{0.0045}{s(4s+1)}\right)\eta_3 \quad (50a)$$

We also have from Equation (30c)

$$z(s) = A(s)\eta(s) = \begin{bmatrix} \dfrac{-15.91}{12s+1} & \dfrac{-4.2}{5s+1} \\ \dfrac{-16.43}{10s+1} & \dfrac{-0.47}{5s+1} \end{bmatrix} \begin{bmatrix} \eta_1(s) \\ \eta_2(s) \end{bmatrix} \quad (50b)$$

The system described by Equation (50) can be realized in the time domain in a number of ways. Following the minimal realization procedure of Gilbert (1963) adapted from Perkins and Cruz (1969), we get

$$\dot{x} = Fx + G\eta \quad (51)$$

with

$$F = \text{diag}\,[-1/12, -1/10, -1/13, -1/5, -1/4]$$

$$G^T = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

$$v(t) = 0.01591\,x_1 - 0.00945\,x_2 + 0.0253\,x_3 - 0.0045\,x_4 + 0.0045\,x_5 \equiv Dx \quad (52)$$

z_1 and z_2 are given by

$$z_1(t) = -1.325\,x_1 - 0.846\,x_4$$
$$z_2(t) = -1.643\,x_2 - 0.094\,x_3$$

Let the observations $\theta(t)$ be corrupted with white Gaussian noise ν of mean zero and covariance

$$E\{\nu(t)\nu(t+\tau)\} = \text{diag}[0.01, 0.01]\delta(t) \equiv Q\delta(t)$$

Since

$$\theta(s) = \frac{z(s)}{s} + \nu(s)$$

We can define two new states x_6 and x_7 as

$$\dot{x}_6 = z_1 = -1.325\,x_1 - 0.846\,x_4$$
$$\dot{x}_7 = z_2 = -1.643\,x_1 - 0.094\,x_3 \quad (53)$$

Adding x_6 and x_7 to the system state, we get

$$\dot{x} = \tilde{F}x + \tilde{G}\eta \quad (54a)$$

$$\theta(t) = \tilde{C}x + \nu \quad (54b)$$

where

$$\tilde{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\tilde{F} = \begin{bmatrix} -0.0834 & & & & & & \\ & -0.10 & & & & & \\ & & -0.077 & & & & \\ & & & -0.2 & & & \\ & & & & -0.25 & & \\ -1.35 & 0 & 0 & -0.846 & 0 & 0 & 0 \\ 0 & -1.643 & 0 & -0.094 & 0 & 0 & 0 \end{bmatrix} \quad \tilde{G} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

The Kalman filter for the above system with observations defined in Equation (54) is given by

$$\dot{\hat{x}} = \tilde{F}\hat{x} + P\tilde{C}^T[\theta - \tilde{C}\hat{x}] \quad (55)$$

where P is the steady state solution of

$$\dot{P}(t) = \tilde{F}P + P\tilde{F}^T - P\tilde{C}^TQ^{-1}\tilde{C}P + \tilde{G}\phi_{\eta\eta}\tilde{G}^T \quad (56)$$
$$P(0) = 0$$

The steady state solution of (56) can be obtained by numerically solving the differential equation until $P(t)$ reaches a constant value. This method proved to be very time consuming owing to the need for small step sizes. (A fourth-order explicit Runge-Kutta algorithm was tried.) A second approach is to solve the discrete Kalman filter for the finite-difference version of Equation (54). The discrete version of the filter, converged in about twenty to forty iterations.*

The expected error in the estimation of the dynamic error $v(t)$ can be calculated as follows. Let $e(t)$ denote the error in the estimation of $v(t)$ and $\epsilon(t)$ denote the error in the estimation of $x(t)$. Then

$$\begin{aligned} E\{ee^T\} &= E\{D\epsilon\epsilon^T D^T\} \\ &= DE\{\epsilon\epsilon^T\}D^T \\ &= DPD^T \end{aligned} \quad (57)$$

The error in the estimation of y can be calculated from

* In order to prevent the divergence of the filter owing to numerical roundoff errors, it was necessary to symmetrize the covariance matrix at every time step.

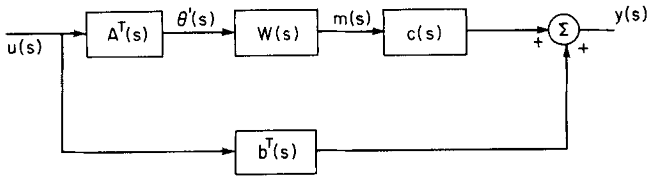

Fig. 2. The control system.

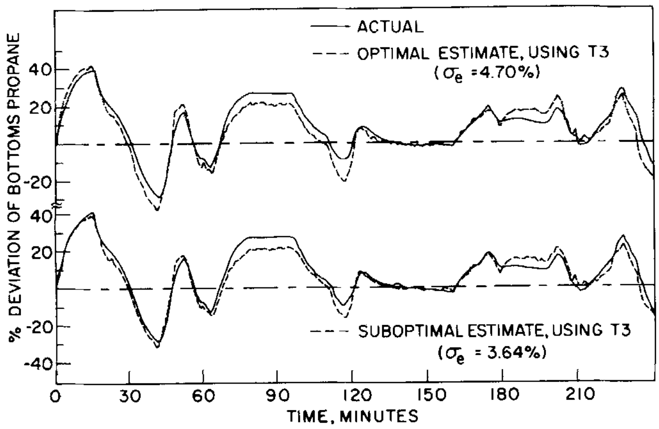

Fig. 3. Optimal and suboptimal estimation using T_3.

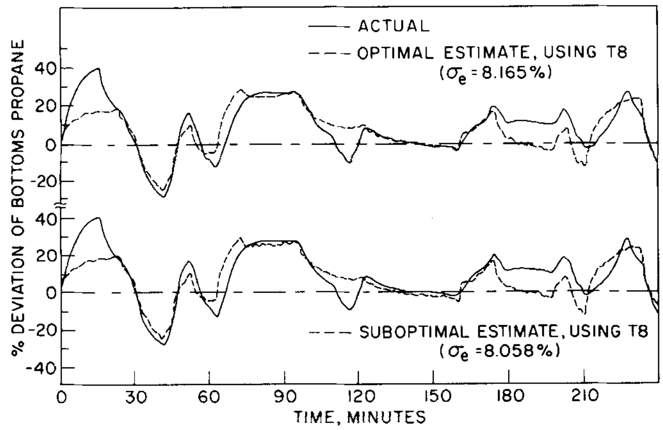

Fig. 4. Optimal and suboptimal estimation using T_8.

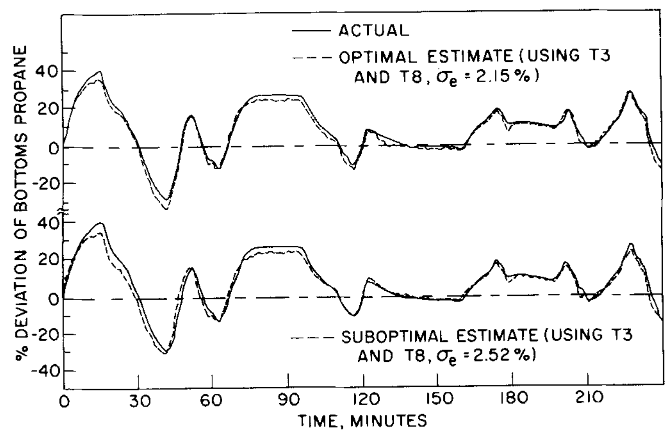

Fig. 5. Optimal and suboptimal estimation using T_3 and T_8.

$$\hat{y}(t) = \alpha^T(0)\theta + v(t) \tag{58}$$

However, since noise in $\theta(t)$ is small, the error in $\hat{y}(t)$ will be closely approximated by the error in $v(t)$.

Results of the Estimation Study

Figures 3, 4, and 5 compare the ability of optimal and suboptimal estimators to track the actual output composition when the column is subject to random step disturbances in the input flow rates of propane and butane. The disturbances u_2 and u_3 were generated with a spectral density $\Phi_{uv}(s) = \text{diag}[0.0116/-s^2, 0.0464/-s^2]$. The temperature measurements were corrupted by Gaussian random noise of standard deviation 0.1°F before feeding to the estimators. The effect of noise in the measurements was not included in the design of the suboptimal estimator since the noise was not significant. The column was run for 250 min of operating time. The average over the 250 min should give a fairly good representation of the estimator performance.

Table 1 compares the mean square error observed from the test runs with the mean square error predicted by Equations (57) and (34). The calculated values contain only the dynamic error in estimation. The mean square errors are reported as a percentage of the steady state value of the mole fraction of propane in the bottoms.

All estimators do a good job of tracking the output composition. There is very little gain in using the optimal estimators over suboptimal estimators. For the two temperature estimators there is no steady state error in estimation, and hence the calculated and experimental errors in estimation can be compared. The observed values are considerably larger. This can be attributed to process nonlinearities and, to a smaller extent, to the limited amount of time that the column was run. Figures 5, 6, and 7 show that most of the error in estimation is incurred when the deviation of the output from the steady state is large. Comparison of the temperature predicted by the linear model and the simulation model showed that when the deviation of the output is large, inaccuracy of the linear model was the major cause of errors in estimation.

In order to see how sensitive the estimator was to changes in input statistics, input disturbances with a spectral density

Table 1. Comparison of Estimators

Estimator	σ_d Calculated (%)	σ_e Observed (%)
A. Optimal estimator		
1. Using T_3	4.3	4.705
2. Using T_8	5.15	8.165
3. Using T_8 and T_3	0.817	2.150
B. Suboptimal estimators		
1. Using T_3	5.08	3.644
2. Using T_8	5.20	8.058
3. Using T_3 and T_8	1.25	2.524

$\sigma_d^2 = E\{e^2(t)\}/x_2^2 \times 10^4$ from Equation (57)

$\sigma_e^2 = E\{e^2(t)\}/x_2^2 \times 10^4$ from simulation studies

Suboptimal estimators

1. Using T_3 $\quad \alpha(s) = -1.39 \times 10^{-3} \left(\dfrac{3.27s + 1}{3.62s + 1}\right)$

2. Using T_8 $\quad \alpha(s) = -1.57 \times 10^{-3} \left(\dfrac{10s + 1}{13s + 1}\right)$

3. Using T_3 and T_8

$$\alpha^T(s) = -10^{-3} \left(\frac{10.3s + 1}{8.7s + 1}, (0.57)\frac{(6.4s + 1)}{(13.6s + 1)}\right)$$

Tong's estimator using T_3 and T_8

$$\alpha^T(s) = -10^{-3}\,[1, (0.57)] \left(\frac{7.5s + 1}{8.5s + 1}\right)$$

$$\Phi_{uu} = \begin{bmatrix} \dfrac{0.0116}{-s^2} & \dfrac{0.0116}{-s^2} \\ \dfrac{0.0116}{-s^2} & \dfrac{0.0116}{-s^2} \end{bmatrix}$$

were fed to the column, and the suboptimal estimator using T_8 and T_3 was used to monitor the composition. The standard deviation of the percent error in estimation (σ_e) was now 3.463 compared to $\sigma_e = 2.324$ for the previous set of input disturbances. Although this test is not conclusive, it indicates that the estimator is not very sensitive to input statistics.

Part II of this series of papers describes an ad hoc procedure for designing suboptimal estimators. For comparison purposes, an estimator following the ad hoc procedure was constructed and tested. The standard deviation of the percent error in estimation for the ad hoc estimator using temperatures T_3 and T_8 was 2.72, compared to σ_e of 1.25 for the suboptimal estimator.

Next, the column was subject to changes in input flow rates of all components with a spectral density given by

$$\Phi_{uu}(s) = \text{diag}[0.0116, 0.0116, 0.0116, 0.0116, 0.0116]/-s^2$$

The average arrival times of all disturbances were assumed to be 19 min. The input flow rate of hexane and ethane varied as much as 100% in this study. A suboptimal estimator using T_1 and T_3 (these two temperatures gave a smaller steady state error than T_3 and T_8) was constructed. The estimate was given by

$$\alpha(s) = \left[0.00155 \frac{10.03s + 1}{9.73s + 1}, -0.00256 \frac{8.08s + 1}{7.63s + 1} \right]$$

Figure 6 compares the actual and estimated compositions in this case. Again, the estimator does a good job of tracking the output composition. The performance is not as good as in the two-input case.

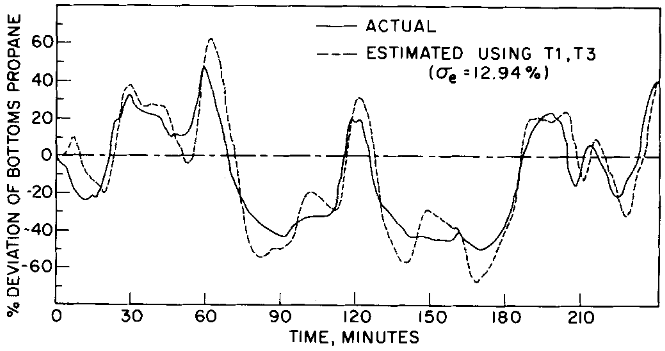

Fig. 6. Suboptimal estimation using T_1 and T_3: all feed component flows varying.

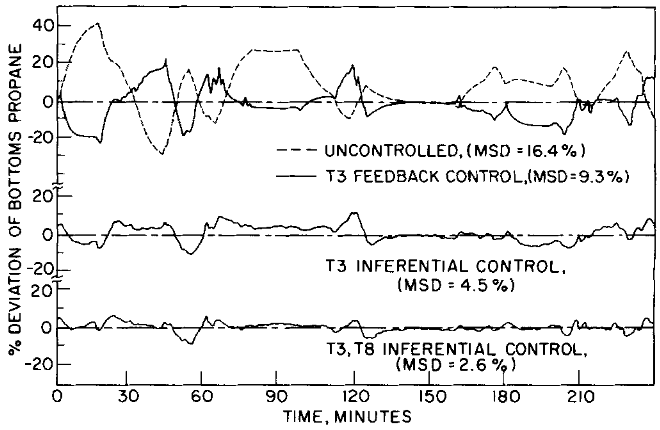

Fig. 7. Comparison of control strategies—two disturbances.

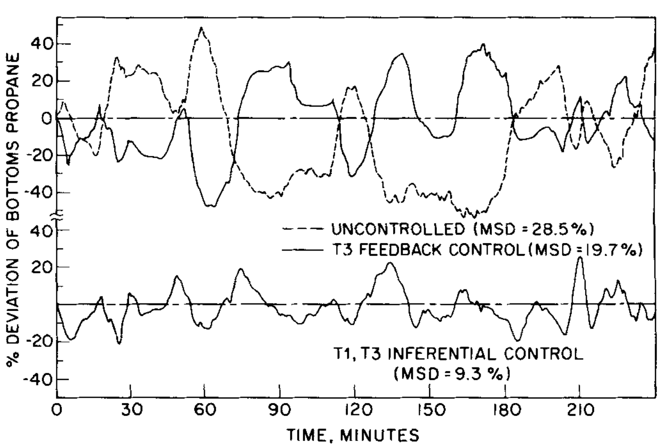

Fig. 8. Comparison of control strategies—five disturbances.

Inferential Control Using the Suboptimal Estimates

In this section, various inferential control schemes are compared against conventional single temperature feedback control. Only suboptimal estimators were used in this study, since the results of the estimation study show that there is little difference in performance between optimal and suboptimal estimators. The single temperature feedback controllers were of the proportional integral type tuned on-line.

The transfer function relating changes in the manipulated variable to changes in output composition was determined to be

$$C(s) = -\frac{0.00768}{7s + 1}$$

A schematic of the inferential control system is given in Figure 1.

The performance of inferential control systems with T_3 feedback control system is compared in Figure 7. Temperature T_3 was selected for feedback because it had the smallest steady state error of all temperature measurements. Only u_2 and u_3 were varied in this study with the same input statistics used in the estimation study. T_3 feedback control is able to reduce the deviation of propane in half. However, the inferential control system using the same temperature (involving two more integrators) does almost twice as good. Using the two-temperature estimator, the deviation of propane is reduced even further. (The two temperature inferential control system requires five integrators.)

Figure 8 compares inferential and T_3 feedback control schemes when all five input disturbances are present. A suboptimal estimator using T_1 and T_3 was used in the inferential control system. Again, the deviation of the output quality is considerably less for the inferential control system.

In all inferential control schemes studied, the temperature measurements were corrupted with Gaussian white noise of mean zero and standard deviation 0.1°F.

An attempt was made to improve the performance of the inferential control system by using a five-temperature measurement set. In order to get a small condition number, these measurements were distributed across the column. However, the resulting inferential control system did worse than the two-temperature control system (MSD

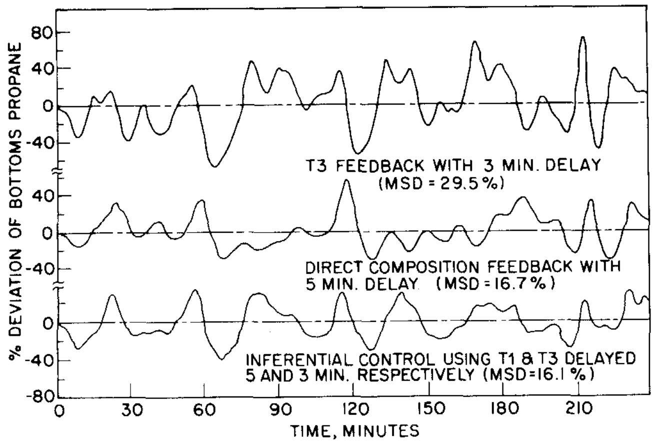

Fig. 9. Effect of measurement delays.

$= 28.1$ compared to 9.1 for the two-temperature control). The reason was traced to the fact that the five-temperature estimator gave undue weight (determined by the steady state estimator) to some measurements which were slow in responding (had large time constants). For this particular input disturbance train, the process is not in steady state for a significant length of time. Hence, it is not necessary to have a good steady state estimation (note that the five-temperature estimator gives perfect estimation in the steady state). For such processes, the input disturbances may be modeled by

$$\Phi_{uu}(s) = \nu\xi^2/(-s^2 + \nu^2)$$

This spectral density also represents a series of random step input disturbances (Chang, 1961). With this model, it is no longer necessary to impose the restriction of perfect steady state estimation in the design of optimal and suboptimal estimators. As $\nu \rightarrow 0$ (when disturbances arrive at slower rates) while keeping $\nu\xi^2$ constant the above model approaches the input disturbance model used in this study.

Effect of Measurement Delays

Although temperature measurement of distillation columns do not have much delay associated with them, time delays were introduced in the measurements in order to see their effect on various control schemes. Arbitrary time delays of 3 and 5 min were introduced in the measurement of T_3 and T_1, respectively. A suboptimal estimator of the form given in Equation (48) was designed to predict the bottoms propane composition. Inferential control was implemented using this estimator. A proportional-integral temperature feedback control was designed using the temperature on stage 3 (delayed by 3 min). In addition, a proportional integral type of direct composition feedback control was designed with a measurement delay of 5 min. Both PI controllers were tuned on-line. The column was run under all three different control schemes on the simulated column. All five input disturbances to the column were perturbed. The results are shown in Figure 9.

The inferential control system is better than the T_3 feedback control and comparable to the direct composition feedback control. Measurement delay has a significant effect on direct composition feedback control, since the square root of the mean squared error of control using composition feedback when no delay was present in the measurement was only 1.9%.

A comparison of Figures 8 and 9 shows that the inferential control scheme with no delays is better than the direct composition feedback control with a 5 min delay.

CONCLUSIONS

Process nonlinearities sufficiently influence the behavior of inferential control systems so that there is little or nothing to be gained by implementing optimal linear estimators. Linear suboptimal estimators are adequate for most systems. These estimators often need be nothing more than lead networks whose parameters are chosen so as to minimize the expected mean square error.

ACKNOWLEDGMENT

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NOTATION

$a_{ik}(s)$ = ik^{th} element of $A(s)$
$A(s)$ = transfer function matrix relating measurements $\theta(s)$ to disturbances $u(s)$
$b(s)$ = transfer function matrix relating outputs $y(s)$ to disturbances $u(s)$
$b_1(s)$ = $b(s) - r(0)$
$C(s)$ = transfer function matrix relating outputs $y(s)$ to disturbances $u(s)$
C = matrix relating measurements $\theta(t)$ to the system state $x(t)$
$d(s)$ = disturbance function $= b^T(s)u(s)$
D = matrix relating outputs $y(t)$ to the system state $x(t)$
$e(\cdot)$ = error in estimation or control
E = expected value of
$E(s)$ = $b_1(s) - A(s)\alpha^*(0)$
F = system matrix relating $x(t)$ to $\dot{x}(t)$
G = matrix relating $u(t)$ to $\dot{x}(t)$
$G(s)$ = transfer function matrix relating the control effort to the error
$m(\cdot)$ = vector of control efforts
$m(s)$ = vector of manipulated variables
MSD = mean square deviation
P = covariance matrix of the state $x(t)$
$P(s)$ = matrix of transfer functions relating the measurements $\theta(s)$ to the control efforts $m(s)$
Q = covariance matrix of measurement noise
$r(s)$ = $b(s) - A(s)\alpha(s)$
s = Laplace transform variable
t = time
$u(\cdot)$ = vector of input disturbances
$u_o(\cdot)$ = unit step function
$v(\cdot)$ = $y_1(\cdot) - \alpha^{*T}(0)\theta(\cdot)$
$x(t)$ = system state
$y(\cdot)$ = system output
$y_1(\cdot)$ = $y(\cdot) - r^T(0)u(\cdot)$
y_d = desired value of y

Greek Letters

$\alpha(s)$ = vector of transfer functions used to estimate the output from measurements
$\delta(t)$ = impulse function
$\eta(t)$ = white noise
$\theta(\cdot)$ = vector of (temperature) measurements
θ' = θ-Pm
$\nu(s)$ = white measurement noise
$\nu(t)$ = measurement noise
ϕ = autocorrelation function of a random variable
$\phi_{\eta\eta}$ = constant matrix
Φ = Laplace transform of ϕ
σ^2 = $10^4E\{e^2(t)\}/x^2(t)$

Superscripts

T = transpose of a matrix
-1 = inverse of a matrix

$\hat{(\cdot)}$ = estimate of $(\cdot)$
$(\cdot)^*$ = optimal value of $(\cdot)$
$\overline{(\cdot)}$ = mean value of $(\cdot)$

Subscripts

e = experimental value
d = calculated value

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Particle Turbulent Diffusion in a Dust Laden Round Jet

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The turbulent diffusion mechanism of particles in a round air jet are studied both theoretically and experimentally, with particular attention to the relative velocity between particles and fluid, overshooting effect of particles, and the distributions of fluid properties in space. The results indicate that the particle diffusivity decreases with the increase of the particle inertia. In general, the turbulent diffusivity of particles in an air jet is smaller than that of fluid scalar quantities. The particle inertia and the fluid large eddies, which are expressed by the Stokes number and the integral scale, respectively, play an important role in the transport mechanism of particles.

SCOPE

Attention has been focused on the diffusion of small particles in dust laden turbulent jets. Such a phenomenon is of interest in rocket engine exhausts, atomized fuel injection systems, spraying and waste disposal plumes, and also applied to such diverse applications as numerous cleaning devices and aerosol production. The principal purpose of the present study is to reveal the mechanism of the particle turbulent diffusion in the dust laden jet by predicting particle turbulent diffusivities theoretically and measuring them experimentally.

Many theoretical investigations of the turbulent diffusion of particles in the stream have been done. Most of the work, however, paid less attention to the effects on the particle diffusion summed up as follows.

1. The effect of the overshooting of particles from one eddy to another.

2. The effect of the relative velocity of particles to fluid due to the interaction between fluid movement and particles.

3. The effect of the various distributions of time averaged fluid velocities and turbulent properties (intensity, time scale, etc.) in space.

Moreover, in experimental works the assumption was also made that time averaged velocities of particles and fluids are equal, so that the turbulent diffusivity of particles may be calculated from the experimental result of concentration distribution.

In order to describe the mechanism of the turbulent diffusion of particles correctly, the factors described above should be taken into consideration, especially in a real situation, such as a jet flow.

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