# Part III: Optimal Selection of Secondary Measurements within the Framework of State Estimation in the Presence of Persistent Unknown Disturbances

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When primary control objectives cannot be measured directly, secondary measurements have to be selected and used in conjunction with estimators to infer the value of the unmeasurable variables. Unmeasured process disturbances (state excitation noise) are assumed to be of major importance, dominating the errors caused by measurement noise. Since the white noise assumption is generally insufficient for the persistent disturbances commonly occurring in the chemical engineering environment, a nonstationary noise model has been employed, and is shown to yield superior estimations under these circumstances. New necessary and sufficient conditions have been developed for the observability of the dynamic system augmented to include the noise model.

A variety of new measurement selection criteria is presented here, with the goal of minimizing estimation error. One class of criteria aims at minimizing the transient estimation error when a static estimator is used. The other class minimizes the measurement error caused by the unobservable subspace. The design of state reconstruction procedures (which are able to handle persistent unmeasured process disturbances) is explained in a stochastic and a deterministic framework. Finally, the synthesis of reduced order control schemes is discussed. The power of the selection criteria and the superiority of a Kalman filter design employing a nonstationary noise model is demonstrated in many examples.

## SCOPE

Frequently, in process control, some important variables are not available for measurement. Secondary measurements have to be selected and used to infer the value of the unmeasurable variables. The proper selection of secondary measurements is a task of paramount importance for the synthesis of control structures. The measurements should be selected to minimize estimation error. The error can be caused by differences between the real system and the process model which forms the basis for the design of the estimator, or by process and measurement noise. Here, the criteria derived consider the influence of those different factors on the error separately: Selection Criterion 1 assumes a steady state model and minimizes the error caused by unmeasurable inputs with normally distributed amplitudes: Selection Criterion 2 (Joseph, Brosilow 1978) minimizes the influence of model inaccuracies. Criteria 3 and 4 minimize the error when a static estimator, which has the advantage of being very simple to implement, is used for the dynamic system.

For a linear dynamic system with white state excitation and measurement noise, the Kalman filter is known to be the best estimator—in the sense of minimum variance, maximum likelihood, etc. If a step change in the inputs to the unit occurs which cannot be measured, or if an unknown change is caused by drifting conditions upstream (so that the process will display a steady state or pseudo steady state behavior under those disturbances), this estimator performs quite poorly. The objective of this article is to present an easily implementable technique which meets those challenges encountered most frequently in practical situations. The method differs from others in the literature through its general applicability, superior performance, simplicity of the construction procedure, and the mathematical rigor of the derivation. The good performance is accomplished using a nonstationary noise model. There are limitations to this approach however, caused by the requirement of observability. Those limitations are overcome here in an optimal fashion: Selection Criterion 1 is proven to minimize the influence of the unobservable subspace on the estimates.

## CONCLUSIONS AND SIGNIFICANCE

Several criteria for the selection of secondary measurements were developed to minimize the mean square estimation error. Simulation examples demonstrated their usefulness and computational ease. The important problem of estimation in the presence of persistent unmeasurable process disturbances is solved in the framework of filtering, with a nonstationary noise model. We began with a simple static estimator which is estimating the unknown inputs using an inverse of the static process model. From this, a dynamic estimation scheme was developed, which combines the features of the static estimator and the Kalman filter, to deal with persistent unknown disturbances in an optimal fashion. It can be regarded as an overdue filling of a significant gap which has probably prevented some practical applications of those more complicated tools. The method is demonstrated on several examples taken from the literature, and is superior in performance to other known techniques. For applications, the presence of nonlinearities might be detrimental when disturbances push the process too far off the state assumed for linearization. Generally, however, a controller will be present, to avoid larger excursions from the steady state by using the corrected state estimates given by the modified Kalman filter.

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In Parts I and II of this series, methods are developed for generating alternative regulatory and optimizing control structures. Economic measures are used to evaluate the benefits of hierarchical control schemes. Extensions of the controllability and observability concepts are utilized to decide on the practical feasibility of the alternatives.

One assumption is present throughout the first two parts: If the measurement of a variable for quality regulation or optimizing control is desirable, it is technically and economically feasible to install a measurement device performing this duty. There are, however, many examples where a specific instrument is notoriously inaccurate, where the time lags associated with the sampling make the direct use of the result in a feedback loop impossible, or where a certain quantity (like catalyst activity) just cannot be measured on line. In those common instances, an estimation device is needed to infer the value of an unmeasurable variable from readily available measurements.

Frequently, many measurements are available as inputs to the estimator. It is rarely technically feasible, desirable or necessary to use all of them. Intuitively it might appear that the quality of the estimate will improve uniformly with the number of measurements. However, as Joseph and Brosilow (1978) show, not even this is necessarily true. The question arises, then, which measurement should be used for the best estimate possible of the important, but unmeasurable, process variables.

Although deterministic state reconstruction procedures for linear dynamic systems are available (e.g. Luenberger observer) it is more natural to view the question of measurement selection in a stochastic environment. This problem has attracted the attention of researchers in many disciplines. We will not present a complete review, but only mention the main sources and the dominant lines of approach.

One group of authors, i.e., Johnson (1969), Müller, Weber (1972), Lückel, Müller (1975), Mehra (1976) assumes that measurement noise is the significant factor making some measurements more desirable than others. By neglecting the state excitation noise, they are able to make decisions on the optimal selection from certain properties of the observability matrix. They take advantage of its relation to the Fisher information matrix.

The second group, Athans (1972), Herring and Melsa (1974), Mellefont and Sargent (1977, 1978) includes both state excitation and measurement noise. They define the performance index of the estimator to be a sum of measurement costs and the integral square estimation error.

In process control, state excitation noise is not only used to account for unmeasured process disturbances but also for the modeling error. Neglecting the state excitation noise would result in a design procedure of dubious value. A selection criterion based on this assumption will be of limited usefulness. Further, it is well known how difficult it is to choose *a priori* values for the weighting matrices in quadratic optimal control or for the covariance matrices for the design of a Kalman filter. Adding a measurement cost term which has rarely any economic significance increases the number of design parameters over which a trial and error search has to be performed. In addition, even for each selected cost parameter, the optimization is an involved numerical procedure.

In this article, quite different methods for measurement selection will be presented. We believe that state excitation noise is of dominant significance, and all our measurement selection criteria are based on that assumption. The basic philosophy has been adopted from Brosilow and coworkers, e.g., Weber, Brosilow (1972), Joseph, Brosilow (1978), Brosilow, Tong (1978), Joseph, Brosilow (1978).

But as it will be pointed out later, some of their derivations are incorrect from a theoretical point of view. Their examples seem to demonstrate that their techniques work. It is likely that their methods are practical and justifiable from an engineering point of view, but the number of test cases to date is insufficient to allow that conclusion. In addition to the significant extension of Brosilow's work, we present a unifying framework by solving the problem in the context of filtering with nonstationary noise. Finally, we claim that our design methods are simpler to apply and subject to less restrictions than others available. Some ideas on the construction of reduced order estimators are also presented. There, the increased design effort has to be balanced against simplicity of implementation. The article concludes with a variety of simulation examples.

## MATHEMATICAL FORMULATION OF THE PROBLEM

We assume the process to be described by a set of linear stochastic differential equations. In the customary engineering notation the model is

$$\begin{pmatrix}\dot{x}\\ \dot{u}\end{pmatrix} = \begin{pmatrix}F & G\\ 0 & L\end{pmatrix}\begin{pmatrix}x\\ u\end{pmatrix} + \begin{pmatrix}H\\ 0\end{pmatrix} m + \begin{pmatrix}w_1\\ w_2\end{pmatrix} \tag{1}$$

$$y = Cx + w_3 \tag{2}$$

$$z = Dx \tag{3}$$

where

$x \in R^n$ = state vector
$u \in R^m$ = colored noise vector
$m \in R^l$ = vector of known system inputs, e.g. manipulated variables
$y \in R^r$ = observation vector
$z \in R^k$ = vector to be estimated
$\begin{pmatrix}w_1\\ w_2\end{pmatrix} \in R^{n+m}$, $w_3 \in R^r$ — zero mean white noise processes with intensities $V$, $V_3$ respectively.

$F$, $G$, $L$, $H$, $C$, $D$ are constant matrices of proper dimensions, which are assumed to have the following properties

$P1$: The eigenvalues of $F$ are distinct and lie in the open left half plane. (The distinctness is not essential and is assumed only to simplify the algebra; stability is necessary for all the following developments. If the system is open loop unstable it has to be stabilized first.)

$P2$: The eigenvalues of $L$ lie in the closed left half plane. (Any meaningful noise model satisfies this property as is discussed below.)

$P3$: The matrix $L$ is partitioned into

$$L = \begin{bmatrix} L_{11} & L_{12} & 0\\ 0 & L_{22} & 0\\ 0 & 0 & L_{33}\end{bmatrix},$$

where $L_{11} \in R^{m_1 x m_1}$, $L_{11} = 0$, $m_1$ is the number of blocks in the Jordan canonical form with zero eigenvalue, the eigenvalues of $L_{22} \in R^{m_2 x m_2}$ are zero and the eigenvalues of $L_{33} \in R^{m_3 x m_3}$ are strictly in the left half plane. (Such a partition is always possible from the Jordan canonical form through permutation operations.) $G$ and $u$ are partitioned accordingly $G = (G_1, G_2, G_3)$, $u^T = (u_1^T, u_2^T, u_3^T)$.

$P4$: The matrix $CF^{-1}G_1$ is of full row rank $r$. It expresses the steady state relationship between the unmeasured disturbances and the observations. If $CF^{-1}G_1$ is not of full rank, some observations $y$ can be neglected without loss of information so that a full rank matrix is obtained. $r \geq m_1$ indicates that more observations than unmeasured disturbances are available. This case offers no difficulties, with regard to observability, has been treated in the steady state case by Weber and Brosilow (1972) and is not emphasized here.

$P5$: The pair $(G, L)$ is completely observable.

If $P5$ is not satisfied redundant linearly dependent components are used in the noise model.

Because the noise model ($\dot{u} = Lu + w_2$) is essential to our development, and because frequent misconceptions in that regard exist in the literature, an explanation is in order. An extensive and lucid discussion of different forms of scalar noise is given by Box and Jenkins (1976) in the context of time series. An extension to the multivariable case is conceptually straightforward. The transformation from discrete time series to continuous time offers no difficulties. The key concept is that any kind of noise can be modeled by a set of linear differential equations with white noise as the input. If the eigenvalues of this set have strictly negative real parts, an autoregressive and/or moving average model results. If some of the eigenvalues are zero the noise is nonstationary.

By a suitable coordinate transformation, we can always separate the stationary ($u_3$) and nonstationary ($u_1$,$u_2$) noise components

$$\dot{u} = Lu + w_2 \rightarrow \begin{pmatrix}\dot{u}_1\\ \dot{u}_2\end{pmatrix} = \begin{pmatrix}0 & L_{12}\\ 0 & L_{22}\end{pmatrix}\begin{pmatrix}u_1\\ u_2\end{pmatrix}$$
$$\dot{u}_3 = L_{33} \; u_3$$

It is possible to identify the noise model from measurements. Very often, however, the parameters are chosen *a priori* or by trial and error to obtain satisfactory properties of the estimator or the controller (Palmor & Shinnar 1976).

Frequently the noise modelling is neglected altogether, and white noise is assumed to enter the system. This habit was adopted from electrical engineering, where it is often sufficient. In chemical engineering, however, the state excitation noise in particular is rarely approximated well by white noise. The process inputs frequently undergo step changes, vary in a trend-like fashion, or are at least correlated with respect to time. If under those circumstances an estimation scheme based on the white noise assumption is designed, it will perform poorly. And, for nonstationary noise, the estimates can be shown to be biased.

An alternate description of stationary noise is the power spectral density matrix. It is defined as the Fourier transform of the covariance matrix, and exists for wide-sense stationary noise only. A development based on a power spectral density for nonstationary noise (Joseph & Brosilow 1978) is incorrect. It is also incorrect to start with stationary noise, carry out a complete derivation, and then take the limit to make the final result valid for nonstationary noise (Chang 1961). Because of the completely different nature of the two processes, the limiting operation is meaningless.

The pertinent feature of our noise model is to permit the presence of constant disturbances $u_1$ through the zero eigenvalues of $L$. Multiple zeroes at the origin allow a polynomial description of the disturbances. If in its simplest form $L$ is a scalar and zero, then $u$ is called Wiener process, independent increment process or simply integrated white noise.

It can be pictured as a sequence of random steps whose amplitude is described by a normal distribution, and the time of occurrence follows a Poisson distribution. If the normal distribution describing the step amplitudes is $N(0,\xi^2)$, and the Poisson distribution has the mean $\nu$, then the covariance is given by

$$\begin{aligned} E\{u(t_3)u(t_2)\} &= E\{u(t_2)^2\} \\ &= E\{(u(t_2)^2 - u(t_1)^2\} + E\{u(t_1)^2\} \\ E\{u(t_3)u(t_2)\} &= \nu\xi^2(t_2 - t_1) + E\{u(t_1)^2\} \end{aligned} \tag{4}$$
$$\text{for} \quad t_3 \geq t_2 \geq t_1 \geq t_0, \quad u(t_0) = 0$$

where we used the fact that the increments are uncorrelated and have zero mean. We also conclude that the white noise process must have intensity $\nu\xi^2$ to result in the Wiener process described by (4) after it has passed through an integrator. The disturbance description which assumes random steps occurring with a certain average frequency seems very suitable for chemical engineering processes.

In this article, we discuss how $z$ can be estimated from observations $y$ when the system is modeled by (1)-(3). If alternative observations $y$ are available, we will develop procedures for selecting the best set of observations.

## ESTIMATORS AND MEASUREMENT SELECTION CRITERIA FOR STEADY STATE CONDITIONS

Often the significant disturbances entering a chemical process vary slowly, compared to the dominant time constant of the process. Then it suffices to use a static estimator and to develop measurement selection criteria on a static basis. Because the value of $m$ is known, we can subtract its effect on the output $y$ by evaluating a convolution integral

$$y' = y - C\int_{t_0}^{t} \exp[F(t-\tau)]Hm(\tau)d\tau \tag{5}$$

This is valid according to the superposition principle for linear equations.

Assuming $w_1 = w_2 = w_3 = 0$ and steady state conditions then the modified outputs are obtained from (1), (2), (3) as

$$y' = -CF^{-1}G_1u_1 \equiv -S^Tu_1 \tag{6}$$

$$z' = -DF^{-1}G_1u_1 \equiv -T^Tu_1 \tag{7}$$

Note that no steady state assumption is needed with respect to $m$, because its influence is subtracted from the observations. The unmeasured output of interest, $z$, can be found by adding the effect of the measured inputs to $z'$

$$\hat{z} = \hat{z}' + D\int_{t_0}^{t} \exp[F(t-\tau)]Hm(\tau)d\tau \tag{8}$$

$y'$ and $z'$ can be regarded as zero mean random variables and our objective is to estimate variable $z'$ by using $y'$. The optimal linear estimator minimizing the error variance

$$E\{(z' - \hat{z}')^T(z' - \hat{z}')\}$$

is

$$\hat{z}' = \phi_{z'y'}\phi_{y'y'}^{-1}y' \tag{9}$$

where $\phi_{ab}$ is the covariance matrix of $a$ and $b$ defined by

$$\phi_{ab} = E\{ab^T\} \tag{10}$$

This well known result is available, for example, from Rhodes (1971). If $u_1$ is also a random variable with zero mean and covariance matrix $\phi_{uu}$ then because of linearity the estimate of $z'$, given by (9), can be rewritten as

$$\hat{z}' = T^T\phi_{uu}S(S^T\phi_{uu}S)^{-1}y' \tag{11}$$

Alternatively if the unknown inputs $u_1$ themselves are to be estimated then

$$\hat{u}_1 = -\phi_{uu}S(S^T\phi_{uu}S)^{-1}y' \tag{12}$$

In the sequel, we assume $\phi_{uu} = I$, which can always be obtained by proper scaling. Then $S(S^TS)^{-1}$ can be recognized as the generalized inverse of $S^T$. This is not a surprise, because all linear estimators can be obtained by orthogonal projection, and the generalized inverse is known to express this projection. Property $P_4$ is necessary for this inverse to exist. If $S$ is a square matrix, the generalized inverse is equal to the regular inverse.

The error covariance matrix is given by

$$E\{(z' - \hat{z}')(z' - \hat{z}')^T\} = T^TT - T^TS(S^TS)^{-1}S^TT \equiv R \tag{13}$$

where the first part is the covariance matrix of $z'$. As a multivariable extension of the projection error by Joseph and Brosilow (1978) we obtain the first measurement criterion.

### Measurement Selection Criterion 1

Select the measurements to minimize the relative estimation error defined by

$$\frac{E\{(z' - \hat{z}')^T(z' - \hat{z}')\}}{E\{z'^Tz'\}} = \frac{\text{trace}(R)}{\text{trace}(T^TT)} \tag{14}$$

A second objective is to make the estimator insensitive to modeling errors. If we define the estimator for the correct model as

$$\Omega \equiv T^TS(S^TS)^{-1} \tag{15}$$

and if we call the estimator determined on the basis of an incorrect model $(\Omega + \Omega_\epsilon)$, then Weber and Brosilow (1972) show that the relative error $\|\Omega_\epsilon\|/\|\Omega\|$ is minimized by using

#### Measurement Selection Criterion 2

To minimize the effect of the modelling error, select the measurements such that the condition number of $S$

$$\text{cond}(S) = \|S\|\,\|S^+\| = \sqrt{\frac{\text{max. eigenvalue of } A^TA}{\text{min. eigenvalue of } A^TA}} \tag{16}$$

is minimized.

These two criteria move in different directions with an increasing number of measurements, and a compromise has to be found. Criteria 1 and 2 give no information about the dynamic performance of the estimator. Under certain conditions, this very simple estimator might perform well (even during the transient). Qualitatively speaking, we are looking for "dynamic similarity" between our measurements $y$ and the variable to be estimated $z$.

In the following development about dynamic similarity, we assume the simplified version of (1)-(3), neglecting the stationary noise component, but allowing for persistent disturbances

$$\dot{x} = Fx + G_1u_1 \tag{17}$$

We also assume that $y$ and $z$ are subsets of the state vector.

If $P$ is the modal matrix ot $F$ containing the eigenvectors $v_i$ of $F$ as columns and $Q^T$ the matrix containing the eigenvectors $w_i$ of $F^T$ as rows then we can use the biorthogonality property for normalization such that

$$w_i^T v_j = \delta_{ij} \tag{18}$$

and

$$Q^TP = I \tag{19}$$

It is generally insufficient to look at the relative magnitude of the elements in $P$ to determine the "content" of the different modes in an observation. This is misleading, because in the extreme case of a mode which is uncontrollable by $u_1$ the contribution of the mode to the observation will be zero, regardless of the magnitude of the elements in $P$. This argument assumes also that the initial conditions are zero, and that all disturbances affecting the system are included in $u_1$. In order to account for those cases, we assume that some information about the "average state" of the system ($x_s$) is available. For modal control Davison and Goldberg (1969) define an average state through

$$x_s = -\frac{1}{m_1} F^{-1} \sum_{i=1}^{m_1} \frac{G_i}{\sqrt{G_i^TG_i}} \tag{20}$$

($G_i$, $i = 1, \ldots m$ denotes a column of $G$) and we can use this definition for our purposes to scale $P$ correctly: Denote by $N$ the matrix

$$N = \text{diag}\,(n_i) \tag{21}$$

where $n_i$ are the different components of

$$n = Q^Tx_s, \tag{22}$$

then the matrix

$$\Gamma = PN \tag{23}$$

can give us a rough indication if it will be possible to find a static estimator with acceptable dynamic behavior. The entry $\Gamma_{ij}$ is a measure of the content of mode $j$ in observation $i$. Note that the relative magnitude of the elements in a row of $\Gamma$ is independent of the scaling of $x$.

#### Measurement Selection Criterion 3

If $z$ contains mostly fast modes, and $y$ mostly slow modes, as determined by $\Gamma$, the dynamic properties of the static estimator are unlikely to be good.

A more detailed check of the dynamic behavior of the static estimator is possible by assuming the frequency spectrum of the anticipated disturbances to be known. In principle, it is possible to determine the frequency spectrum of the disturbances through on-line measurements. It is questionable, however, if this effort is justified.

A simpler approach is to assume changes in the disturbance inputs (upstream conditions, environment) to have a certain amplitude and to occur with a period of one hour, eight hours, one day, etc. A gross estimate of period and amplitude can be obtained without a detailed analysis from a knowledge of the overall process. Moreover, very fast disturbances can usually be neglected, because they are attenuated by the system and not reflected in the outputs.

Let the Laplace transform of the system described by (17), (2), (3) be given by

$$y'(s) = -S^T(s)\, u_1(s) \tag{24}$$

$$z'(s) = -T^T(s)\, u_1(s) \tag{25}$$

The dynamic estimation error of the static estimator can be expressed by

$$e(s) = z'(s) - \hat{z}'(s) = (-T^T(s) + T^T(0)\, S(0)(S^T(0)S(0))^{-1}S^T(s))u_1(s) \tag{26}$$

For a pure sinusoid ($a \sin \omega t$) signal the mean square deviation is calculated to be $a^2/2$. If we model the disturbances as

$$u_1 = \sum_j a_j\, e^{i\omega_j t} \tag{27}$$

with the disturbance amplitude $a_j \epsilon R^{m_1}$ the mean square error is given by

$$\{e^2\} = \frac{1}{2} \sum_j \| (-T^T(i\omega_j) + T^T(0)\, S(0)(S^T(0)S(0))^{-1}S^T(i\omega_j))\, a_j\|^2 \tag{28}$$

Furthermore, if the power spectral density matrix $\Phi(i\omega)$ of the disturbances is given, the mean square error can be computed as

$$\{e^2\} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \Phi(i\omega)(-T^T(i\omega) + T^T(0)S(0)(S^T(0)S(0))^{-1}S^T(i\omega))\Phi^T(-i\omega)d\omega \tag{29}$$

but the necessary computational effort makes it impossible to use (29) as a measurement selection criterion. Equation (28) corresponds to the assumption of a discrete power spectral density consisting of δ-functions with areas $a_j\sqrt{\pi}$ at the frequencies $\omega_j$. In several examples, the ordering of the measurement sets based on (28) was very insensitive to the particular frequencies chosen, i.e., a gross approximation to the satistics of the inputs was sufficient.

Defining

$$\{z^2\} = \frac{1}{2} \sum_j \| -T^T(i\omega_j)\, a_j\|^2 \tag{30}$$

we can state the fourth criterion.

#### Measurement Selection Criterion 4

To minimize the relative dynamic error of the static estimator, the measurements should be selected to minimize

$$\{e^2\}/\{z^2\} \tag{31}$$

defined by (28), (30).

Remark: The steady state (projection error) can be accounted for heuristically by including a term for $\omega_j = 0$ in (28), (30). Because the power spectral density is not defined for nonstationary noise it is recommended however to test for the dynamic and the steady state error separately.

## DYNAMIC ESTIMATOR—STOCHASTIC APPROACH

The mathematical problem is to find an estimator for the system described by (1)-(3) such that the mean square estimation error

$$E\{(z(t)-\hat{z}(t))^T (z(t)-\hat{z}(t))\}$$

is minimized for all $t$. It is well known that this optimal estimator is the Kalman filter. But for the filter to have a finite gain as time progresses, the system (1), (2) must be at least detectable. Standard linear state space theory states that (1), (2) is observable if—and only if—the matrix

$$\left[\begin{pmatrix} C^T \\ 0 \end{pmatrix}, \begin{pmatrix} F^T & 0 \\ G^T & L^T \end{pmatrix}\begin{pmatrix} C^T \\ 0 \end{pmatrix}, \begin{pmatrix} F^T & 0 \\ G^T & L^T \end{pmatrix}^2\begin{pmatrix} C^T \\ 0 \end{pmatrix}, \ldots \begin{pmatrix} F^T & 0 \\ G^T & L^T \end{pmatrix}^{m+n-1}\begin{pmatrix} C^T \\ 0 \end{pmatrix}\right]$$

has full rank $m + n$. This criterion is computationally awkward and does not yield any insight into the structural requirements for observability. We were able to prove the alternate condition:

*Theorem 1*: The pair

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

is completely observable if and only if

$$\text{a)}\ \left\{(C, 0), \begin{pmatrix} F & G_3 \\ 0 & L_{33} \end{pmatrix}\right\}$$

is completely observable

$$\text{b) rank} \begin{pmatrix} F & G_1 \\ C & 0 \end{pmatrix} = n + m_1$$

For proof, see Morari and Stephanopoulos (1979). Requirement a) means that the original system with the stationary noise has to be observable. Trivially, b) is not satisfied when $r < m_1$, i.e., when the number of independent persistent disturbances exceeds the number of measurements.

*Corollary 1:* The pair

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

is not detectable if $r < m_1$. (For proof, see Morari and Stephanopoulos (1980).)

We conclude that in the case of primary interest in chemical engineering ($r < m_1$) the standard filter design method fails because of the presence of an undetectable subspace. Qualitatively, we have to proceed in two steps:

1) Transform the system described by the pair

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

into an observable one such that the error caused by the unobservable subspace is minimized.

2) Construct a Kalman filter for the new transformed system.

Mathematically, only one step is really necessary: We derive the estimator minimizing the mean square estimation error by using the Orthogonal Projection Theorem for Hilbert spaces. This extends the arguments by Kalman in the original derivation (Kalman & Bucy 1961) and is given in detail for lumped parameter systems by Morari and Stephanopoulos (1979) and for distributed parameter systems by Morari and O'Dowd (1978). The results can be summarized in a theorem and a corollary:

*Theorem 2:* The mean square estimation error for the system (1), (2) caused by the unobservable subspace is minimized by constructing a Kalman filter for the transformed completely observable system

$$\begin{pmatrix} \dot{x} \\ \dot{u}^* \end{pmatrix} = \begin{pmatrix} F & G\Sigma \\ 0 & \Sigma^+ L\Sigma \end{pmatrix}\begin{pmatrix} x \\ u^* \end{pmatrix} + \begin{pmatrix} H \\ 0 \end{pmatrix} m + \begin{pmatrix} w_1 \\ w_2^* \end{pmatrix} \tag{32}$$

$$y = (C\ 0)\begin{pmatrix} x \\ u^* \end{pmatrix} + w_3 \tag{33}$$

where

$$\Sigma = \begin{pmatrix} S & 0 \\ 0 & I_{m_2+m_3} \end{pmatrix}, \Sigma^+ = \begin{pmatrix} S^+ & 0 \\ 0 & I_{m_2+m_3} \end{pmatrix}, S^+ = (S^TS)^{-1}S^T \tag{34}$$

$$u^* = \Sigma^+ u \tag{35}$$

$(w_1, w_2^*)$ white noise process of intensity

$$V^* = \begin{pmatrix} I_n & 0 \\ 0 & \Sigma^+ \end{pmatrix} V \begin{pmatrix} I_n & 0 \\ 0 & \Sigma^+ \end{pmatrix}^T$$

The filter has the form

$$\begin{pmatrix} \dot{\hat{x}} \\ \dot{\hat{u}}^* \end{pmatrix} = \begin{pmatrix} F & G\Sigma \\ 0 & \Sigma^+ L\Sigma \end{pmatrix}\begin{pmatrix} \hat{x} \\ \hat{u}^* \end{pmatrix} + K(y - C\hat{x}) + \begin{pmatrix} H \\ 0 \end{pmatrix} m \tag{36}$$

and the steady state optimal filter gain $K$ is computed from the matrix Riccati equation, i.e., $K = QC^TV_3^{-1}$, where $Q$ is the solution of

$$\begin{pmatrix} F & G\Sigma \\ 0 & \Sigma^+ L\Sigma \end{pmatrix} Q + Q\begin{pmatrix} F^T & 0 \\ \Sigma^T G^T & \Sigma^T L^T (\Sigma^+)^T \end{pmatrix} + V^* - QC^TV_3^{-1}C\,Q = 0 \tag{37}$$

A common solution procedure for (37) is to integrate the associated matrix differential equation, i.e., the right-hand side of (37) being equal to $\dot{Q}$, until a steady state value is reached.

*Corollary 2:* In the absence of noise, and in the steady state the estimates obtained by the filter (36), are equal to those obtained by the static estimator (11).

We would like to interpret the results and to put them in perspective with other work. For an estimator to perform well in the presence of persistent disturbances, a non-stationary noise model has to be used. If the number of nonstationary noise components ($m_1$) exceeds the number of observations ($r$), detectability of the system is lost through the noise model poles at the origin.

Instead of simply neglecting some noise components, we combine them optimally in $u^*$. By using Measurement Selection Criterion 1, we minimize the influence of the nonobservable subspace, and our estimates are optimal in the static and dynamic sense. The disadvantage of using a colored noise model instead of white noise is that the order of the estimator is increased.

There are other approaches to deal with the bias caused by persistent unknown process disturbances. In particular, a comparison with the work by Hamilton et al. (1973) is instructive. We would like to draw a parallel to the associated control problem: If only proportional control is available in a specific situation, then the offset can be reduced by increasing the feedback gain. Essentially this approach is used by the aforementioned authors to reduce the bias in the estimate. By assuming white state excitation noise of artificially high intensity, the filter gain is increased and the bias reduced. The disadvantages are obvious. The high gain allows most of the measurement noise to pass through the filter, and bias reduction has to be balanced against increase of noise in the estimates.

On the other hand, drawing a parallel to the associated control problem again, integral control allows elimination of offset without requiring an increase in gain. Essentially this approach is used in our work. The nonstationary noise model leads to integral action in the estimator. It is possible to reduce the bias down to the minimum set by the lack of observability by using this integral action without increasing the gain.

These arguments imply that the superiority of one method over the other depends on the particular application. If the measurement noise is significant, a nonstationary noise model and consequently a filter of high dimension ($>n$) should be used to reduce the bias in the estimate. If the measurement noise is small, it will suffice to use a higher filter gain (obtained by assuming state excitation noise of high intensity). But we cannot endorse the latter method. With negligible measurement noise, an observer should be used which will have the dimension $n$, i.e.

same dimension as the filter, when it *includes* integral compensation for the bias error. This is explained in the next section.

## STATE RECONSTRUCTION—DETERMINISTIC APPROACH

Significantly more research is reported on observer theory in the presence of unmeasurable disturbances than on the stochastic equivalent of this problem which was discussed in the last section. The earliest results are probably due to Johnson and are summarized in Johnson (1975). They are reviewed below.

Basile and Marro (1969) and Guidorzi and Marro (1971) state geometric existence conditions for unknown input observers. Several papers are based on a theorem by Wonham and Morse (1970), in which existence of an observer feedback matrix is proved which eliminates the influence of unknown inputs. The theorem is stated for control and not state reconstruction, but it can be interpreted in both ways.

Harunoglu and Bankoff (1974) as well as Wang et al. (1975) use this theorem and attempt to reconstruct a linear combination of the states which is chosen such that the differential equation describing the error between the estimate, and the actual value is not affected by the unmeasured inputs. In principle, this method is ideal, because the effect of the disturbances can be eliminated completely, independent of their magnitude and frequency of occurrence. A drawback, mentioned by the authors, is that the placement of the observer poles is not arbitrary. Indeed, not even the stability can be guaranteed.

One fact was overlooked by Harunoglu and Bankoff (1974), however: Their major reason for introducing the observer was to gain freedom in assigning the eigenvalues of the system through the use of feedback when the complete state vector is not available for measurement. This observer property is completely independent of the estimation bias due to unknown inputs. The standard observer works perfectly well without any modifications. A better constructive method with the same goal as Harunoglu and Bankoff (1974) is presented by Bhattacharyya (1977).

If an unknown input observer in the sense of the theorem by Wonham and Morse (1970) can be constructed, it is generally preferable to the methods discussed in this section because of its better performance and reduced dimensionality. The existence conditions are quite stringent however, are not statisfied in many practical situations, and other approaches have to be chosen in most cases. Seborg et al. (1975) proceed in the deterministic case in the same fashion as in the stochastic one: They reduce the bias error by increasing the gain of the observer. For multivariable systems, there are different ways to increase the "overall gain" and by trial and error the most efficient way can be found.

The model used by Johnson (1975) for his unknown input observer is slightly more general than

$$\begin{pmatrix} \dot{x} \\ \dot{u} \end{pmatrix} = \begin{pmatrix} F & G \\ 0 & L \end{pmatrix} \begin{pmatrix} x \\ u \end{pmatrix} \tag{38}$$

$$y = Cx \tag{39}$$

where the symbols and dimensions have been defined above. In the deterministic case $L$ is more difficult to interpret. If $L$ is singular, persistent disturbances can be compensated for. For the design of a Luenberger observer (Luenberger 1964, 1966) the system (38), (39) has to be detectable. Theorem 1 and Corollary 1 state the conditions under which this is true. We recognize immediately that we encounter difficulties when $r < m_1$. The same approach as in theorem 2 can be used to circumvent them.

*Corollary 3:* If a Luenberger observer is constructed for the modified completely observable system

$$\begin{pmatrix} \dot{x} \\ \dot{u}^* \end{pmatrix} = \begin{pmatrix} F & G\Sigma \\ 0 & \Sigma^+ L\Sigma \end{pmatrix} \begin{pmatrix} x \\ u^* \end{pmatrix} + \begin{pmatrix} H \\ 0 \end{pmatrix} m \tag{40}$$

$$y = (C0) \begin{bmatrix} x \\ u^* \end{bmatrix}$$

in the steady state the estimate of $x$ is equal to that obtained by the static estimator (11). The reduced order observer has dimension $n$.

*Proof:* The steady state properties can be demonstrated easily by setting the left hand side of (40) equal to zero and performing some algebraic manipulations. For the observer design we refer to Luenberger (1964, 1966).

## THE DESIGN OF REDUCED ORDER ESTIMATORS

Following the construction procedures described above, the necessary order of the Kalman filter is $n + r$, the reduced order Luenberger observer will be just an $n$ dimensional dynamic system, an advantage for implementation, especially when the measurements are essentially noise free. It is often quite simple to achieve an acceptable observer response through the placement of the poles alone. From our limited number of example calculations, we conclude that the particular structure of the extended system matrix makes the task more difficult.

It is well known that even lower order observers can be found, if not the whole state (but only a linear function of the state) is to be estimated. For our particular problem, we could use the numerical procedure of Sirisena and Choi (1977) to find the minimal-order observer for the unknown output $z$. The application of their algorithm to our case is straightforward and will not be described further.

The estimate of $z$ and $u^*$ which we obtain by one of the discussed methods can be used for optimizing or regulatory control. For the special case of regulation, alternative techniques exist to eliminate the influence of unmeasured inputs (e.g., Fabian & Wonham 1975).

We would like to discuss a different approach combining the ideas of the minimal observer with reduced order control laws. For full order estimators and controllers, the design of the estimator and the controller can proceed separately based on the separation principle. For reduced order schemes, the two tasks have to be handled jointly.

Our goal consists of two parts: *Goal 1:* Estimation of $u^*$; elimination of the effect of the observable part of $u$ on the output $z$. *Goal 2:* Design of a feedback controller to improve system behavior toward general unmeasured disturbances not included in $u$. For Goal 1, a minimal order observer for the reconstruction of $u^*$ has to satisfy the following properties stated in

*Theorem 3:* (Fortmann and Williamson 1972):

The observer

$$\begin{aligned} \dot{p} &= Ap + By + Em \\ w &= Pp \end{aligned} \tag{41}$$

tracks the system (40) in the sense that

$$\lim_{t\to\infty} \| u^* - w \| \to 0,$$

if and only if there exists a matrix $M$ satisfying the following equalities:

$$M\begin{pmatrix} F & G\Sigma \\ 0 & L\Sigma \end{pmatrix} - AM = B(C \quad 0) \tag{42a}$$

$$E = M\begin{pmatrix} H \\ 0 \end{pmatrix} \tag{42b}$$

$$PT = (0 \quad I_r) \tag{42c}$$

and the eigenvalues of $A$ are strictly in the left half plane. (42b) does not represent a constraint, (42a,c) restrict the possible choices of the observer matrices $A$ and $B$.

Assume that a feedback law was found to satisfy Goal 2: $m = -\bar{K}p$. Instead of formally deriving a control law to eliminate the effect of $u^*$ on $z$ we can solve (40), (41) jointly for $m$, assuming steady state conditions and $z = 0$. For a solution to exist it is necessary that $l \geq k$. We assume $l = k$ for simplicity, the extension to the inequality case being straightforward,

$$m = -\left(D\bar{F}^{-1}\begin{pmatrix}H\\0\end{pmatrix}\right)^{-1} D\bar{F}^{-1}\begin{pmatrix}G(S^+)^T\\O\end{pmatrix}\hat{u}_1^* \equiv -\bar{K}Pp \qquad (43)$$

where

$$\bar{F} = \begin{pmatrix}F & -H\tilde{K}\\ BC & A-E\tilde{K}\end{pmatrix} \quad \text{and} \quad \hat{u}_1^* = Pp$$

In summary: To satisfy Goal 1, an observer has to be found satisfying the conditions of Theorem 3. The control action necessary to eliminate the effect of the unmeasured persistent disturbance $u_1^*$ is expressed by (43).

For Goal 2, combine (32), (41) into one stochastic vector differential equation neglecting the terms involving $u^*$, $\dot{u}^*$ and setting $m = -\tilde{K}p$:

$$\dot{\bar{x}} = \bar{F}\bar{x} + \bar{B}\begin{pmatrix}w_1\\w_3\end{pmatrix} \qquad (44)$$

where

$$\bar{x} = \begin{pmatrix}x\\p\end{pmatrix}, \quad \bar{B} = \begin{pmatrix}I_n & 0\\0 & B\end{pmatrix}$$

The usually stated objective is to minimize the expected value of the error norm, augmented by a quadratic penalty term, to avoid excessive control action:

$$\min \lim_{t_0 \to -\infty} E\{x^T(t)R_1x(t) + m^T(t)R_2m(t)\} \qquad (45a)$$

where $R_1$ and $R_2$ are positive definite weighting matrices. In the case of Gaussian white noise this stochastic optimization problem can be translated into an equivalent deterministic one (Kwakernaak & Sivan, section 5.7, 1972)

$$\min \text{trace } (\bar{S}_{11}R_1 + \bar{S}_{22}\tilde{K}^TR_2\tilde{K}) \qquad (45b)$$

where $S$ is the solution of the linear matrix Lyapunov equation

$$M\bar{S} + \bar{S}M^T + NVN^T = 0 \qquad (46)$$

and

$$\bar{S} = \begin{pmatrix}\bar{S}_{11} & \bar{S}_{12}\\ \bar{S}_{21} & \bar{S}_{22}\end{pmatrix}; \ \bar{S}_{11} \in R^{nxn}, \qquad \bar{S}_{22} \in R^{pxp}$$

The feedback controller

$$\dot{x} = Fx + Gu + Hm \qquad (47)$$

$$m = -(\tilde{K} + \bar{K}L)p \qquad (48)$$

$$\dot{p} = AP + By + Em \qquad (49)$$

is designed in the following fashion

(i) assume dim (p)
(ii) find $A$, $B$, $\tilde{K}$ in order to minimize (45b) under the constraints (42a) and (42c)
(iii) if (45b) cannot be made sufficiently small, increase dim (p) and go to (i).

It has the following properties

(i) the steady state least square optimal estimate of $u$ is given by $u^* = Lp$
(ii) The steady state effect of the unknown disturbance is eliminated apart from a remainder term caused by the unobservability:

$$z = -(D \quad 0)\ \bar{F}^{-1}\ G(I - SS^+)^T u_1 \qquad (50)$$

*Remarks:* (1) For the constrained optimization (ii) the algorithm of Kwakernaak and Sivan (section 5.7, 1972) and Sirisena and Choi (1977) have to be combined. The gradient of (45b) with respect to the unknown matrices $A$, $B$, $\tilde{K}$ can be computed explicitly and a gradient projection method appears to be the most primising.

(2) There exists no theoretical result for determining the minimal dimension of $p$ such that a solution exists.

(3) To minimize numerical difficulties due to the non-uniqueness of the optimum, canonical forms (which have a minimum number of independent parameters) should be used for $A$, $B$, $\tilde{K}$. For the general multivariable case, they are given by Bucy and Ackermann (1970). Even then, the optimization problem can be formidable. It has to be weighed off against the disadvantages caused by the implementation of higher order estimators and control systems.

(4) The feedback term $\tilde{K}p$ decreases the steady state error caused by unmeasured disturbances not modeled by $u$.

(5) The eigenvalues of the (full order) observer and the system under feedback can be selected independently, regardless of unmeasured inputs (see the remark on the work by Harunoglu and Bankoff (1974) above). This fact is rather trivial and a proof will be outlined only. Defined the estimation error as

$$e = x - \hat{x}$$

then a representation of system and observer combined which is equivalent with respect to the eigenvalues (similarity transform) is

$$\begin{pmatrix}\dot{x}\\ \dot{e}\end{pmatrix} = \begin{pmatrix}F-H\tilde{K} & H\tilde{K}\\ 0 & F-KC\end{pmatrix}\begin{pmatrix}x\\e\end{pmatrix} + \begin{pmatrix}G\\0\end{pmatrix}u$$

where $K$ is the observer feedback matrix. Because of the block diagonal form of the matrix the separation of the eigenvalues is obvious. This is also true when a compensation for the disturbances is introduced (augmentation by $\dot{u}^* = 0$).

## EXAMPLE 1: DOUBLE EFFECT EVAPORATOR (10TH ORDER MODEL)

We would like to demonstrate our measurement selection criteria on an example studied extensively in the literature: A double-effect evaporator (DEE). It was chosen mainly because the model was shown in numerous studies to represent the physical system well, and it offers the possibility for a comparison of our results with the large amount of data available in the references cited above. A diagram of the system is given in Part II of this series. The detailed modelling and a variety of control studies are collected in Fisher and Seborg (1976). The variables used in the model are deviation variables which are normalized by dividing by the steady state value. Their meaning is

*TS* = steam temperature ($x_1$)
*TW*1 = first effect tube wall temperature ($x_2$)
*W*1 = first effect holdup ($x_3$)
*C*1 = first effect concentration ($x_4$)
*H*1 = first effect enthalpy ($x_5$)
*TW*2 = second effect tube wall temperature ($x_6$)
*W*2 = second effect holdup ($x_7$)
*C*2 = second effect concentration ($x_8$)
*H*2 = second effect enthalpy ($x_9$)
*TW*3 = condenser tube wall temperature ($x_{10}$)

Because of the two poles at the origin the system has to be stabilized first for a static estimator to exist. (This is explained in Example IV.)

The objective of the study was to find out if it is possible to use any subset of the six available temperatures in the 10th order model to estimate the outlet concentration $C2$ through a static estimator. The detailed computation of the error criterion (31) and simulation studies showed that it is impossible to obtain an estimate with acceptable dynamic properties*.

This conclusion can also be drawn immediately based on Measurement Section Criterion 3: When "weak" stabilizing feedback is applied, the modal matrix $P$ is approximately equal to the modal matrix $P$ without stabilization whose entries are listed in Fisher, Seborg (1976). We assumed the average deviation of the variables to be 10%, i.e. $x_{si}$ = .1 in Eqn. (22). The normalization matrix $N$, Eqn. (21), is then diag (−2., 2., −.3, .2, −.2, .02, .07, .03, .02, −.02). The matrix Γ is shown in Table I. (In each row the elements of dominating magnitude are marked.) The temperatures contain predominantly fast modes

*It is interesting to note that the system is also "barely observable" using these measurements. We are grateful to D. E. Seborg for pointing out this fact.

Table 1: Normalized Modal Matrix for the Double Effect Evaporator.

| Eigen-values | 0. | 0. | −.04 | −.08 | −.29 | −1.7 | −8.4 | −46 | −49 | −309 |
|---|---|---|---|---|---|---|---|---|---|---|
| TS | +6.8E-8 | −2.2E-7 | −8.4E-7 | −3.3E-5 | +7.8E-2 | −3.8E-3 | −1.7E-3 | −2.6E-2 | 1.6E-3 | −1.9E-2 |
| TW1 | +6.5E-8 | −2.3E-7 | −1.8E-6 | −3.4E-5 | +8.4E-2 | −4.1E-3 | +2.2E-3 | 1.3E-2 | −2.5E-3 | −3.8E-4 |
| W1 | +1.5 | −1.4 | +5.8E-4 | −7.6E-6 | +1.6E-2 | −1.1E-3 | +9.4E-5 | 1.1E-5 | −3.6E-5 | −5.7E-6 |
| C1 | +3.4E-4 | 3.3E-4 | +2.9E-6 | 1.4E-1 | −2.1E-2 | 1.2E-3 | −9.6E-5 | 1.1E-5 | 3.6E-5 | +5.7E-6 |
| H1 | +3.1E-6 | −3.1E-6 | −2.9E-6 | −1.3E-3 | +1.0E-1 | −4.7E-3 | −1.6E-4 | −3.6E-3 | 7.2E-4 | +3.0E-4 |
| TW2 | +1.2E-6 | −1.4E-6 | −3.0E-6 | −4.0E-5 | +7.4E-2 | 8.6E-3 | −4.7E-3 | 6.0E-3 | 9.9E-3 | +9.9E-4 |
| W2 | −1.3 | 1.4 | −1.1E-4 | −9.2E-5 | +3.2E-2 | 8.9E-4 | −9.5E-4 | −6.9E-6 | 1.4E-6 | +2.4E-7 |
| C2 | +6.8E-4 | −7.6E-4 | +3.0E-1 | −1.4E-1 | −3.4E-2 | −9.4E-4 | 9.5E-4 | 4.4E-6 | −9.0E-7 | −1.4E-7 |
| H2 | −1.2E-5 | 1.3E-4 | −6.1E-3 | 2.8E-3 | +8.9E-2 | 1.5E-2 | −7.3E-3 | −5.7E-4 | −1.0E-3 | −1.1E-4 |
| TW3 | +5.4E-7 | −6.0E-7 | −9.0E-7 | −1.3E-5 | +2.3E-2 | 4.9E-3 | 7.0E-2 | 3.0E-4 | −1.1E-4 | −1.6E-5 |

while there are slower modes present in $C2$. Any static estimator employing temperatures will exhibit strong phase lead.

**EXAMPLE II**

$$\dot{x} = Ax + Bu$$

with

$$A = \begin{bmatrix} -2.4 & -.175 & -.245 & -.188 & .393 \\ 3.2 & -.6 & 2.69 & -1.667 & -10.903 \\ 0 & 0 & -4.811 & -.344 & -.084 \\ 0 & 0 & .351 & -5.676 & -.068 \\ 0 & 0 & .270 & -.135 & -6.014 \end{bmatrix}$$

$$B = \begin{bmatrix} 6.55 & 2 \\ -8 & 20 \\ 2.75 & 16 \\ 5.5 & 16 \\ 0 & 12 \end{bmatrix}$$

The eigenvalues of $A$ are −1, −2, −5, −5.5 and −6. The transfer function and modal matrix can be found with other details in Morari (1977). Our objective is to estimate $x_3$ using two other state vairables as observations. The condition numbers (16) were computed for the six possible pairs:

| Measurements | Condition Number |
|---|---|
| $(x_1,x_2)$ | 1.323 |
| $(x_1,x_4)$ | 1.686 |
| $(x_1,x_5)$ | 1.326 |
| $(x_2,x_4)$ | 6.143 |
| $(x_2,x_5)$ | ∞ |
| $(x_4,x_5)$ | 6.712 |

To avoid the amplification of modelling errors, $(x_1,x_2)$ could be chosen as measurements. The condition numbers of $(x_1,x_2)$, $(x_1,x_4)$ and $(x_1,x_5)$ differ very little and the dynamic indices (28), (31) were computed for those three pairs at $\omega = 2$ with $a = 1$.

| | $\{e^2\}$ | $\{e^2\}/\{z^2\}$ |
|---|---|---|
| $(x_1,x_2)$ | 2.374 | .171 |
| $(x_1,x_4)$ | .159 | .011 |
| $(x_1,x_5)$ | .195 | .014 |

The dynamic index predicts a better estimator using $(x_1,x_4)$ or $(x_1,x_5)$. The result was confirmed using simulation and the striking difference is depicted in Fig. 1.

**EXAMPLE III**

The operation, control and modeling of an FCC unit have been described elsewhere (Kurihara 1967; Gould, Evans and Kurihara 1970). The linearized form of the state equation was developed by Schuldt and Smith (1971), using a state variables $C_{rc}$, $C_{cat}$, $C_{sc}$, $T_{ra}$, $T_{rg}$ with the following interpretation

$C_{rc}$ = carbon on regenerated catalyst
$C_{cat}$ = catalytic carbon on spent catalyst
$C_{sc}$ = total carbon on spent catalyst
$T_{ra}$ = temperature in reactor
$T_{rg}$ = temperature in regenerator

The amount of oxygen in the flue gas $O_{fg}$ is a function of $C_{rc}$, $T_{rg}$ and $R_{ai}$, the air rate. Kurihara (1967) termed maintaining the carbon balance to be the "most vexing problem". The amount of carbon on the catalyst is of the order of 1 wt % and cannot be measured on line. It is, however, one clear indication of the overall FCC performance allowing conclusions about the feedstock conversion to be made.

We are trying to select the pair of measurements ($C_{rc}$, $T_{ra}$; $C_{rc}$, $T_{rg}$; $T_{ra}$, $T_{rg}$) that yields the best estimate of $C_{sc}$ when used in the static estimator. Changes in the composition of the feed crude cannot be measured on-line, and are assumed to be disturbances expressing themselves through changes in the kinetic constants $k_{cr}$ and $k_{cc}$ in the model.

The modal matrix constructed for the normalized linearized model (the state variables represent percentage deviations from the steady state) points out the theoretical possibility for the use of a static estimator

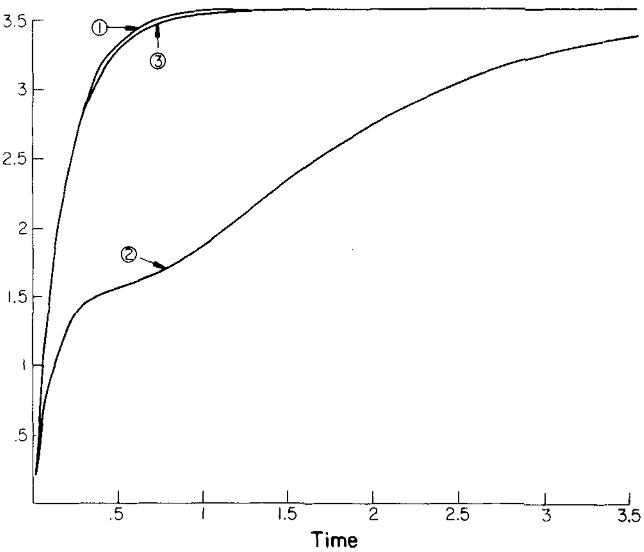


Figure 1. Example II. ① Response of $x_3$ as computed from the system equations, ② estimator $[x_1,x_2]$, ③ estimator $[x_1,x_5]$; $u$ = (1,1).

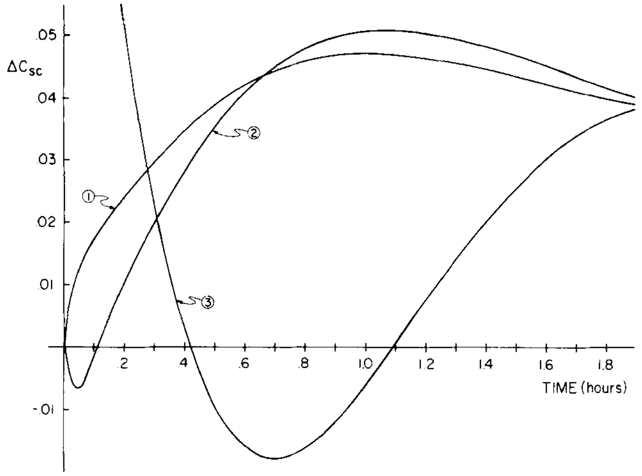


**Figure 2. Step response: $\Delta k_{cr}$ = 25%, $\Delta k_{cc}$ = 5%. ① system response, ② estimate $C_{sc} = f_1(C_{rc},T_{ra})$, ③ estimate $C_{sc} = f_2(T_{rg},T_{ra})$.**

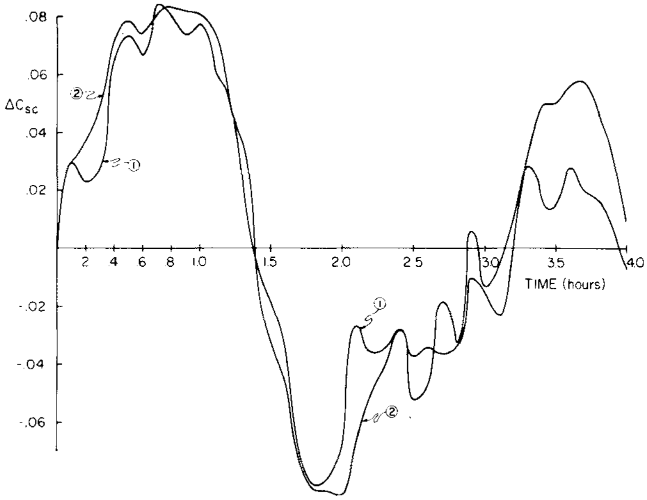


**Figure 3. Response to random step input to 1st order lag $t_c$ = 1 hour, period = .05 hour, $\sigma_{k_{cr}}$ = 25%, $\sigma_{k_{cc}}$ = 5%, ① system response, ② estimate $C_{sc} = f_1(C_{rc},T_{ra})$.**

| Eigen-values: | −.36 | −3.74 | −62.37 | −81.77 | −122.67 |
|---|---|---|---|---|---|
| $C_{rc}$ | .9899 | .9928 | −.667 | −.434 | −.276 |
| $C_{cat}$ | .0057 | −.0908 | .033 | .617 | .712 |
| $C_{sc}$ | .1396 | .065 | .744 | .652 | .645 |
| $T_{ra}$ | .0165 | −.027 | .0025 | .0696 | −.039 |
| $T_{rg}$ | .0166 | −.0330 | $5.6 \times 10^{-4}$ | $4 \times 10^{-3}$ | .0017 |

Modal Matrix of the Fluid Cat Cracker

For the computation of the mean square error the following amplitudes were used $\Delta k_{cr}$ = 25% and $\Delta k_{cc}$ = 5%, at frequencies corresponding approximately to the eigenvalues of this system: .34, 3.75, 60., 80. and 120.

| Measurements | $\{e^2\}$ | $\{e^2\}/\{z^2\}$ |
|---|---|---|
| $[C_{rc}, T_{ra}]$ | $7.8 \times 10^{-3}$ | .015 |
| $[C_{rc}, T_{rg}]$ | $7.8 \times 10^{-3}$ | .015 |
| $[T_{ra}, T_{rg}]$ | $4.5 \times 10^{-2}$ | .087 |

The transfer functions were computed from the system matrix using the Leverrier algorithm (Melsa & Jones 1973). It was found to be extremely sensitive to round off errors. The responses of the system and the estimators to different disturbances in the kinetic constants are shown in Figs. 2, 3, and 4. The merit of the dynamic index can clearly be seen. We must conclude that temperature measurements alone are insufficient from a dynamic point of view to obtain estimates of $C_{sc}$ through the use of the static estimator.

#### EXAMPLE IV: DOUBLE EFFECT EVAPORATOR (5TH ORDER MODEL)

For most control studies, Fisher and Seborg (1976) use a reduced-order model of the double effect evaporator. A fifth-order model was regarded as the best compromise between accurate representation and complexity.

The numerical values used in the model are omitted here for brevity. They are easily obtainable from the original source. A few specifics should be mentioned, however, so the reader can get some feeling about the dynamic characteristics of the system. The mass balances around the two tanks give rise to two poles at the origin. For a static estimator to exist, all the poles have to be strictly in the left half plane. This was obtained by introducing two single loop unity gain feedback controllers, regulating the levels by manipulating the corresponding outlets.

The resulting system (see Appendix), which formed the basis of our studies, has five real eigenvalues: −.0380, −.0381, −.0766, −.0766, −.773. The dominant time constant in the system is therefore approximately 26 minutes. We assume throughout the study that our objective is to obtain an estimate of the concentration in the first tank $C1$, which is not measured in the experimental setup. For the three available measurement pairs the following relative errors defined in (14) were found

| Measurement | $(\text{trace}(R)/\text{trace}(T^TT))^{\frac{1}{2}}$ |
|---|---|
| $(W1, W2)$ | .89 |
| $(W1, C2)$ | .19 |
| $(W2, C2)$ | .16 |

For those calculations, uncorrelated disturbances of feed rate, feed composition and feed temperature of identical variances were assumed. The measurement pair ($W1$, $W2$) would be desirable from a practical point of view, the large error clearly renders it infeasible. The main contribution is arising from changes in the feed concentration, which is poorly sensed by the levels. The combination $W2$, $C2$, level and concentration in the second tank, was the selected alternative.

Changes in the feed temperature are the main cause of the deviation. It should be emphasized that this is a measure of the mean square error. The actual error depends on how the disturbance vector is positioned in the three dimensional disturbance space. For particular cases, a larger or even a zero error can be obtained.

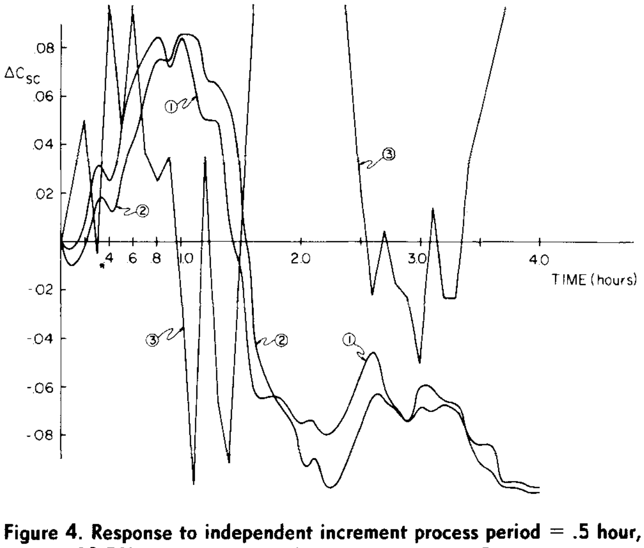


**Figure 4. Response to independent increment process period = .5 hour, $\sigma_{k_{cr}}$ = 12.5%, $\sigma_{k_{cc}}$ = 2.5%, ① system response, ② estimate $C_{sc} = f_1(C_{rc},T_{ra})$, ③ estimate $C_{sc} = f_2(T_{rg},T_{ra})$.**

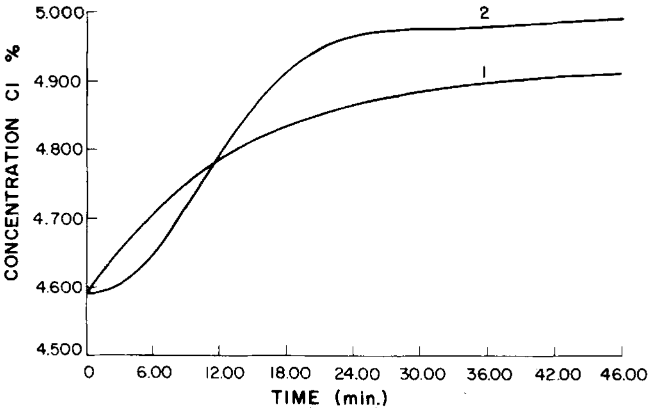


**Figure 5. Example IV: Response of system (1) and filter (2) to an unknown step change ($F$ = .1, $C_F$ = .1, $h_F$ = .1).**

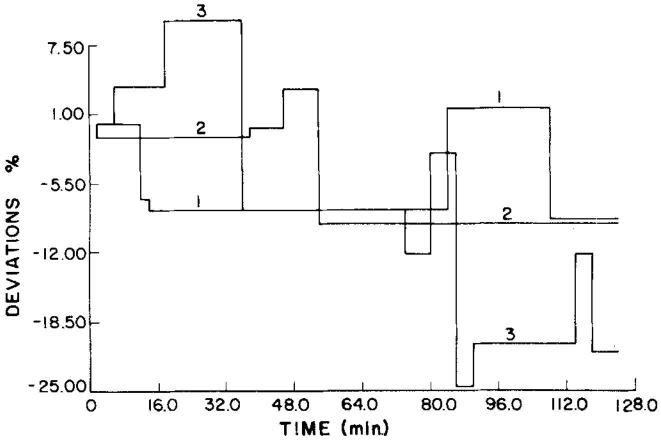


**Figure 6. Example IV: State excitation noise used in the simulation; 1 = $F$, 2 = $C_F$, 3 = $h_F$.**

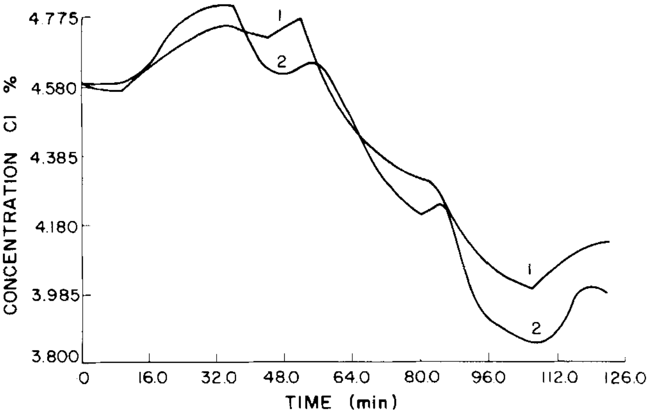


**Figure 7. Example IV: Response of system (1) and filter (2) to the disturbances in Fig. 4; ($V_2$ = 0).**

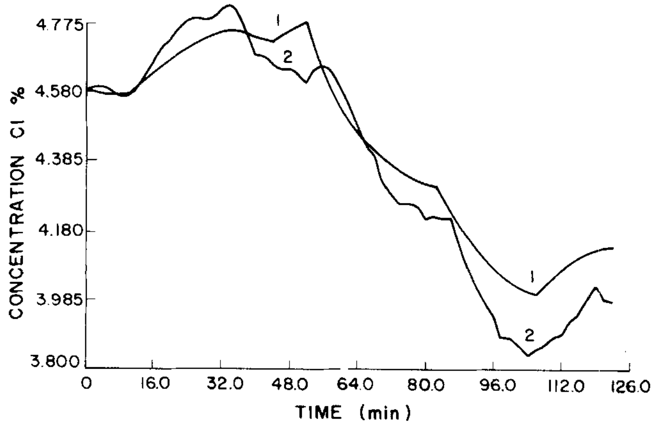


**Figure 8. Example IV: Response of system (1) and filter (2) to the disturbances in Fig. 4; ($V_2$ = diag (2 × $10^{-6}$)).**

To find the optimal filter gains according to Theorem 2, parameters describing the disturbances had to be chosen. The three disturbances were assumed to arrive on the average every twenty minutes. In view of the dominant time constant of 26 minutes, that frequency violates the steady state assumption used for the derivation of the relative error criterion. We wanted to see how our estimator performs when pushed to the extreme, to get a feel of the performance in a practical situation. Both measurements were subjected to error. The optimal steady state filter gain was determined by integrating the matrix Riccati equation until the solution was constant within an error bound. White noise of intensity $V_1$ = diag(5 × $10^{-4}$), and $V_2$ = diag(2.5 ×$10^{-5}$), lead to filter eigenvalues with real parts between −.11 and −.78. The state equations (augmented by the two equations for the disturbances), and the filter gain are listed in the Appendix. Figure 5 gives the response of the system and the filter to a +10% step change in all three disturbances. Figure 6 shows the input disturbances forming the basis of the simulation runs pictured in Figures 7, 8, and 9. The influence of different amounts of measurement noise on the estimate can be seen in Figure 7 ($V_2$ = diag(0)), Figure 8 ($V_2$ = diag(2 × $10^{-6}$) and Figure 9 ($V_2$ = diag(5 × $10^{-5}$)). The filter tracks the system response very well, despite unmeasured changes in the input variables with magnitudes up to 25%.

Simulation experiments with the Luenberger observer were carried out as well and are available in Morari (1977). For insignificant measurement noise, the results parallel those obtained with the filter. Difficulties were encountered in the attempts to obtain a satisfactory observer response solely through the specification of the eigenvalues.

## EXAMPLE V: DISTILLATION COLUMN

This example was chosen in order to compare our results with the work by Joseph and Brosilow (1978), who have chosen a different approach to the problem of estimation under the influence of sustained disturbances. The model of the $C_{\bar{3}}$ splitter used was discussed first by Amundson and Pontinen (1958). A linear input output model, constructed by step input tests, is given by Brosilow and Tong (1974). The relevant part of the model is

$$\theta_3 = \frac{-15.91}{12s + 1} \bar{u}_2 + \frac{-4.23}{5s + 1} \bar{u}_3$$

$$\theta_8 = \frac{-16.43}{10s + 1} \bar{u}_2 + \frac{-.47}{5s + 1} \bar{u}_3$$

$$y = \frac{.0253}{13s + 1} \bar{u}_2 + \frac{.0045}{4s + 1} \bar{u}_3$$

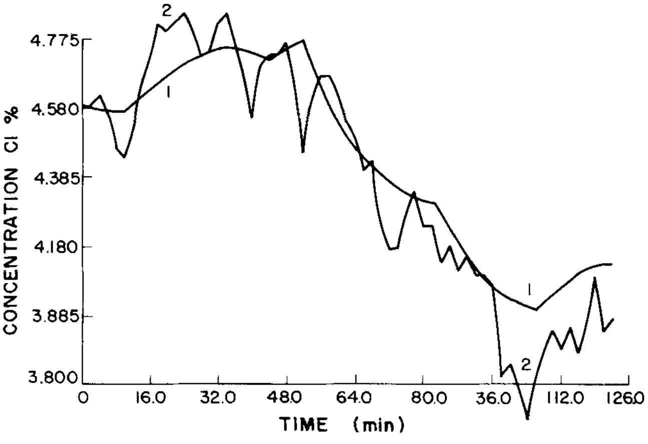


**Figure 9. Example IV: Response of system (1) and filter (2) to the disturbances in Fig. 4; ($V_2$ = diag (5 × $10^{-5}$)).**

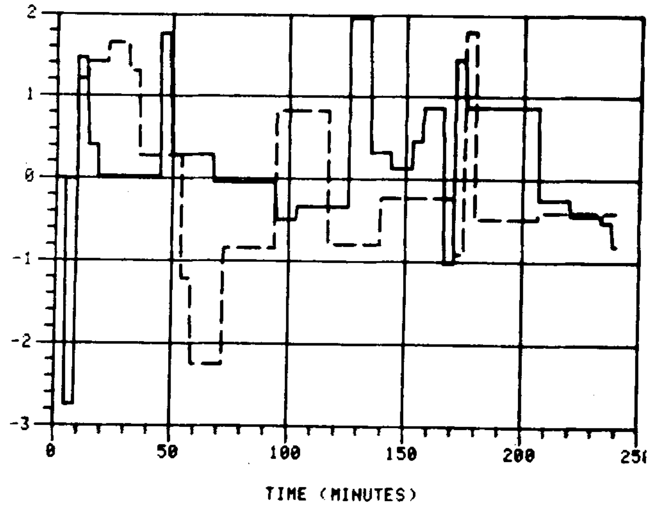


Figure 10. The disturbances used in the simulation of example 5.

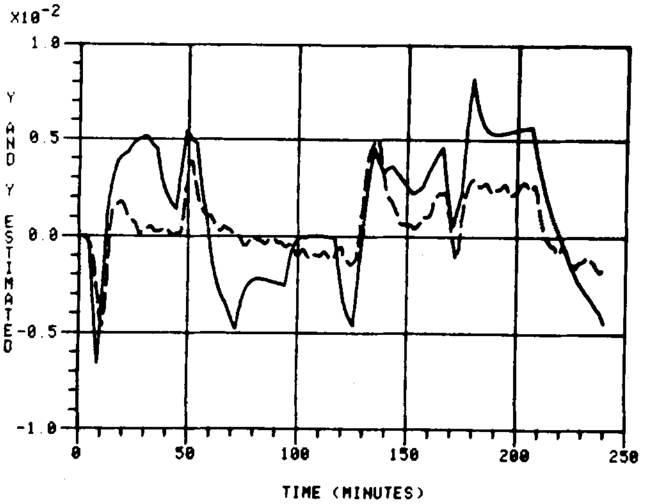


Figure 12. Example 5: y (solid line) and y estimated from measurement $\theta_8$ (dashed line).

where

$\theta_3$ temperature on 3rd tray (available for measurement)
$\theta_8$ temperature on 8th tray (available for measurement)
$\bar{u}_2$ $C_2$ fraction feed flow change
$\bar{u}_3$ $C_3$ fraction feed flow change
$y$ $C_3$ bottom composition (to be estimated)

$\bar{u}_2$ and $\bar{u}_3$ are modeled as sequences of steps with normally distributed amplitudes ($\sigma_2 = .34$, $\sigma_3 = .68$) occurring at an average frequency of $\nu = 0.1\ \text{min}^{-1}$. In order to use the standard formulae developed in the main part of the paper we normalize the inputs first, i.e.,

$$u = \phi_{\bar{u}\bar{u}}^{-\frac{1}{2}}\, \bar{u}$$

such that

$$\phi_{uu} = I$$

This necessary step was omitted by Joseph and Brosilow (1978).

$$\theta_3 = \frac{-5.409}{12s + 1}\, u_2 + \frac{-2.876}{5s + 1}\, u_3 \tag{51}$$

$$\theta_8 = \frac{-5.586}{10s + 1}\, u_2 + \frac{-0.320}{5s + 1}\, u_3 \tag{52}$$

$$y = \frac{.0086}{13s + 1}\, u_2 + \frac{.0031}{4s + 1}\, u_3 \tag{53}$$

The measurement selection criterion 1 (14) indicates that $\theta_3$ is preferable to $\theta_8$ for the estimation of $y$:

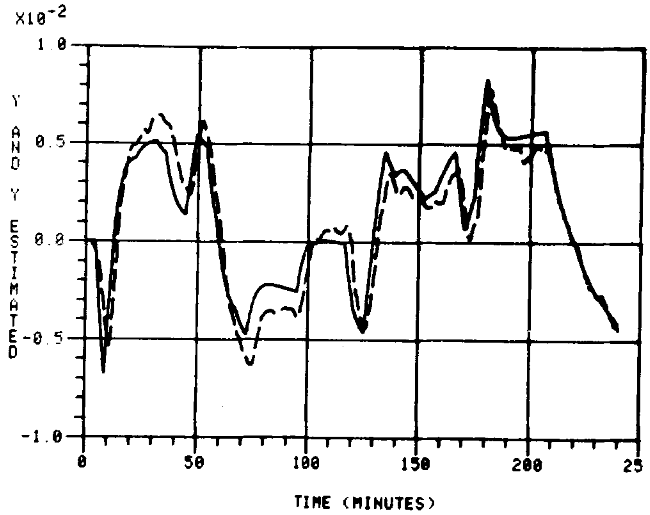


Figure 11. Example 5: y (solid line) and y estimated from measurement $\theta_3$, (dashed line).

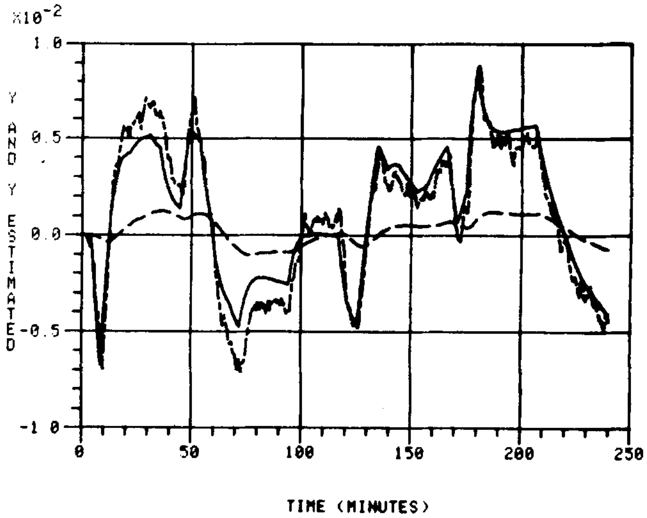


Figure 13. Example 5: System response (solid line), estimate from Kalman filter (---) ($V_1$ = diag (.001)) and modified Kalman filter (—·—·).

| Measurement | trace($R$)/trace($T^TT$) |
|---|---|
| $\theta_3$ | .146 |
| $\theta_8$ | .278 |

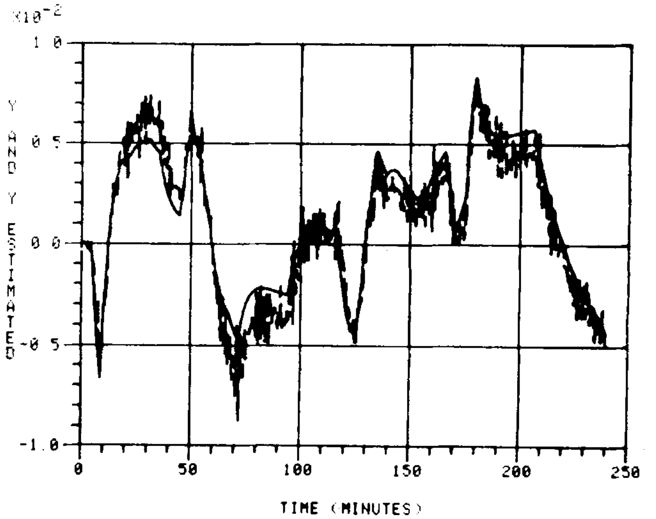


Figure 14. Example 5: System response y (solid line) and estimate from Kalman filter (dashed line) ($V_1$ = diag (.1)).

Using standard techniques (Athans & Falb 1966) a state variable representation can be found for (51)-(53). Because the system as defined is unobservable we proceed as follows: $u_2$, $u_3$ are estimated based on (51) or (52) using the modified Kalman filter (36). The results are substituted in (53) to obtain an estimate of the unknown composition $y$. The measurement noise was approximated by white noise of intensity $V_2 = .123$ which corresponds to a standard deviation of about 15% of the average temperature measurements $\theta_3$, $\theta_8$. $V_1$ was calculated based on Theorem 2. The steady state filter gain is reproduced in the Appendix, the response of the system and the estimates to changes in $u_2$, $u_3$ (Figure 10) is shown in Figure 11 and Figure 12, respectively.

Because of unobservability, we cannot construct the unmodified Kalman filter for (51)-(53) and compare it with the results of our modified filter. Therefore we lumped the poles, and keeping the steady state gains constant, we arrived at an approximate representation of (51)-(53) where all the long time constants associated with the action of $u_2$ are replaced by 11.6, and all the short ones associated with the action of $u_3$ by 4.6.

Figure 13 compares the estimates obtained from our modified filter (augmented state vector) and the unmodified filter without state vector augmentation. As was explained earlier, the offset can be reduced by increasing the assumed state excitation noise for the filter design. The resulting estimates become quite noisy, however (Figure 14). Equivalent results were obtained through measurement $\theta_8$ and are not reproduced here. The assumed parameters and the filter gains can be found in the appendix. A comparison of Figures 13 and 14 demonstrate the superiority of our scheme.


## ACKNOWLEDGEMENT

Financial assistance from the National Science Foundation, Grant ENG 75-11165 is gratefully acknowledged. We also wish to thank M. J. O'Dowd for performing the numerical computations for Example V and D. E. Seborg for the valuable comments in his review.


## NOTATION

$a$ = $\epsilon R^{m_1}$ disturbance amplitude defined in (27)
$C$ = $\epsilon R^{rxn}$ observation matrix
$D$ = $\epsilon R^{kxn}$ observation matrix for $z$
$E\{\}$ = expected value operator
$e$ = estimation error defined in (26)
$F$ = $\epsilon R^{nxn}$ system model matrix
$G$ = $\epsilon R^{nxm}$ matrix describing influence of $u$ on system
$H$ = $\epsilon R^{nxl}$ matrix describing influence of $m$ on system
$I$ = identity matrix (a subscript denotes the dimension)
$K$ = feedback gain matrix
$L$ = $\epsilon R^{mxm}$ noise model matrix
$m$ = $\epsilon R^{l}$ vector of known system inputs, e.g. manipulated variables
$N$ = normalization matrix defined in (21)
$P$ = modal matrix of $F$; the columns of $P$ are the eigenvectors of $F$
$Q$ = modal matrix of $F^T$; the columns of $Q$ are the eigenvectors of $F^T$
$R$ = defined in (13)
$S$ = defined in (6)
$S^+$ = $(S^TS)^{-1}S^T$ generalized inverse of S
$T$ = defined in (7)
$u$ = $\epsilon R^m$ colored noise vector
$u^*$ = defined in (34)
$V$ = white noise intensity $E\{w(t_1)\, w^T(t_2)\} = V\delta(t_1 - t_2)$
$(w_1^T, w_2^T)^T$ $\epsilon R^{n+m}$, $w_3$ $\epsilon R^r$ } zero mean white noise processes with intensities $V$, $V_3$ respectively
$x$ = $\epsilon R^n$ state vector
$y$ = $\epsilon R^r$ observation vector
$z$ = $\epsilon R^k$ vector to be estimated

### Greek Letters

$\Gamma$ = normalized modal matrix defined in (23)
$\delta_{ij}$ = Kronecker delta $\delta_{ij} = 1 \quad i = j$; $= 0 \quad i \neq j$
$\phi_{ab}$ = covariance matrix of vectors $a$, $b$: $\phi_{ab} = E\{ab^T\}$
$\Phi$ = power spectral density matrix
$\Sigma$ = defined in (35)
$\Omega$ = defined in (15)

### Superscripts

$\hat{}$ = estimate
$T$ = transpose

The symbols referring specifically to quantities used in the examples are defined in the example section.

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## APPENDIX

I. Numerical data used in the simulation of the double effect evaporator (Example IV).
5th order state space representation of the model of the double effect evaporator after feedback stabilization

$$X^T = (W1, C1, H1, W2, C2)$$
$$u^T = (B1, B2)$$
$$y^T = (W2, C2)$$
$$\dot{x} = \bar{A}x + Bu$$

where

$$\bar{A} = A + B\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$y = Cx$

$$\bar{A} = \begin{bmatrix} -.7658 \times 10^{-1} & -.1085 \times 10^{-2} & -.1254 & 0 & 0 \\ 0 & -.7549 \times 10^{-1} & .1254 & 0 & 0 \\ 0 & -.6036 \times 10^{-2} & -.7740 & 0 & 0 \\ .7945 \times 10^{-1} & -.1219 \times 10^{-2} & -.1447 & -.3808 \times 10^{-1} & .1258 \times 10^{-3} \\ -.4135 \times 10^{-1} & .3930 \times 10^{-1} & .1447 & 0 & -.3796 \times 10^{-1} \end{bmatrix}$$

$$B = \begin{bmatrix} -.7658 \times 10^{-1} & 0 \\ 0 & 0 \\ 0 & 0 \\ .7945 \times 10^{-1} & -.3808 \times 10^{-1} \\ -.4135 \times 10^{-1} & 0 \end{bmatrix}$$

Eigenvalues of $\bar{A}$: $-.3796E\text{-}1$, $-.3808E\text{-}1$, $-.7658E\text{-}1$, $-.7658E\text{-}1$, $-.7729$

Augmented matrix $A'$ including the effect of the unmeasured disturbances:

| | | | | | | |
|---|---|---|---|---|---|---|
| −.7658E-1 | −.1085E-2 | −.1254 | 0. | 0. | −.3729E-1 | −.6899E-2 |
| 0. | −.7549E-1 | .1254 | 0. | 0. | −.3926E-1 | −.6918E-1 |
| 0. | −.6036E-2 | −.7740 | 0. | 0. | −.1424E-2 | −.1998E-1 |
| .7945E-1 | −.1219E-2 | −.1447 | −.3808E-1 | .1258E-3 | 0. | 0. |
| −.4135E-1 | .3930E-1 | .1447 | 0. | −.3796E-1 | 0. | 0. |
| 0. | 0. | 0. | 0. | 0. | 0. | 0. |
| 0. | 0. | 0. | 0. | 0. | 0. | 0. |

Filter gain used in the simulation

$$K^T = \begin{pmatrix} .1983E1 & .5124 & -.1479 & .5399 & -.1549 & -.1286E2 & .6909E1 \\ -.6650 & .2039E1 & .1965 & -.1549 & .4616 & .6967E1 & -.9039E1 \end{pmatrix}$$

II. Numerical data used in the simulation of the distillation column (Example V)

Filter gain used to obtain Fig. 11:
$K^T = (-1.354 \quad -0.646 \quad -5.558)$
for $V_1 = \text{diag}(0, 0, 3.8)$; $V_2 = .123$
Filter gain used to obtain Fig. 12:
$K^T = (-0.081 \quad -1.614 \quad -5.020)$
for $V_1 = \text{diag}(0, 0, 3.1)$, $V_2 = .123$
Filter gain used to obtain Fig. 13:
$K^T = (-1.107 \quad -0.520 \quad -4.032)$
for $V_1 = \text{diag}(0, 0, 3.8)$, $V_2 = .123$
$K^T = (-0.044 \quad -0.023)$
for $V_1 = \text{diag}(0.001, 0.001)$, $V_2 = .123$
Filter gains used to obtain Fig. 14:
$K^T = (-4.393 \quad -2.338)$
for $V_1 = \text{diag}(0.1, 0.1)$, $V_2 = .123$

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# Statistical Analysis of Constrained Data Sets

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Practical, comprehensive computer-based methods for analyzing data sets are developed. Methods for calculating data adjustment, parameter values, variance-covariance of adjusted data and parameters and for detecting aberrant data are presented. A simple calculation algorithm and application of the methods for design of experimental measurements are proposed.

## SCOPE

Least squares analysis, commonly used to fit regression equations to sets of experimental data, also provides powerful techniques for analyzing the measured data themselves, when these data can be interrelated through constraining physical laws. Least squares parameter estimation problems are typically "parameter—rich" in the sense that the data set is constrained by a single regression equation. (In this article, the term "parameter" is used in the engineering sense of a quantity to be estimated from other data, rather than in the statistical sense, wherein it applies to all estimated quantities.)

In another frequently met situation of particular interest in this work, a large set of data is interrelated by physical laws such as heat balances, material balances or kinetic equations. This situation may be thought of as being "constraint-rich", and is typical of many laboratory experiments, pilot unit tests, and commercial unit performance tests. Constraints, together with estimates of the variances of the measured data, can be used to adjust data to more accurate values and to draw conclusions about their credibility.

The data estimation techniques discussed here greatly facilitate analysis of constrained data sets by providing maximum likelihood estimates of the measured data and any parameters, by assessing the probability that there are extraordinary errors, and by providing error information about the calculated quantities for use in subsequent analysis. Further, the techniques can be used to develop experiments producing data with improved accuracy. The method can be thought of as an extension of the averaging process to situations, in which each measured quantity may enter into one or a number of physical constraints, and by which alternative values can be inferred. It can be applied, if necessary, to detect gross measurement errors and to isolate any such by using data redundancies, much as a skilled analyst would. And, replicates or near replicates are not required to judge credibility of the data values.

The net effect can be significantly increased efficiency of experimentation, offering the happy choice of either obtaining more accurate data for a given cost, or of achieving the same accuracy in the final results with less experimental cost. Because the techniques are general, they can handle data sets described as a typical linear or nonlinear regression problem, a parameter-free data adjustment problem, or any combination of these.

The basic data correction algorithm was first derived for and applied to surveying problems (Demming 1946). Data adjustment techniques were applied in the chemical engineering literature by Kuhn and Davidson (1961). They handled nonlinear problems, but did not address either estimates of the error in the adjusted data, or criteria for assessing consistency of the measured data set.

Gross errors in measured data, if undetected, tend to be spread out among the calculated adjustments to the measured data. Ripps (1967) considered the possibility of gross measurement error and suggested an algorithm for computing data adjustments when gross errors are suspected. Nogita (1972) added an univariate statistical criterion for judging the probability that a blunder exists in the data set. The specific case of simultaneous chemical reactions has been discussed, with emphasis on computational aspects, by Murthy (1973, 1974).

Madron et al. (1977) also address simultaneous chemical reactions. Of particular note in their work is the multidimensional chi-square test used to test for consistency of measured values, and the calculation of the variance-covariance matrices for all estimated data. A chi-square test can, however, be applied to the general data adjustment problem, both in detecting gross measurement error and in locating likely aberrant measurements. Further, unnecessary restriction is placed on the applicability of the test in their work. In good treatment of the general estimation problem, Britt and Leucke (1973) calculated the error structure of estimated parameters and placed special emphasis on parameter estimation in nonlinear problems.

This study attempted to develop practical and comprehensive computer based tools for analyzing data sets and planning of experimental measurements. Essential elements include the ability to handle general linear and nonlinear cases, estimates of the variance of and covariance between all estimated data, generally applicable methods for detecting inconsistency in the measured data set and for isolating any aberrant measurements, and efficient methods of computation.

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