27
5/14/79
2460771 c,

UCID- 18116

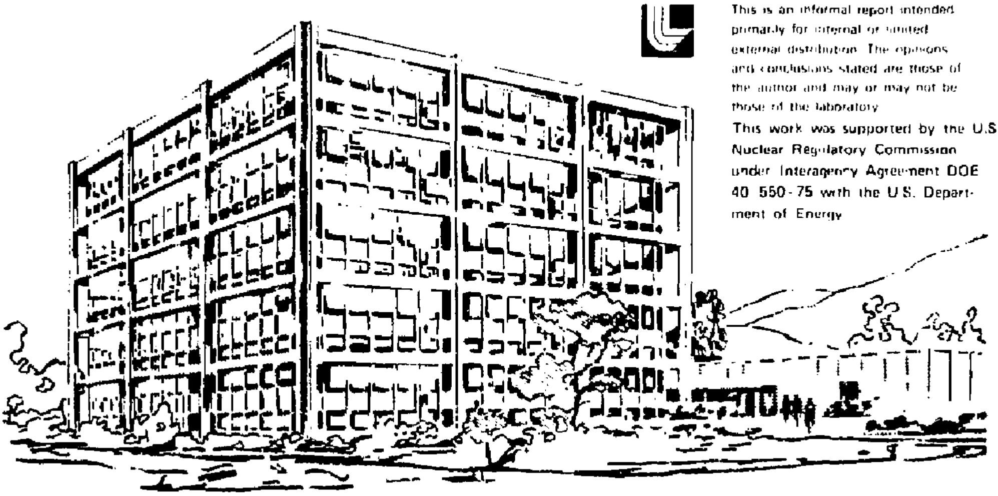
Lawrence Livermore Laboratory

DESIGN TECHNIQUES FOR LARGE SCALE LINEAR MEASUREMENT SYSTEMS

James V. Candy

March 1979

MASTER



This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the laboratory.

This work was supported by the U.S. Nuclear Regulatory Commission under Interagency Agreement DOE 40 550-75 with the U.S. Department of Energy

FORWARD

The NRC Safeguards Program at LLL is directed toward developing a methodology for assessing the effectiveness of material control and accounting systems at processing/reprocessing facilities for special nuclear material. The methodology under development requires many types of mathematical models including performance models of safeguard components. Included in the class of safeguard components are real-time measurement systems which incorporate on-line estimators/detectors for the timely detection of material losses.

Performance modeling generally involves mathematical model development and simulation of the physical process being measured. This paper discusses the development of design techniques for large scale measurement systems. These techniques are applicable to any processing units which can be adequately represented by linear or linearized models in state space form. Although this work is discussed in the context of a plutonium extraction column and a plutonium nitrate storage tank, they are representative of two classes of safeguard components which are generic to any fuel cycle involving chemical separations/purifications.

TABLE OF CONTENTS

LIST OF FIGURES

ABSTRACT

In this report we primarily discuss some techniques to design measurement schemes for systems modeled by large scale linear time invariant systems, i.e., physical systems modeled by a large number (>5) of ordinary differential equations. The techniques are based on transforming the physical system model to a coordinate system facilitating the design and then transforming back to the original coordinates. An example of a three-stage, four-species, extraction column used in the reprocessing of spent nuclear fuel elements is presented.

The basic ideas are briefly discussed in the case of noisy measurements. An example using a plutonium nitrate storage vessel (reprocessing) with measurement uncertainty is also presented.

I. INTRODUCTION

In order to control a large-scale dynamical system, one is inevitably faced with the problem of making measurements of various process variables directly or indirectly. The choice of which variables to measure, the number of measurements to make, selecting the proper instrumentation, and finally deciding whether or not the scheme selected achieves the measurement requirements is difficult.

In this report, we discuss the measurement system design problem for processes modeled by linear deterministic and stochastic systems. The basic question of observability, i.e., the ability (loosely) to choose measurement variables enabling the reconstruction of process variables which cannot be measured directly, is investigated. Suppose we are interested in the volume of a liquid in a chemical processing unit, but we have no means of measuring this desired process variable directly. Instead, we know that (physically) the volume is related (mathematically) to the pressure and temperature which can be measured. Thus, from these measurements and their mathematical relation with volume, we are able to "reconstruct" the volume. This example emphasizes the basic concept of observability--a reconstruction process.

In this report, we develop techniques to design (simply) measurement systems for large scale processes modeled by linear systems. Although these results may not appear realistic to the practicing engineer, they can provide useful guidelines and have been used to design estimators for linearized systems.[1] These results are useful for design purposes as well as analyses of proposed large scale measurement schemes.

The necessary theoretical development of the design techniques is presented. The design algorithm evolves from this development. The algorithm is applied to a realistic large scale model of a three-stage, four-species extraction column. Some theoretical results for columns in general are also presented.

The basic question of observability of linear systems is defined and resolved in Section II. In Section III, the question of how to design a large scale measurement system is addressed. The results we arrive at are applied to a N stage M species extraction column which is used in the chemical reprocessing of spent nuclear fuel elements. The deterministic concepts developed are then briefly extended to include stochastic linear models. Stochastic observability is defined and applied to a plutonium-nitrate storage vessel.

II. OBSERVABILITY OF LINEAR SYSTEMS

We are concerned basically with examining the inherent properties of a system which can be utilized to aid in the design or analysis of measurement systems. We restrict our attention to linear systems because they can be used to represent a large class of physical systems and also because this restriction enables us to obtain some meaningful results. We define a continuous linear dynamical system in state form by the model

$$\dot{x}(t) = F_t x(t) + G_t u(t) \tag{2.1}$$

where x, u are the n-state, m-input vectors and F_t, G_t are appropriately dimensioned matrices. Suppose we wish to design a linear measurement system

$$y(t) = H_t x(t) \tag{2.2}$$

where $y \epsilon R^p$ and H_t is the measurement distribution matrix.

We ask ourselves, what properties must (2.2) or H_t contain in order for us to be able to determine or reconstruct x(t) from measurements y(t)! This is really an analysis question, but the answer ultimately leads to design. This question is one of observability, i.e., the system of (2.1, 2) is observable if for any $x(t_0)$ in the state space, there exists a finite $t_1 > t_0$ such that knowledge of u(t) and y(t) over $t_0 \leq t \leq t_1$ is sufficient to specify $x(t_0)$. If p = n and H_t is nonsingular over $[t_0, t_1]$ then

$$x(t) = H_t^{-1} y(t) \tag{2.3}$$

and we recall that

$$x(\alpha) = \Phi(\alpha,t_0)x(t_0) + \int_{t_0}^{\alpha} \Phi(\alpha,\beta)G_\beta u(\beta)d\beta \quad \alpha > t_0 \qquad (2.4)$$

where $\Phi(\alpha,t_0)$ is the well-known <u>state transition matrix</u> (see [2]). Clearly, letting $t = \alpha$ in (2.3) and using (2.4) we obtain

$$H_\alpha^{-1}y(\alpha) = \Phi(\alpha,t_0)x(t_0) + \int_{t_0}^{\alpha} \Phi(\alpha,\beta)G_\beta u(\beta)d\beta$$

or solving for $x(t_0)$ (using the property $\Phi^{-1}(\alpha,t_0) = \Phi(t_0,\alpha)$)

$$x(t_0) = \Phi(t_0,\alpha)[H_\alpha^{-1}y(\alpha) - \int_{t_0}^{\alpha} \Phi(\alpha,\beta)G_\beta u(\beta)d\beta] \qquad (2.5)$$

Clearly, since u and y are known over this interval, the "constraint" on our measurement system H_α is that it be nonsingular, one obvious choice is $H_\alpha = H = I_n$, i.e., measure every state independently.

Unfortunately, H is singular--typically we have many more states than measurements! Even if the states are accessible for measurement, we may not be able to afford the cost of instrumentation that is required. So, the more realistic case exists when $p \neq n$. The answer to this problem is also well-known, using the results in Meditch[3] we have

<u>Lemma 2.1</u>. The system in (2.1,2) is completely observable on $[t_0,t_1]$ if the symmetric nxn matrix

$$V(t_0,t_1) := \int_{t_0}^{t_1} \phi^T(\alpha,t_0)H_\alpha^T H_\alpha \phi(\alpha,t_0)d\alpha$$

is positive definite for some $t_1 > t_0$ (2.6)

The proof of this lemma is straightforward, but the sufficiency part is instructive and will be used later so we develop it briefly.

From (2.5) we have

$$y(t) = H_t \, \phi(t,t_0)x(t_0) + \int_{t_0}^{t} \phi(t,\beta)G_\beta u(\beta)d\beta$$

or since u(•) is known we can examine

$$\bar{y}(t) = y(t) - \int_{t_0}^{t_1} \phi(t,\beta)G_\beta u(\beta)d\beta = H_t\phi(t,t_0)x(t_0). \tag{2.7}$$

Now multiplying both sides of (2.7) and integrating from t_0 to t_1, we have

$$\int_{t_0}^{t_1} \phi^T(\alpha,t_0)H_\alpha^T\bar{y}(\alpha)d\alpha = \left\{\int_{t_0}^{t_1} \phi^T(\alpha,t_0)H_\alpha^T H_\alpha \phi(\alpha,t_0)d\alpha\right\}x(t_0)$$

or

$$x(t_0) = V^{-1}(t_0,t_1)\int_{t_0}^{t_1} \phi^T(\alpha,t_0)H_\alpha^T\bar{y}(\alpha)d\alpha \qquad .8)$$

So analogous to (2.5), we see that V must be nonsingular; thus, our design problem becomes that of assuring that (2.6) is satisfied. Consider the following corollary to the lemma, which indicates the well-known time invariant case

Corollary 2.2 Let $\Sigma_t := (F_t, G_t, H_t)$ of (2.1,2) be time invariant, i.e., $\Sigma = (F,G,H)$, then the corresponding system is completely observable if

$$\rho(V_n) = n$$

where $V_n^T := [H^T | (HF)^T | \ldots | (HF^{n-1})^T]$ is the observability matrix and $\rho(\cdot)$ is the rank of $\cdot$.

The proof of this corollary can be found in [2].

We will now digress slightly and work with the linear time invariant version of (2.1,2) to answer some fundamental questions and then return to the time varying case in a later section.

III. DESIGN OF LINEAR TIME INVARIANT MEASUREMENT SYSTEMS

In this section, we restrict our examination to linear time invariant systems and ask two basic questions. What is the minimal number of outputs required to assure system observability? What is the minimal number of sensors required to achieve observability? The answer to the first question requires some mathematical machinery which we briefly describe.

First, we define two systems (F_1,G_1,H_1) and (F_2,G_2,H_2) to be <u>equivalent</u> if there exists a nonsingular coordinate transformation T such that for $x_1 = Tx_2$

$$(F_2,\ G_2,\ H_2) = (TF_1T^{-1}, TG_1, H_1T^{-1}). \tag{3.1}$$

Let's consider a specific coordinate representation of (F,G,H) - the Jordan canonical form. Following Chen[4] we define a system to be in Jordan form when

$$\underset{(n\times n)}{F_J :=} \begin{bmatrix} F_1 & & 0 \\ & \ddots & \\ 0 & & F_q \end{bmatrix}, \quad \underset{(n\times m)}{G_J :=} \begin{bmatrix} G_1 \\ \vdots \\ G_q \end{bmatrix}, \quad \underset{(p\times n)}{H_J :=} [H_1 \ \dots \ H_q]$$

where corresponding to each eigenvalue, say λ_i, we have submatrices

$$\underset{(n_i\times n_i)}{F_i :=} \begin{bmatrix} F_{i1} & & 0 \\ & \ddots & \\ 0 & & F_{ir_i} \end{bmatrix}, \quad \underset{(n_i\times m)}{G_i :=} \begin{bmatrix} G_{i1} \\ \vdots \\ G_{ir_i} \end{bmatrix}, \quad \underset{(p\times n_i)}{H_i :=} [H_{i1} \dots H_{ir_i}]$$

and

$$\underset{(n_{ij}\times n_{ij})}{F_{ij} =} \begin{bmatrix} \lambda_i & 1 & & 0 \\ & \lambda_i & \ddots & \\ & 0 & \ddots & \lambda_i \quad 1 \\ & & & \lambda_i \end{bmatrix}, \quad \underset{(n_{ij}\times m)}{G_{ij} =} \begin{bmatrix} g_{1ij} \\ \vdots \\ g_{n_{ij}ij} \end{bmatrix} \quad \underset{(p\times n_{ij})}{H_{ij} =} [h_{1ij} \dots \ h_{n_{ij}\ ij}] \tag{3.2}$$

Note that the Jordan structure enables one to decompose a system into decoupled or noninteracting subsystems. Consider the following simple example

Example 3.1 Let a system (F_1, G_1, H_1) be transformed to (F_J, G_J, H_J) such that $n_1 = 3$, $n_{11} = 2$, $n_{12} = 1$ and $n_2 = 1$, $n_{21} = 1$. Construct the Jordan form representation.

For λ_1:

$$F_{11} = \begin{bmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{bmatrix}, \quad G_{11} = \begin{bmatrix} g_{111} \\ g_{211} \end{bmatrix}, \quad H_{11} = [h_{111} \; h_{211}]$$

$$F_{12} = [\lambda_1], \quad G_{12} = [g_{112}], \quad H_{12} = [h_{112}]$$

For λ_2:

$$F_{21} = [\lambda_2], \quad G_{21} = [g_{121}], \quad H_{21} = [h_{121}]$$

Thus,

$$F_J = \left[\begin{array}{cc|c|c} \lambda_1 & 1 & & 0 \\ & \lambda_1 & & \\ \hline & & \lambda_1 & \\ \hline 0 & & & \lambda_2 \end{array}\right], \quad G_J = \left[\begin{array}{c} g_{111} \\ g_{211} \\ \hline g_{112} \\ \hline g_{121} \end{array}\right], \quad H_J = [h_{111} h_{211} | h_{112} | h_{121}]$$

If one were to construct a block diagram of this system, then we have[†]

$$\dot{x}_1 = \lambda_1 x_1 + x_2 + \underline{g}_{111}\underline{u}$$

$$\dot{x}_2 = \lambda_1 x_2 + \underline{g}_{211}\underline{u}$$

$$\dot{x}_3 = \lambda_1 x_3 + \underline{g}_{112}\underline{u}$$

$$\dot{x}_4 = \lambda_2 x_4 + \underline{g}_{121}\underline{u}$$

[†] Here we use the underline to distinguish vector from scalar quantities.

and the measurement scheme

$$\underline{y} = (\underline{h}_{111}x_1 + \underline{h}_{211}x_2) + \underline{h}_{112}x_3 + \underline{h}_{121}x_4 = \underline{y}_{11} + \underline{y}_{12} + \underline{y}_{21} \qquad (3.3)$$

The system is depicted in Figure 1. Note that each of the three subsystems are state-decoupled from one another, i.e., none of the states of one subsystem interact with another subsystem . For example, we can rewrite (3.3) as the subsystems $\{S_1\}$, i = 1,2,3

$$S_1 := \begin{cases} \dot{x}_{11} = F_{11}x_{11} + G_{11}u \\ y_{11} = H_{11}x_{11} \end{cases} \qquad \text{for } x_{11}^T = [x_1 \;\; x_2]$$

$$S_2 := \begin{cases} \dot{x}_{12} = F_{12}x_{12} + G_{12}u \\ y_{12} = H_{12}x_{12} \end{cases} \qquad \text{for } x_{12} = x_3$$

$$S_1 := \begin{cases} \dot{x}_{21} = F_{21}x_{21} + G_{21}u \\ y_{21} = H_{21}x_{21} \end{cases} \qquad \text{for } x_{21} = x_4$$

Thus, the Jordan form enables us to decouple the system, by a coordinate transformation. Note that the system responds identically to the original system--only an "equivalent" internal structure has been formed. The transmission T^{-1} is conventionally designated M_F the

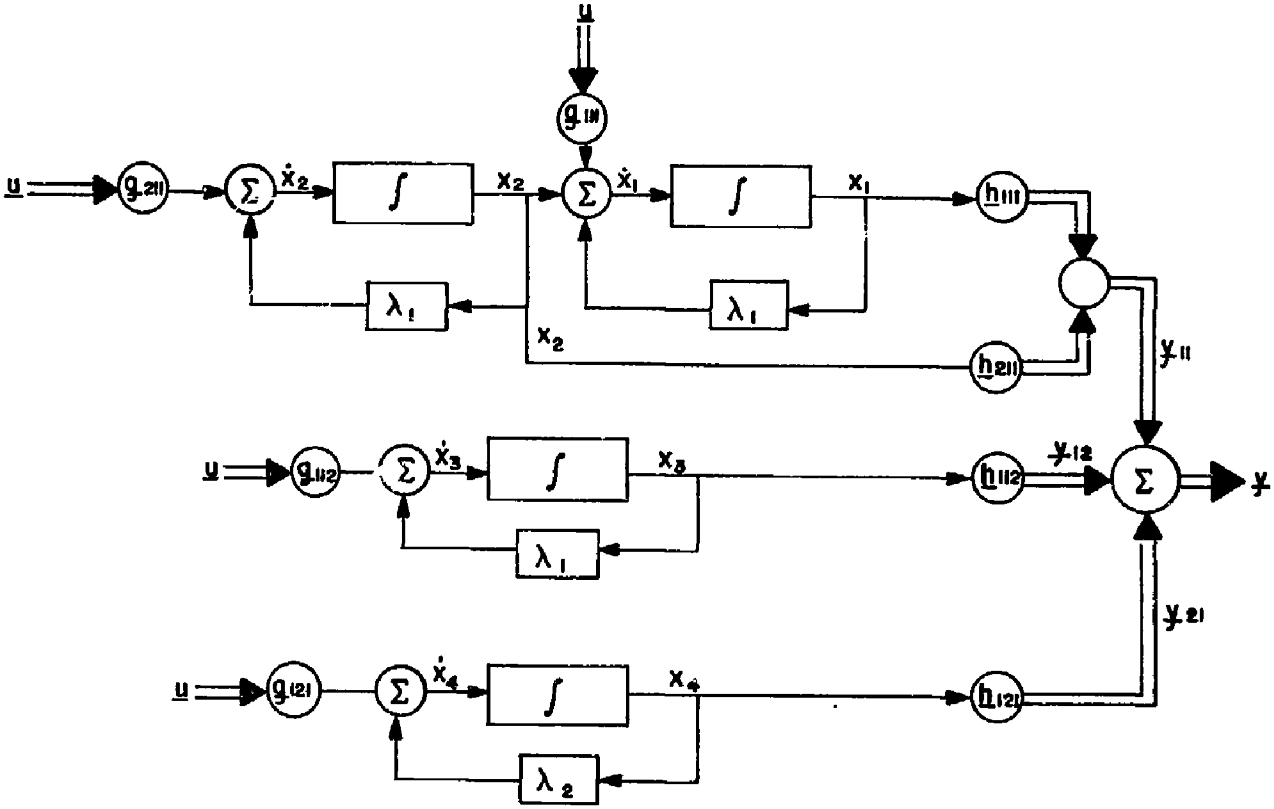


FIGURE I. JORDAN FORM REPRESENTATION OF LINEAR SYSTEM modal matrix of F and is made up of the eigenvectors and generalized eigenvectors that correspond to distinct eigenvalues (see Chen[4] for details), i.e.,

$$M_F = [\underline{v}_1 | \cdots | \underline{v}_q] \tag{3.4}$$

where $\underline{v}_i$ satisfies the eigenvector equation

$$(F-\lambda_i I)v_i = \underline{0} \tag{3.5}$$

or $\underline{v}_i$ is a generalized eigenvector of rank k of F associated with λ_i if and only if

$$(F-\lambda_i I)^k \underline{v}_i = \underline{0}$$

and

$$(F-\lambda_i I)^{k-1} \underline{v}_i \neq \underline{0} \tag{3.6}$$

Thus, the modal matrix is always guaranteed to be nonsingular by construction; therefore, we can be assured that the transformation $T = M_F$ always exists.

The importance of the Jordan canonical form in the design of control systems has been well known for a long time, and its significance in a more general geometric setting has been discussed in Wonham[5]. Thus, the Jordan form is the matrix representation of a linear operator which decomposes the state space into cyclic subspaces. (See Wonham[5] for details). This decomposition is unique and it enables us to easily determine such important properties as stability, controllability, and observability.

Consider the situation where the dimension of F is large (n>5). To check observability we merely must check the rank of V_n in Corollary 2.2; however, this step is not necessarily an easy task even on a computer. Also, the rank check is not enlightening as a design aid; therefore, we consider the following lemma which employs the Jordan form,

Lemma 3.1 Given the system $\Sigma_J = (F_J, G_J, H_J)$ in Jordan form, Σ_J is observable iff for each $i \epsilon \underline{q}$,[†] the columns of the $p x r_i$ matrix

$$V_i^* = [h_{1i1} h_{1i2} \cdots h_{1ir_i}]$$

are linearly independent.[††]

The proof of this lemma is given in Chen[4] and it follows directly from properties of invariant subspaces. It merely means that we need only find a single vector which generates the subspace, i.e., the vector which corresponds to each independent eigenvector associated with a particular eigenvalue. To see this, let's construct the observability matrix presented in Example 3.1. Here we have

---

[†] This notation means i = 1,2,...,q.

[††] Similar results hold for the controllability of the system (see Chen[4]).

$$V_n = \left[\begin{array}{cc|c|c} h_{111} & h_{211} & h_{112} & h_{121} \\ \lambda_1 h_{111} & h_{111}+\lambda_1 h_{211} & \lambda_1 h_{112} & \lambda_2 h_{121} \\ \lambda_1^2 h_{111} & 2\lambda_1 h_{111}+\lambda_1^2 h_{211} & \lambda_1^2 h_{112} & \lambda_2^2 h_{121} \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_1^{n-1} h_{111} & (n-1)\lambda_1^{n-2} h_{111}+\lambda_1^{n-1} h_{211} & \lambda_1^{r-1} h_{112} & \lambda_2^{n-1} h_{121} \end{array}\right] \tag{3.7}$$

Clearly, column 2 is linearly independent of column 1 for any h_{211}; therefore, the independence of columns 1 and 3 are determined by the values of h_{111} and h_{112} exclusively. Column 4 is always linearly independent due to λ_2; thus, $\rho V_n = n = 4$ and the system is observable. Thus, one only need check the independence of h_{111} and h_{112} to assure observability. For large scale systems and design, this technique is extremely useful. Now applying the lemma directly to this example, we obtain for $i = 1,2$, $r_1 = 2$, $r_2 = 1$

$$\rho V_1^* = [h_{111} \; h_{112}] = r_1 = 2$$

$$\rho V_2^* = [h_{121}] = r_2 = 1 \tag{3.8}$$

So, we see that (3.7) and (3.8) yield the same results and in fact these *results indicate immediately* the minimum number of outputs required to assure observability. The following theorem summarizes this.

Theorem 3.1 Given a linear time invariant system, $\Sigma = (F,G,H)$. The minimum number of outputs required to assure complete observability, i.e., $\rho V_n = n$ is given by $p = \max \{r_i\}$, $i \epsilon \underline{q}$, where r_i is the number of Jordan blocks associated with λ_i.

The proof this theorem follows by applying the duality theorem to results of Vogt and Cullen [6] where they show that the max $\{r_i\}$ can be used to design a system for the minimum number of inputs to assure controllability. We formally state this as a Corollary, i.e.,

Corollary 3.2 The minimum number of inputs required to assure controllability, i.e., to assure that each state can be driven to the origin by a given input and the analogous condition $\rho W_n = \rho[G|FG|...|F^{n-1}G] = n$ is given by $m = \max \{r_i\}$, $i \epsilon \underline{q}$ above and W_n is the controllability matrix.

We summarize these results in the measurement system design algorithm presented in Table I. This algorithm will be applied to an extraction column in Section III-2.

III-1 N-Stage, M-Species Extraction Column Structural Models

We now apply these results to a large scale physical system utilized in nuclear reprocessing operation--an extraction column. In a Purex process, plutonium and uranium nitrates are complexed with tribatylphosphate then separated from other fission products by extraction with a suitable organic solvent (see Alspach[7] for details). The liquid-liquid pulsed extraction column is a chemical processing unit to bring

TABLE I: MEASUREMENT DESIGN ALGOPITHM

Step 1: Transform $F \longrightarrow F_J$, using an available eigenvalue-eigenvector routine.

Step 2: Set $p = \max \left\{r_i\right\}$ $i \varepsilon \underline{q}$ - this is the minimum number of outputs to assure obervability.

Step 3: Form the set of matrices $\left\{V_i^*\right\}$, $i \varepsilon \underline{q}$ and select the elements of H to assure the rank condition $\rho V_i^* = \min \left\{p, r_i\right\}$.

Step 4: Transform (F_J, G_J, H_J) back to the original system (F, G, H).

two immiscible phases (aqueous and organic) into better than usual contact, enhancing the transfer of mass between them by the hydraulic pulsation of the liquid through holes in plates spaced throughout the column. A state space model of a simple 3-stage extraction column was reported in Candy, et.al [8], the dynamic state equations take the form

$$\dot{x}(t) = Fx(t) + Gu(t) + \psi(x(t)) \tag{3.9}$$

In steady state, simulation runs indicate that the state trajectory is dominated by the linear time invariant part[†], therefore, we assume that the column can be adequately modeled by

$$\dot{x}(t) = Fx(t) + Gu(t) \tag{3.10}$$

where the state vector of the N stage, M species column can be written by stages as

$$\begin{aligned} x^T := [&C_1^o(2)\ldots C_M^o(2)|\ldots|C_1^o(N+1)\ldots C_M^o(N+1)|C_1^a(2)\ldots \\ &C_M^a(2)|\ldots|C_1^a(N+1)\ldots C_M^a(N+1)|T(2)\ldots T(N+1)]^T \end{aligned} \tag{3.11}$$

where $C_i^o(j)$ is the organic concentration of the i-th species at the j-th stage

$C_i^a(j)$ is the acqueous concentration of the i-th species at the j-th stage

$T(j)$ is the stage temperature.

[†] This can be checked formally using a Taylor series expansion (see Athans[9]).

Note that there are two ideal stages assumed when modeling the column -- an input and output stage; thus, the actual stage numbers start at (2) and end at (N+1). See Figure 2 for a 3-stage column.

The input to the column is defined by the first and last stages, 1 and N+2, with the feed solution appearing at the N^*-th stage ($2 \leq N^* \leq N+1$). The input vector is given by

$$U^T := [C_1^o(1)\ldots C_M^o(1)|C_1^f(N^*)\ldots C_M^f(N^*)|C_1^a(N+2)\ldots$$

$$C_M^a(N+2)|T(1)T^f(N^*)T(N+2)] \qquad (3.12)$$

where $C_i^f(N^*)$ is the feed concentration of the i-th species at the N^* stage.

The matrix F in (3.9,10) takes the following form for an N stage, M species column when defining the state as in (3.11) with $F \epsilon R^{N(2M+1)xN(2M+1)}$ and

$$\underset{N(2M+1)xN(2M+1)}{F =} \begin{array}{cccl} \underbrace{\text{Organic}} & \underbrace{\text{Aqueous}} & \underbrace{\text{Temperature}} & \\ \left[\begin{array}{c} F_{11} \\ F_{12} \\ 0_{N,MN} \end{array}\right. & \begin{array}{c} 0_{MN} \\ F_{22} \\ 0_{N,MN} \end{array} & \left.\begin{array}{c} 0_{MN} \\ 0_{MN,N} \\ F_{33} \end{array}\right] & \begin{array}{l} \}\ \text{Organic phase} \\ \}\ \text{Aqueous phase} \\ \}\ \text{Temperature} \end{array} \end{array} \qquad (3.13)$$

for F_{11}, F_{12}, F_{13} ϵR^{MNxMN}; $F_{33} \epsilon R^{NxN}$ for an N stage.

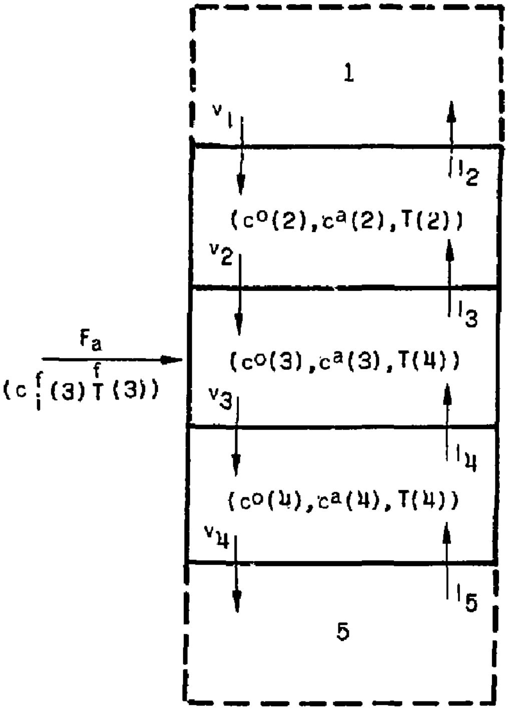


FIGURE 2. EXTRACTION COLUMN MODEL

The submatrices are given by

$$F_{11} = \begin{bmatrix} -(\kappa_2^0+\nu_{22})I_M & & & & \bigcirc \\ \nu_{23}I_M & -(\kappa_3^0+\nu_{33})I_M & & & \\ & \nu_{34}I_M & -(\kappa_4^0+\nu_{44})I_M & & \\ \bigcirc & & \ddots & \ddots & \\ & & \nu_N(N+1)I_M & & -(\kappa_{N+1}^0 + \nu_{(N+1)(N+1)})I_M \end{bmatrix}$$

$$F_{21} = \mathrm{diag}(\kappa_i^a I_M) \quad i = 2,\ldots,(N+1)$$

$$F_{22} = \begin{bmatrix} -\gamma_{22}I_M & \gamma_{32}I_M & \bigcirc \\ & -\gamma_{33}I_M & \gamma_{43}I_M \\ \bigcirc & \ddots & \ddots \\ & -\gamma_{NN}I_M & \end{bmatrix}$$

$$F_{33} = \begin{bmatrix} -\zeta_2\alpha_2 & \ell_3\alpha_2 & & & \\ \nu_2\alpha_3 & -\zeta_3\alpha_3 & \ell_4\alpha_3 & & \bigcirc \\ \ddots & \ddots & \ddots & & \\ \bigcirc & & \nu_{(N-1)N}\alpha_N & \zeta_N\alpha_N & \ell_{N+1}\alpha_N \\ & & & \nu_{N(N+1)} & -\zeta_{N+1}\alpha_{N+1} \end{bmatrix}$$

where V_j^o, V_j^a is organic and acqueous phase volumes at the j-th stage

v_j, ℓ_j is organic and acqueous phase flow rates at the j-th stage

K is a rate constant

and

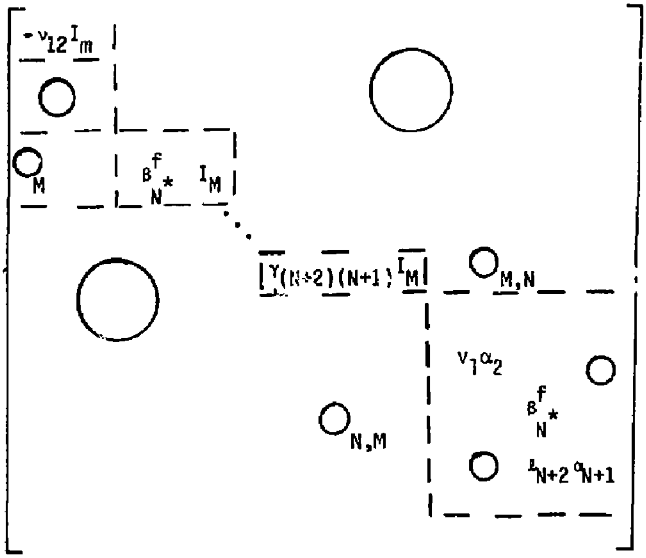
$$\kappa_j^o = K/V_j^o \quad , \quad \nu_{ij} = v_i/V_j^o$$

$$\kappa_j^a = K/V_j^a \quad , \quad \gamma_{ij} = \ell_i/V_j^a \quad \text{for } 2 \le i,j \le N$$

$$\zeta_j = (v_j + \ell_j) \quad , \quad \alpha_j = 1/(V_j{}^o + V_j{}^a)$$

The input distribution matrix G takes the following form

G =
$N(2M+1)x(N_fM+N)$



where $\beta^f_{N^*}$ is the aqueous phase feed flow rate at that $N=N^*$ stage

N_f is the number of input stages

Let us briefly note a few properties about the structure of F which will be useful in future discussions. From (3.12) we see that the F matrix has a block lower triangular structure which means that the

$$|F| = |F_{11}|\cdot|F_{22}|\cdot|F_{33}|$$

Similarily for the eigenvalues we see that

$$|\lambda I-F| = |\lambda I-F_{11}|\cdot|\lambda I-F_{22}|\cdot|\lambda I-F_{33}|$$

Note also that F_{11} has an upper triangular structure; therefore, its eigenvalues are obtained by inspection of the diagonals which is

$$|\lambda I-F_{11}| = |\lambda I_M + (\kappa_2^o + \nu_{22})I_M|\cdot|\lambda I_M + (\kappa_3^o + \nu_{33})I_M|\ldots|\lambda I_M + (\kappa_{N+1}^o + \nu_{(N+1)(N+1)})I_M|$$

$$\text{or} \quad \lambda_{k_i} = -(\kappa_i^o + \nu_{ii}) \qquad i = 2,\ldots,(N+1)$$

Also, since F_{22} is upper triangular, we have

$$|\lambda I-F_{22}| = |\lambda I_M + \gamma_{22}I_M|\cdots|\lambda I_M + \gamma_{(N+1)(N+1)}I_M|$$

or

$$\lambda_{ji} = -\gamma_{jj} \qquad i = 2,\ldots,(N+1)$$

Unfortunately, the N remaining eigenvalues of F_{33} must be calculated, but of course this can be done separately, since it is decoupled from F_{11}, F_{22}. Thus, we summarize this result as

Lemma 3.3 Given an N stage, M species extraction column model as in (3.10), then the eigenvalues are $\left\{\lambda_{ki}, \lambda_{ji}, \lambda_i\right\}$ i=2,..., N+1 for

$$\lambda_{ki} = -(\kappa_i^0 + \nu_{ii}) \quad \text{of multiplicity M for each i}$$

$$\lambda_{ji} = -\gamma_{ii} \quad \text{of multiplicity M for each i}$$

The remaining N eigenvalues are found by solving

$$|\lambda I - F_{33}| = 0 \quad \text{for } \lambda_i$$

Note that guaranteeing the eigenvalues are negative insures stability of the system of (3.10) as well as (3.9), if (3.10) is an adequate linearization of (3.9) (see Theorem 1.16 of Kwakernaak and Siven[10]).

This completes the theoretical development for general extraction system design. In the next section, we discuss the algorithm and apply it to a 3-stage, 4-species extraction column.

III-2 Design Example: 3-Stage, 4-Species, Extraction Column

Now let us investigate the simple 3-stage/4-species column used in [5]. The model parameters are duplicated in Table II for easy reference. Using these values we find that, so N = 3, M = 4

$$F_{11} = \begin{bmatrix} -55.166\ I_4 & & \bigcirc \\ 5.166\ I_4 & -55.166\ I_4 & \\ \bigcirc_4 & 5.166\ I_4 & -55.166\ I_4 \end{bmatrix}$$

TABLE II: SIMULATION PARAMETERS

Time (minutes)	0.0 - 10.0	($\Delta T = 0.02$)
No. of Stages/Species/States	3 / 4 / 27	
Feed Stage	3	
Feed Concentration		
U (gm/ℓ)	200.0	
Pu (gm/ℓ)	7.0	
HNO_3 (moles/ℓ)	2.9	
Salts (moles/ℓ)	0.0	
TBP Concentration (in hydrocarbon)	15%	
Rate Constant	100.0	
Temperature (°C)	25.0	
Phase Volumes (liters)	2.0	
Flow Rates (ℓ/m)		
Feed	6.0	
Aqueous Solvent	4.33	
Organic Solvent	10.33	

$$F_{12} = 50\, I_{12}$$

$$F_{22} = \begin{bmatrix} -5.166\, I_4 & 5.166\, I_4 & 0_4 \\ & -5.166\, I_4 & 2.166\, I_4 \\ \bigcirc & & -5.166\, I_4 \end{bmatrix}$$

$$F_{33} = \begin{bmatrix} -5.166 & 2.583 & 0 \\ 2.583 & -5.166 & 1.083 \\ 0 & 2.533 & -3.666 \end{bmatrix}$$

and

$$G = \left[\begin{array}{ccc|c} -5.166\, I_4 & & & \\ 0_4 & \bigcirc & & \\ 0_4 & & & \bigcirc_{24,3} \\ 0_4 & & & \\ 0_4 & 6\, I_4 & 0_4 & \\ 0_4 & 0_4 & 2.1666\, I_4 & \\ \hline & \bigcirc_{3,12} & & \begin{array}{c|c} 2.583 & \bigcirc \\ 6 & \\ \bigcirc & 1.083 \end{array} \end{array}\right]$$

Since we would like to "design" a measurement system with the minimum number of output terminals to be instrumented, we apply the algorithm of Table I.

To our simple 3-stage extraction column.

<u>Example 3.2</u>

<u>Step 1</u>: The transformed F matrix is given by

$$F_j = \begin{bmatrix} F_1 & & & & & \\ & F_2 & & \bigcirc & & \\ & & F_3 & & & \\ & & & F_4 & & \\ & & & & F_5 & \\ & \bigcirc & & & & F_6 \end{bmatrix}$$

where $F_1 \epsilon R^{12x12}$; $F_2 \epsilon R^{8x8}$; $F_3 \epsilon R^{4x4}$; F_4, F_5, $F_6 \epsilon R^{1x1}$

$$F_1 = \begin{bmatrix} F_{11} & & \bigcirc & \\ & F_{12} & & \\ & & F_{13} & \\ \bigcirc & & & F_{14} \end{bmatrix}, \; F_2 = \begin{bmatrix} F_{21} & & \bigcirc & \\ & F_{22} & & \\ & & F_{23} & \\ \bigcirc & & & F_{24} \end{bmatrix}, \; F_3 = \begin{bmatrix} F_{31} & & \bigcirc & \\ & F_{32} & & \\ & & F_{33} & \\ \bigcirc & & & F_{34} \end{bmatrix}, \; F_1 = F_{i1}; i=4,5,6$$

and $F_{1i} \epsilon R^{3x3}$; $F_{2i} \epsilon R^{2x2}$; $F_{3i} \epsilon R^{1x1}$; F_4, F_5, $F_6 \epsilon R^{1x1}$

$$F_{1j} = \begin{bmatrix} -55.167 & 1 & 0 \\ & -55.167 & 1 \\ \bigcirc & & -55.167 \end{bmatrix}, \; j \epsilon \underline{4}$$

$$F_{2j} = \begin{bmatrix} -5.167 & 1 \\ 0 & -5.167 \end{bmatrix}, \; j \epsilon \underline{4}; \; F_{3j} = 2.1667, \; j \epsilon \underline{4}$$

$F_{41} = -8.086$, $F_{42} = -1.751$, $F_{43} = -4.163$

Step 2: $\left\{r_i\right\} = \left\{4,4,4,1,1,1\right\}$ which implies $p = \max \left\{r_i\right\} = 4$

Step 3: First construct the general pxn, H_J matrix as in (3.2)

Here we have $\left\{n_i\right\} = \left\{12,8,4,1,1,1\right\}$

and $\left\{n_{ij}\right\} = \left\{(3,3,3,3),(2,2,2,2),(1,1,1,1),1,1,1\right\}$

Thus,

$$H = [H_1 | H_2 | H_3 | H_4 | H_5 | H_6]$$

or

$$= [H_{11}\ H_{12}\ H_{13}\ H_{14} | H_{21}\ H_{22}\ H_{23}\ H_{24} | H_{31}\ H_{32}\ H_{33}\ H_{34} | H_{41} | H_{51} | H_{61}]$$

or

$$H = [h_{111}\ h_{211}\ h_{311}\ h_{112}\ h_{212}\ h_{312}\ h_{113}\ h_{213}\ h_{313}\ h_{114}\ h_{214}\ h_{314} |$$
$$h_{121}\ h_{221}\ h_{122}\ h_{222}\ h_{123}\ h_{223}\ h_{124} | h_{224}\ h_{131}\ h_{132}\ h_{133}\ h_{134} |$$
$$h_{141} | h_{151} | h_{161}]$$

$$\rho V_1^* = [h_{111}\ h_{112}\ h_{113}\ h_{114}]$$

$$\rho V_2^* = [h_{121}\ h_{122}\ h_{123}\ h_{124}]$$

$$\rho V_3^* = [h_{131}\ h_{132}\ h_{133}\ h_{134}]$$

$$\rho V_4^* = [h_{141}]$$

$$\rho V_5^* = [h_{151}]$$

$$\rho V_6^* = [h_{161}]$$

Now, since $h_{ijk} \epsilon R^4$ the rank conditions required for observability are:

$$\rho V_1^* = 4$$

$$\rho V_2^* = 4$$

$$\rho V_3^* = 4$$

$$\rho V_4^* = 1$$

$$\rho V_5^* = 1$$

$$\rho V_6^* = 1$$

Thus, if we select (arbitrarily) unit vectors for each required independent column we obtain

$$H_J = [\underline{e}_1\ \underline{0}\ \underline{0}\ e_2\ \underline{0}\ \underline{0}\ e_3\ \underline{0}\ \underline{0}\ e_4\ \underline{0}\ \underline{0} | \underline{e}_1\ \underline{0}\ \underline{e}_2\ \underline{0}\ e_3\ \underline{0}\ e_4\ \underline{0} |$$

$$e_1\ e_2\ e_3\ e_4 | e_1 | e_1 | e_1]$$

where e_i is the unit vector with 1 in the i-th position

$\underline{0}$ is the p-null vector

Note that this choice indicates which outputs must be measured simultaneously on an output terminal, e.g., $y_1^J(t)$ requires measurements of

$$\left\{x_1^J(t),\ x_{13}^J(t),\ x_{21}^J(t),\ x_{25}^J(t),\ x_{26}^J(t),\ x_{27}^J(t)\right\}$$

Step 4 Transforming $H_J \longrightarrow H$, we must first determine the modal matrix by constructing chains of generalized eigenvectors (as in (3.6)).

The modal matrix is given by

$$M_F = [M_{11}\ M_{12}\ M_{13}\ M_{14} | M_{21}\ M_{22}\ M_{23}\ M_{24} | M_{31}\ M_{32}\ M_{33}\ M_{34} | M_{41} | M_{51} | M_{61}]$$

where

$$\sigma_{j-1} M_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 5.166 \\ \underline{0}_3 & \underline{0}_3 & \underline{0}_3 \\ 0 & 26.69 & 0 \\ \underline{0}_3 & \underline{0}_3 & \underline{0}_3 \\ 1.03 & 4955.6 & 101.3 \\ \underline{0}_3 & \underline{0}_3 & \underline{0}_3 \\ -.03781 & 57.74 & -2.92 \\ \underline{0}_3 & \underline{0}_3 & \underline{0}_3 \\ -.4753 & -133.5 & -25.19 \\ \underline{0} & \underline{0} & \underline{0} \end{bmatrix}, \ j=1,2,3,4; \quad \sigma_{k-1} M_{2k} = \begin{bmatrix} \underline{0}_{12} & \underline{0}_{12} \\ 1 & 1 \\ \underline{0}_3 & \underline{0}_3 \\ 1 & 5.166 \\ \underline{0} & \underline{0} \end{bmatrix} \ k = 1,2,3,4;$$

$$\sigma_{k-1} M_{3k} = \begin{bmatrix} \underline{0}_{21} \\ \underline{1} \\ \underline{0} \end{bmatrix}, \ k = 1,2,3,4; \quad M_{41} = \begin{bmatrix} \underline{0}_{24} \\ .659 \\ -.744 \\ .435 \end{bmatrix}; \quad M_{51} = \begin{bmatrix} \underline{0}_{24} \\ -.601 \\ -.795 \\ -1.07 \end{bmatrix}; \quad M_{61} \begin{bmatrix} \underline{0}_{24} \\ -.609 \\ -.237 \\ 1.233 \end{bmatrix}$$

and σ_k is a shift operator which shifts each matrix element down k rows with $\sigma_0 := 1$

The original measurement matrix is given by

$$H = H_J M_F^{-1}$$

which gives

$$H = \begin{bmatrix} 0.45 & 0 & 0 & 0 & -24.45 & 0 & 0 & 0 & -229.7 & 0 & 0 & 0 & 1.24 & 0 & 0 & 0 & -.24 & 0 & 0 & 0 & . & 0 & 0 & -.35 & -1.46 & .35 \\ 0 & .19 & 0 & 0 & 0 & -19.6 & 0 & 0 & 0 & -179.7 & 0 & 0 & 0 & 1.24 & 0 & 0 & 0 & -.24 & 0 & 0 & 0 & 1 & . & . & . & 0 \\ 0 & 0 & .19 & 0 & 0 & 0 & -19.6 & 0 & 0 & 0 & -179.7 & 0 & 0 & 0 & 1.24 & 0 & 0 & 0 & -.24 & 0 & 0 & 0 & 1 & . & . & . & 0 \\ 0 & 0 & 0 & .19 & 0 & 0 & 0 & -19.6 & 0 & 0 & 0 & -179.7 & 0 & 0 & 0 & 1.24 & 0 & 0 & 0 & -.24 & 0 & 0 & 0 & 1 & . & .. & 0 \end{bmatrix}$$

This completes the design example.

We note that in the Jordan measurement system we required six sensors on output 1, 3 on outputs 2, 3, 4, while in the actual system this becomes (thru M_F^{-1}) 8 on 1, and 6 on outputs 2, 3, 4. This leads us to the following question. What is the minimal number of sensors required to instrument a system and be assured of its observability? Before we discuss this point, let us note that if we make more output ports (entries in H) available in the Jordan system, then we need only require one sensor per port. The following corollary to Theorem 3.1 points this out.

Corollary 3.4 Given the conditions of Theorem 3.1, the minimum number of outputs ports required to admit one and only one measurement and be completely observable is $p^* = \sum_{i=1}^{q} r_i$.

The proof of this corollary follows easily from the theorem when the system is in Jordan form - all that it states is that we only allow one entry per row of H_J and therefore we decouple the output space. Reconsider the previous example.

Example 3.3

Let's redesign the extraction column measurement system of Example 3.2 to meet the requirement of this corollary. We see that $p^* = 15$, thus

$$H_J^* = [e_1\underline{00}e_2\underline{00}e_3\underline{00}e_4\underline{00}| e_5\underline{0}e_6\underline{0}e_7\underline{0}e_8\underline{0}| e_9e_{10}e_{11}e_{12}| e_{13}| e_{14}| e_{15}]^\dagger$$

Now we require 15 output channels each with one sensor. Transforming this back to the original system, we have

$$H^* = \begin{bmatrix}
1 & 0 & & & & & & & & & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & .04 & 0 & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & 0 & 0 & 0 & .19 & 0 & & & & & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & 1 & 0 & & & & & & & & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & & \cdot & \cdot & \cdot & & & & 0 & .04 & 0 & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & & \cdot & \cdot & \cdot & 0 & .19 & 0 & & & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & 0 & 0 & 0 & & & & & & & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & & \cdot & \cdot & \cdot & & & & & 0 & .04 & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & & \cdot & \cdot & \cdot & & 0 & .19 & 0 & & & \cdot & \cdot & \cdot & & & & & & & & 0 \\
0 & 0 & 0 & 1 & 0 & & \cdot & \cdot & \cdot & & 0 & .04 & \cdot & \cdot & \cdot & & & & & & & 0 \\
0 & & \cdot & \cdot & \cdot & & & & 0 & .19 & 0 & \cdot & \cdot & \cdot & & & & & & & & 0 \\
-1.29 & 0 & 0 & 0 & -24.45 & 0 & 0 & 0 & -229.7 & 0 & 0 & 0 & 1.24 & 0 & 0 & 0 & -.24 & 0 & & \cdot & \cdot\ \cdot & 0 \\
0.26 & 0 & 0 & 0 & 4.84 & 0 & 0 & 0 & 44.05 & 0 & 0 & 0 & -.29 & 0 & 0 & 0 & .24 & 0 & & \cdot & \cdot\ \cdot & 0 \\
0 & 1.29 & 0 & 0 & 0 & -24.45 & 0 & 0 & 0 & -229.7 & 0 & 0 & 0 & 1.24 & 0 & 0 & 0 & -.24 & 0 & \cdot & \cdot\ \cdot & 0 \\
0 & .26 & 0 & 0 & 0 & 4.84 & 0 & 0 & 0 & 44.05 & 0 & 0 & 0 & -.24 & 0 & 0 & 0 & .24 & 0 & \cdot & \cdot\ \cdot & 0
\end{bmatrix}$$

This completes the example.

[†] Here the asterisk denotes independent sensor location design.

The particular choice of unit vectors in H_J and H_J^* are not important as long as they are independent. Selecting outputs according to this corollary is merely selecting the rows of M_A^{-1} which means that the "best" we could hope to do in the physical system is to require only p^* sensors -- a judicious choice of eigenvectors (if possible) may yield this immediately! In the next section, we consider the design of measurement systems within the minimum number of sensors.

IV. DESIGN OF MINIMUM SENSOR MEASUREMENT SYSTEMS

To answer the final question of the minimum number of sensors, we require another form termed the "Bucy canonical form" [11]. In this paper, the concept of minimal observability was introduced. It means that there are no redundancies in the measurement system with respect to observability, i.e., the system would cease to be observable if one of the sensors were eliminated. The Bucy row form is given by

$$F_{BR} = \begin{bmatrix} L_{11} & & & 0 \\ L_{21} & L_{22} & & \\ \vdots & \vdots & \ddots & \\ L_{p1} & L_{p2} & \cdots & L_{pp} \end{bmatrix} \; ; \quad H_{BR} = \begin{bmatrix} e_1^T \\ e^T_{\tilde{\nu}_1+1} \\ \vdots \\ e^T_{\tilde{\nu}_1+\ldots+\tilde{\nu}_{p-1}+1} \end{bmatrix}$$

where

$$L_{ii} = \left[\begin{array}{cc} 0 & I_{\tilde{\nu}_i-1} \\ \hline \multicolumn{2}{c}{\tilde{\beta}^T_{ii}} \end{array}\right] \; ; \qquad L_{ij} = \left[\begin{array}{c} 0^{\tilde{\nu}_i-1}_{\tilde{\nu}_j} \\ \hline \tilde{\beta}^T_{ij} \end{array}\right] \; ; \qquad (4.1)$$

$\tilde{\nu}_i > 0$ and satisfy $\sum_{s=1}^{p} \tilde{\nu}_s = n$;

$\tilde{\beta}^T_{ii}$, $\tilde{\beta}^T_{ij}$ are $\tilde{\nu}_i, \tilde{\nu}_j$ - row vectors containing $\{\beta_{ist}\}$ invariants.

The transformation, T_{BR}, required to obtain the pair (F_{BR}, H_{BR}) is

$$T_{BR}^T = [T_{B_1}^T \mid , , , \mid T_{B_p}^T] \tag{4.2}$$

where $T_{B_i}^T = [h_i^T (h_i F)^T \dots (h_i F^{\tilde{\nu}_1 - 1})^T]$, $i \epsilon \underline{p}$.

Note that the pair is completely observable by construction and that

$\sum_{s=1}^{p} \tilde{\nu}_s = n$ assuring this property.

Unfortunately, there does not appear to be any direct relationship between the Jordan form indices $\{r_i\}$ which indicate state structural information (F_J) and the Bucy form indices $\{\nu_i\}$ which indicate output structural information (H_{BR}). Note also that the characteristic polynomial of a system in Bucy form is obtained by inspection as

$$x_{FBR}(s) = \det (Is - F_{BR}) = x_{L_{ii}}(s) \dots x_{Lpp}(s) \tag{4.3}$$

Where

> $x_{L_{ii}}(s)$ are the polynomials associated with the L_{ii} companion matrix, i.e.,
>
> $$x_{L_{ii}}(s) = (s^{\tilde{\nu}_i} - \beta_{jk\ell} s^{\tilde{\nu}_i - 1} - \dots - 1)$$

These are <u>not</u> the irreducible polynomials associated with F_J.

The tradeoff between forms is now obvious. The Jordan form enables us to decouple the state space into invariant subspaces (subsystem decomposition) with coupled input and output distribution matrices, while the Bucy form enables us to decouple the output space with some coupling between subsystems. Let's re-examine Example 3.1.

Example 4.1 Transform the Jordan system (F_J, G_J, H_J) to (F_{BR}, G_{BR}, H_{BR}).

(i) Construct the observability matrix as in (3.7) for n=3. Choose $H_J = [\underline{e}_3 | \underline{0} | \underline{e}_1 | \underline{e}_2]$ and we see that

$$\left\{\nu_i\right\} = \left\{1,1,2\right\} \text{ and}$$

$$F_{BR} = \left[\begin{array}{c|c|cc} \lambda_1 & & \multicolumn{2}{c}{\bigcirc} \\ \hline & \lambda_2 & & \\ \hline & & 0 & 1 \\ \bigcirc & & \left(1-\lambda_1^2\right) & 2\lambda_1 \end{array}\right], \quad H_{BR} = \begin{bmatrix} \underline{e}_1^T \\ \underline{e}_2^T \\ \underline{e}_3^T \end{bmatrix} \qquad G_{BR} = \left[\begin{array}{c} g_{112} \\ \hline g_{121} \\ \hline g_{111} \\ \lambda_1 g_{111} + g_{211} \end{array}\right]$$

The interconnection diagram for the system in Bucy form is shown in Figure 3. Comparing this with Figure 1 we see that the output interconnection have been simplified greatly at the price of more complex state coupling. In general, we can expect more coupling between states as indicated in (4.1). We have selected the minimum number of outputs as well as the minimum number of sensors. The following lemma implied in Bucy[11] resolves the question

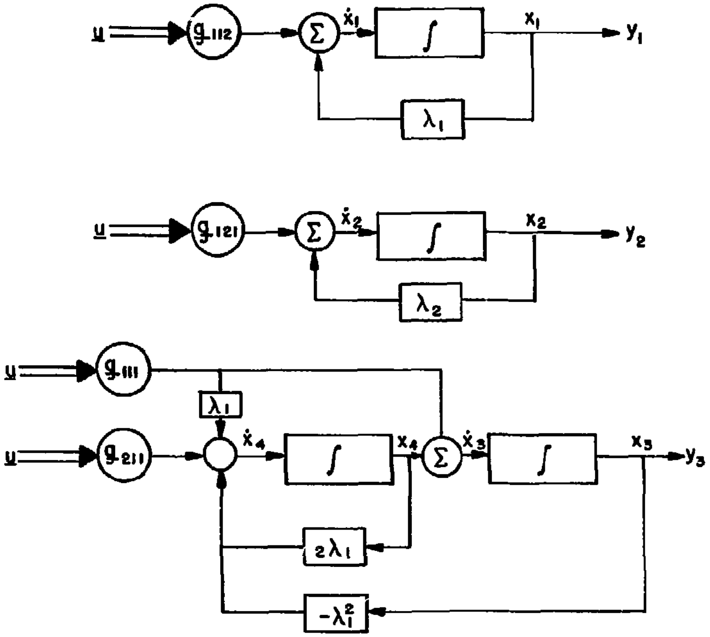


FIGURE 3. BUCY REPRESENTATION OF A LINEAR SYSTEM

<u>Lemma 4.1</u> Let the system $\Sigma = (F,G,H)$ be represented in Bucy form $\Sigma_{BR} = (F_{BR}, G_{BR}, H_{BR})$. Then the minimum number of sensors required to assure observability is $n_s = p_{min}$.

The proof of this resides in the fact that the Bucy form yields the minimum number of sensors required for any p' measurement channels and therefore selecting $p' = p_{min}$ gives the desired results. The Bucy form can be obtained for linear time varying systems, i.e., $\Sigma(t) = (F_{BR}(t), G_{BR}(t), H_{BR}(t))$, while the Jordan form cannot (see Wiberg[12]). This completes our discussion for the deterministic case. In the next section we consider the more realistic case with measurement noise at the output terminals.

V. LINEAR STOCHASTIC MEASUREMENT SYSTEMS

In this section we consider the design/analysis of linear stochastic systems. As before, in the deterministic case, it is important to investigate what, if anything, can be gained by filtering of data. Obviously, the amount of (state) information available in the data is related to the precision (variance) of the particular measurement instrumentation employed as well as any signal processing devices or algorithms employed to improve the estimates. As we utilize more and more information about our knowledge of the physical principles underlying the given data set, we expect to improve our estimates (decrease estimation error) significantly. Referring to Figures 4 through 6, we see a hierarchial description of this process. In Figure 4, the ideal measurement instrument and a more realistic model of the measurement process are depicted. If we were to use z to estimate ($\hat{x}$) x, we have the noise superimposed on the signal y. The "best" estimate of x we can hope for is only within the accuracy (bias) and precision (variance) of the instrument. If we next include a model of the measurement instrument (see Figure 5) as well as its associated uncertainties, then we can improve on the (above) noisy measurements. This technique is the removal or filtering of noise from the signal based on our model of the instrument and noise. We can also specify the estimation error variance (P) of this filter (e.g., least squares filter) in estimating x. Finally, if we incorporate not only instrumentation knowledge, but also knowledge of the physical process, then we expect to do even better, i.e., we expect the estimation error ($\tilde{x} = x_{TRUE} - \hat{x}$) variance to be smaller as we incorporate more and more knowledge (see Figure 6). In fact, this is the case, because (see Candy [13])

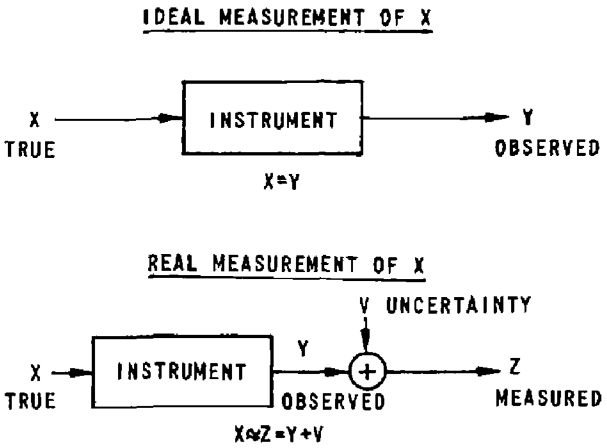
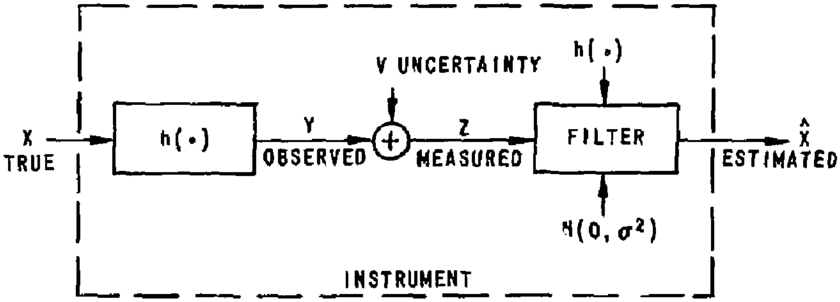


FIGURE 4 SIMPLE MEASUREMENT SYSTEMS

INCORPORATE KNOWLEDGE OF INSTRUMENT AND UNCERTAINTY

$y=h(x)$ (Instrument model)

$V\sim N(0,\sigma^2)$ (Measurement uncertainty model)



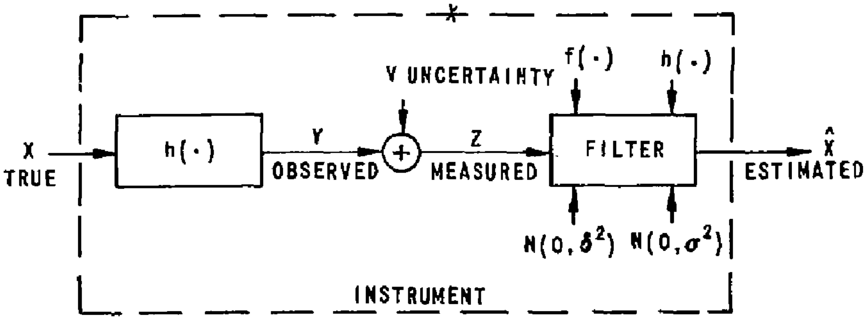
$$X\approx\hat{X} \text{ WITH } P=COV(\tilde{X})$$

$$\text{WHERE } \tilde{X}=X_{TRUE}-\hat{X}$$

FIGURE 5 MEASUREMENT INSTRUMENT MODELING

INCORPORATE KNOWLEDGE OF PHYSICAL PROCESS AND UNCERTAINTY

$\dot{X}=f(x,w)$ (Process model)
$W \sim N(0,\delta^2)$ (Process uncertainty model)
$y=h(x)$ (Instrument model)
$V \sim N(0,\sigma^2)$ (Measurement uncertainty model)



$X \approx \hat{X}$ WITH $\pi = \mathrm{COV}(\tilde{X})$

WHERE $\tilde{X} = X_{TRUE} - \hat{X}$

FIGURE 6 MEASUREMENT UNCERTAINTY AND PROCESS MODELING

$$\sigma^2 > P > \pi$$

The basic idea in applying a Kalman type estimator is to improve measurement system precision. The Kalman filter incorporates process as well as measurement instrumentation knowledge into its algorithm to (decrease) obtain the minimum error variance.

Before filtering, etc., commences, one may ask questons of a more pertinent nature before expending a lot of effort. How much information about the state of a system is in the data? Can the state actually be determined from the data? To answer these questions we must review concepts typically associated with deterministic systems and extend them to the stochastic systems. Most of this discussion is taken from [13,14]. Recall from linear system theory [2], that the question of observability arises when one attempts to discover under what conditions it is possible to establish the time history of the state x(k), given the corresponding history of the measurements over the same finite time interval. To be more precise, a discrete deterministic system is <u>completely observable</u>, if $x(t_0)$ can be determined from the set of measurements Z(N) for N finite and any t_0. For a linear system of p outputs, we have

$$z(k) = H(k)x(k) = H(k)\phi(k,0)x(0)^{\dagger} \tag{5.1}$$

Let k vary to N, then

$$\underset{(pNx1)}{\begin{bmatrix} z(1) \\ \\ z(N) \end{bmatrix}} = \underset{(pNxn)}{\begin{bmatrix} H(1)\phi(1,0) \\ \\ H(N)\phi(N,0) \end{bmatrix}} x(0) \text{ or } z_N = H_N x(0). \tag{5.2}$$

---

† Here ϕ is the state transition matrix (see Jazwinski [14]).

Solving for x(o) we obtain

$$x(o) = (H_N^T H_N)^{-1} H_N^T z_N, \qquad (5.3)$$

but from (4.2) we see that

$$M(N,0) := \sum_{i=1}^{N} \Phi^T(i,o)H^T(i)H(i)\Phi(i,o) = H_N^T H_N. \qquad (5.4)$$

Thus, for deterministic systems M(N,0) must be positive definite for complete observability. With this we use Jazwinski's [14] definition of stochastic observability: a discrete stochastic system given by

$$\begin{aligned} x(k+1) &= \Phi(k+1,k)x(k)^{\dagger} \\ z(k) &= H(k)x(k) + v(k) \quad , \ v(k) \sim N(o,R(k)) \end{aligned} \qquad (5.5)$$

is said to be completely stochastically observable with respect to z(ℓ),...,z(ℓ+N) if the information matrix J_T is

$$J_T(N,\ell) > 0 \qquad (N \geq \ell) \qquad (5.6)$$

where $J_T(N,\ell) := \sum_{i=\ell}^{k} \Phi^T(i,k)H^T(i)R^{-1}(k)\Phi(i,k)$.

Similarily, a system is completely (stochastically) controllable with respect if

$$C(N,\ell) > 0 \text{ for } (N \geq \ell) \qquad (5.7)$$

where C(•,•) is the controllability matrix given by

$$C(N,\ell) := \sum_{i=\ell}^{N-1} \Phi(N,i+1)Q(i+1)\Phi^T(N,i+1) \qquad (5.8)$$

---

† These results can be extended to include additive process noise also (see Candy [13]).

It is possible to now use (5.6) and (5.8) to develop bounds on the error covariance. Jazwinski [14] shows that for (5.5) completely stochastically controllable and observable with $\tilde{\pi}_0 \geq 0$ then

$$\tilde{\pi}(k|k) \leq J_T^{-1}(k,k-N) + C(k,k-N) \qquad k \geq N \qquad (5.9)$$

where $\tilde{\pi} := \text{Cov}(\tilde{X})$ and $\tilde{X} := x - \hat{x}$.

And under these assumptions, the system is also uniformly asymptotically stable. Thus, the link on the information matrix to the fundamental system concepts of observability and controllability is established.

As an example, consider the diversion of material from a plutonium-nitrate storage area as reported in [15].

Example 5.1

Consider the following linear state model of a plutonium-nitrate storage tank in the static mode (see Dunn [15] for modeling details). The continuous discrete model is given by

$$\dot{x}_t = \begin{bmatrix} -\lambda_r P_t & -\lambda_r P_t(\alpha/\beta) & -1/\beta \\ — & — & — \\ & 0_3^2 & \end{bmatrix} x_t + \begin{bmatrix} -1/\beta \\ — \\ 0_2^T \end{bmatrix} u_t + \begin{bmatrix} -\alpha/\beta & 0 \\ — & — \\ & I_2 \end{bmatrix} w_t$$

$$z(t_k) = \begin{bmatrix} g & 0 & 0 \\ 0 & g\cdot\ell & 0 \end{bmatrix} x(t_k) + v(k) \qquad (5.10)$$

where $x_{t_o} \sim N(0,\tilde{\pi}_{t_o})$, $w_t \sim N(0,Q_t)$, $v(k) \sim N(0,R(k))$.

It is easy to show that the state-transition matrix for $P_t = P \; \forall t$ satisfies

$$\Phi(t,\tau) = \Phi(t-\tau) = \begin{bmatrix} e^{-\lambda_r(P(t-\tau)} & -\alpha/\beta(1 - e^{-\lambda_r P(t-\tau)}) & -1/\beta\lambda_r P(1 - e^{-\lambda_r P(t-\tau)}) \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$(5.11)$$

Assume there is no process noise ($Q_t = 0$), then we would like to check observability of (5.10) on [k,k-1]. Recall that the <u>symmetric</u> information matrix is,

$$J(k,k-1) = \sum_{i=k-1}^{k} \phi^T(i,k)H^T(i)R^{-1}(i)H(i)\phi(i,k)$$

$$= \sum_{i=k-1}^{k} \begin{bmatrix} \left(g^2 e^{-2\lambda_r P(i-k)} r_1(i)\right) & \left(-g^2\alpha/\beta e^{-\lambda_r P(i-k)}\left(1 - e^{-\lambda_r P(i-k)}\right) r_1(i)\right) & \left(-\frac{g^2 e^{-\lambda_r P(i-k)}}{\beta\lambda_r P}\left(1 - e^{-\lambda_r P(i-k)}\right) r_1(i)\right) \\ (*) & \left(r_1(i)\left(g\alpha/\beta(1 - e^{-\lambda_r P(i-k)}\right)^2 + (g\ 1)^2 r_2(i)\right) & \left(\frac{g^2}{\beta^2\alpha\lambda_r P} \left(1 - e^{-\lambda_r P(i-k)}\right)^2 r_1(i)\right) \\ (*) & (*) & \left(\left(\frac{g}{\beta\lambda_r P}\right)^2 \quad 1 - e^{-\lambda_r P(i-k)\ 2} r_1(i)\right) \end{bmatrix}$$

(5.12)

where $R(i) := \text{diag}(r_1(k), r_2(i))$

or

$$J(k,k-1) = g^2 \begin{bmatrix} \left(r_1(k) + r_1(k-1)e^{2\lambda_r P}\right) & \left(-\left(\frac{\alpha r_1(k-1)}{\beta}\right)e^{\lambda_r P}(1 - e^{\lambda_r P})\right) & \left(-\left(\frac{r_1(k-1)}{\beta\lambda_r P}\right)e^{\lambda_r P}(1 - e^{\lambda_r P})\right) \\ \left(-\left(\frac{\alpha r_1(k-1)}{\beta}\right)e^{\lambda_r P}(1 - e^{\lambda_r P})\right) & \left(\left[(\alpha/\beta)r_1(k-1)(1 - e^{\lambda_r})\right]^2 + 1^2(r_2(k) + r_2(k-1))\right) & \left(\frac{r_1(k-1)}{\alpha\beta^2\lambda_r P}(1 - e^{\lambda_r P})^2\right) \\ \left(-\left(\frac{r_1(k-1)}{\beta\lambda_r P}\right)e^{\lambda_r P}(1 - e^{\lambda_r P})\right) & \left(\frac{r_1(k-1)}{\alpha\beta^2\lambda_r P}(1 - e^{\lambda_r P})^2\right) & \left(\left(\frac{1}{\beta\lambda_r P}\right)^2 r_1(k-1)(1 - e^{\lambda_r P})^2\right) \end{bmatrix}$$

(5.13)

The total information matrix, $J_T(k,k-1)$ is given as

$$J_T(k,k-1) = \pi_{t_o}^{-1}(k) + J(k,k-1) = I_3 + J(k,k-1) \tag{5.14}$$

This implies that for stochastic observability J-(k,k-1) > 0 or

$$1 + g^2(r_1(k) + r_1(k-1)e^{2\lambda_r P}) > 0$$

$$\left(1 + g^2(r_1(k) + r_1(k-1)e^{2\lambda_r P}\right) \left\{1 + \left|g(\alpha/\beta)r_1(k-1)(1 - e^{\lambda r^P})\right|^2 + (g\ell)^2(r_2(k) + r_2(k-1))\right\}$$

$$-\left(\frac{\alpha r_1(k-1)}{\beta}\right)^2 \quad e^{2\lambda_r P}(1 - e^{\lambda_r P})^2 g^4 > 0$$

$$|J_T(k,k-1)| > 0 \tag{5.15}$$

If we use the data in (5.14), i.e.,

$\lambda_r = 9.4 \times 10^{-10} \frac{\text{kg } H_2O}{\text{sec}} / \text{kg Pu}$, $\alpha = .0209\ m^3$, $\beta = 0.329\ m^2$,

$P = 0.173$ kg Pu/kg soln, $g = 9.8\ m/sec^2$, $\ell = 0.254$

$r_1 = 2641\ kg/msec^2$, $r_2 = 81\ kg\ /m\ sec^2$, then

Since $e^{\lambda_r P} \rightarrow 1$, we have approximately

$$J_T(k,k-1) = \begin{bmatrix} (1 + g^2(r_1(k) + r_1(k-1)) & 0 & 0 \\ 0 & 1 + (g^2(r_2(k) + r_2(k-1)) & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 5.07 \times 10^5 & 0 & 0 \\ 0 & 1.005 \times 10^3 & 0 \\ 0 & 0 & 1 \end{bmatrix} > 0$$

or the given system is stochastically observable on [k,k-1].

V. CONCLUSIONS

This report has discussed the concept of observability for large scale linear deterministic and stochastic systems. It has presented design algorithms based on the Jordan and Bucy canonical forms. The algorithm was applied to a three stage extraction column model used in reprocessing of nuclear fuels. Some general results for an N stage, M species column were presented. The linear stochastic case was briefly discussed.

ACKNOWLEDGMENTS

We would like to thank F. Deadrick for computing eigenvalues/eigenvectors in the given examples and Drs. D. Dunn, I. Sacks, J. Sherman, and D. Siljak for their motivation as well as technical discussions on this subject.

REFERENCES

[1] J. V. Candy, R. A. Emmert, and G. K. Patterson, "Process Monitor Design for an Extraction Column--An Application of Estimation/Detection," Lawrence Livermore Laboratory Report to be published circa March 1979.

[2] P. Padulo and M. Arbib, System Theory. Phila: Saunders, 1974.

[3] J. S. Meditch, Stochastic Optimal Linear Estimation and Control, New York: McGraw Hill Co., 1969.

[4] C. T. Chen, Introduction to Linear System Theory. New York: Holt, Rinehart and Winston, Inc., 1970.

[5] W. M. Wonham, Linear Multivariable Control A Geometric Approach, New York: Springer-Verlag, 1974.

[6] W. G. Vogt and C. G. Cullen, "The Minimum Number of Inputs Required for the Complete Controllability of a Linear Stationary Dynamical System," (correspondence) IEEE Trans. on Autom. Contr., 1967.

[7] D. L. Alspach, "Estimation Theory and Safeguards Accounting," Lawrence Livermore Laboratory Report, UCRL-13641, 1975.

[8] J. V. Candy, R. A. Emmert, and G. K. Patterson, "Material Accounting in a Complex Chemical Processing Unit--An Application of Estimation/Detection," Proc. of Lawrence Symposium on Systems and Decision Sciences, 1977.

[9] M. Athans, "The Role and Use of Stochastic Linear-Quadratic-Gaussian Problem in Control System Design," IEEE Trans. on Autom. Contr., Vol. AC-16, 1971.

[10] H. Kwakernaak and R. Sivan, Linear Optimal Control Systems, New York: Wiley, 1972.

[11] R. S. Bucy, "Canonical Forms for Multivariable Systems," IEEE Trans. on Autom. Contr., 1968.

[12] D. M. Wiberg, State Space and Linear Systems, Schaums Outline, New York: McGraw Hill, 1971.

[13] J. V. Candy, "The Cramer-Rao Bound: A Measure of Estimator Quality," Lawrence Livermore Laboratory Report, UCID-17660, 1977.

[14] A. Jazwinski, Stochastic Processes and Filtering Theory, New York: Academic Press, 1970.

[15] D. Dunn, Dynamic Models, "Estimation and Detection Concepts for Safeguarding $Pu(NO_3)_4$ Storage Tanks," Lawrence Livermore Laboratory Report, UCRL-79216, 1977.