OPTIMAL DESIGN OF DISTRIBUTED PARAMETER MEASUREMENT SYSTEMS

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This thesis is dedicated
to my parents.

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ABSTRACT

The measurement system design for a process governed by partial differential equations (so called distributed parameter system) consists of the choice of state variables to be measured, the frequency of measurements, and the optimal location of sensors. In this work, we consider the problem of optimal location of sensors in distributed parameter systems.

The optimal sensor location problem is approached from the point of view of estimation theory. The objective chosen is the estimation of the system state variables with maximum possible accuracy. An upper bound for the error covariance of the state estimate is derived. Optimal sensor locations are determined by minimizing this upper bound of the error covariance. This approach offers significant savings in computation time over the conventional approaches based on direct minimization of the error covariance. A one-dimensional heat conduction system is considered as an example. The effect of process dynamics on optimal sensor locations is studied in detail for that example. The optimal locations are found to vary for spatially varying measurement noise.

To apply the theory to a technologically important system we consider the optimal location of measurements for tubular reactors. The state of this system is described by two variables — concentration and temperature—and is governed by two nonlinear partial differential equations. For the first time, the optimal sensor location problem for a system with two state variables has been studied. For this problem, an approach based on discretization of the system equations is developed.

The feasibility of estimating both concentration and temperature profiles from temperature measurements only is demonstrated. The effect of process noise and measurement noise on optimal sensor locations was studied and it was found that optimal sensor locations move towards region of lower measurement error variance. For the particular set of parameters chosen, it was found that two optimally located temperature sensors can give a sufficiently accurate estimate of the concentration and temperature profiles.

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CHAPTER 1

INTRODUCTION

The general problem of estimation and control of dynamic systems can be described with the help of Figure 1.1. In practice, it is often desired that the system state follow a particular path, and control action is necessary to guide the system along this specified path. Before one can decide on the required control action, it is necessary that adequate knowledge of the system state be available. Knowledge of the system state can be acquired through comparison of the predictions of a system model and measurements on the system. Since most physical systems are subject to random disturbances and uncertainties in system parameters, deterministic models are often inadequate. A common approach to account for the stochastic nature of a system is to include a random dynamical disturbance in the system equations. In addition measurements of the system state contain errors that can be described as a random process.

The process of obtaining an estimate of the system state from noisy measurements is known as filtering and the algorithm used for obtaining the estimate is called a filter. If a performance measure is introduced into the estimation problem, we can define an optimal estimate obtained from an optimal filter. Mathematical models of physical systems can be classified as lumped parameter or distributed parameter. Systems described by ordinary differential equations are termed lumped parameter systems. (These systems are also known as finite-dimensional.) On the other hand, systems whose state varies spatially as well as temporally are described by partial differential equations or integral equations and are called distributed parameter systems. (These systems are known as infinite-dimensional.)

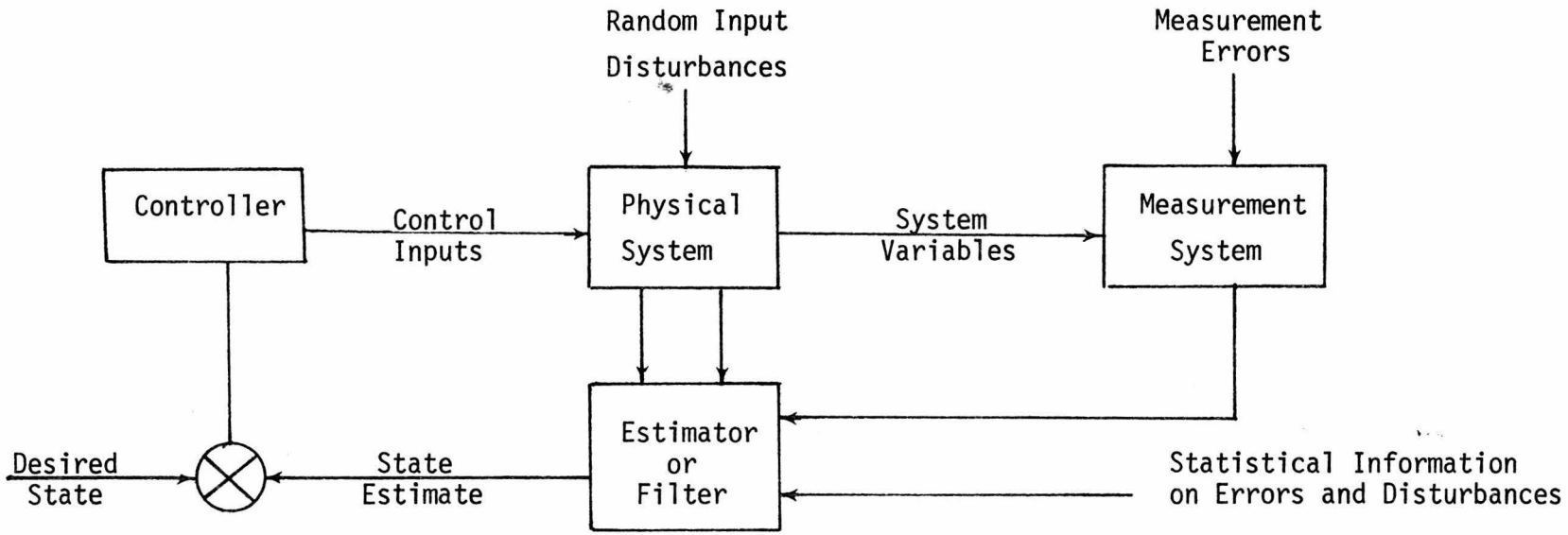

FIGURE 1.1: BLOCK DIAGRAM DESCRIPTION OF THE GENERAL PROBLEM OF ESTIMATION AND CONTROL OF DYNAMIC SYSTEMS

Kalman and Bucy (1961) developed the optimal filter for linear lumped parameter systems. The state estimate depends on the system dynamics and the measurements. The estimate error is measured by the error covariance which is governed by a Riccati differential equation. Balakrishnan and Lions (1967), Falb (1967) and Kushner (1970) extended the Kalman-Bucy filter for linear distributed systems. Tzafestas and Nightingale (1968a, 1968b, 1969), Thau (1969), Meditch (1970), and Sakawa (1972) obtained filters for linear distributed systems using various approaches. Estimation of states in nonlinear distributed systems has been considered by Seinfeld et al. (1971) and Hwang et al. (1972). Yu et al. (1974) also derived filters for nonlinear time-delay systems.

The accuracy of the state estimate obtained from optimal filters depends on the measurements available on the system. The measurement system design problem in lumped system is concerned basically with the question of which states are to be measured. On the other hand for distributed systems, the measurement system design problem is more complicated. Since it is physically impossible to measure the state over the entire spatial domain, the question of just where to locate these sensors is an important one. In addition, to specify the measurement system design completely, the questions of choice of states to be measured, frequency of measurements, and number of measurement sensors should also be dealt with. In most physical processes, however, there will normally be little choice in the states to be measured because of the difficulty in continuously measuring certain state variables. The number of sensors is usually governed by economic considerations. Assuming that the state variables

being measured can be measured continuously, the major question in measurement system design is the selection of sensor locations.

Let us discuss briefly two engineering systems of interest to be considered in this work. The first system is a bar undergoing heat conduction in which heat is lost to the surroundings along the length of the bar. The unsteady state temperature u is described by (Section 2.8 defines the nomenclature)

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} - \beta u$$

We assume that this idealized model does not represent the physical process exactly. The temperature profile in the bar is to be estimated by measuring the temperature at certain points. Recognizing that the temperature measurements are not necessarily perfect, we wish to select the location of temperature sensors so that a "best" estimate of the system state (i.e. the temperature) is obtained. Some interesting questions are:

- Should the sensors be located near the ends of the bar or near the middle?
- Do the locations change if the boundary conditions on the system change?
- How do the measurement locations change if the measurement errors and model errors are functions of space?

The second system to be considered is a non-adiabatic tubular reactor in which an exothermic chemical reaction is taking place. In this system, there are two state variables — concentration and temperature. The equations defining the system are nonlinear and coupled (and will be given

in Chapter 3). Assuming the model and the measurements to be imperfect, we wish to estimate the concentration and temperature profiles in the reactor. Since we can make measurements at only a finite number of points along the reactor length, the choice of sensor locations is very important. In general, it is difficult to make continuous concentration measurements and therefore we would like to explore the possibility of estimating both concentration and temperature profiles based on temperature measurements only. Measurement system design encompasses all these and other related questions.

The optimal design of lumped parameter measurement systems has received considerable attention although comparatively little work has been directed towards the specific problem of measurement locations in distributed parameter systems. For distributed parameter systems Bensoussan (1972) derived necessary conditions for optimality of sensor locations. He posed the problem as an optimal control problem with the state described by the infinite dimensional Riccati equation and the sensor locations considered as control variables. Based on a modal (eigenfunction expansion) approach, Yu and Seinfeld (1973) developed an algorithm for determining suboptimal sensor locations. Brewer and Moore (1974) considered the use of estimation theory for minimizing the cost of measurements while meeting certain estimate accuracy criteria. Pimentel (1975) considered the infrequent sampling problem and employed a modal representation of the distributed system to determine optimal sensor locations. Chen and Seinfeld (1975) derived necessary conditions for optimal sensor locations for a general linear distributed system and developed an algorithm for determining the set of optimal locations. Aidarous (1976) considered discrete-time

measurements and determined sensor locations such that a scalar measure of the error covariance matrix over one time increment is minimized.

The problem of optimal sensor locations, approached as an estimation problem, involves a finite dimensional approximation at some point. There are basically two approaches. The distributed parameter system can be approximated right at the beginning, and the sensor location problem is attempted by employing finite-dimensional filters. This approach can be called approximation at the beginning. On the other hand, one can retain the distributed nature of the problem by employing infinite-dimensional filters and use finite-dimensional approximation for numerical implementation. This approach can be termed approximation at the end. Of course, the techniques for finite-dimensional approximation in both the cases are the same. Figure 1.2 illustrates the concepts of approximation at the beginning and approximation at the end. Various techniques that can be used for finite-dimensional approximation are finite-difference methods, orthogonal collocation, Galerkin method and eigenfunction expansion. Seinfeld and Koda (1977) have discussed these techniques for numerical implementation of distributed parameter filters.

The basic problem in determining optimal sensor locations is the computational requirement. In all the approaches available, it has been necessary to solve the infinite-dimensional Riccati equation. In this work, our objective is to develop computationally attractive approaches for the optimal sensor location problem. In Chapter 2, we consider a general stochastic linear distributed parameter system and develop an upper bound for the estimate error covariance matrix. The optimal sensor locations are

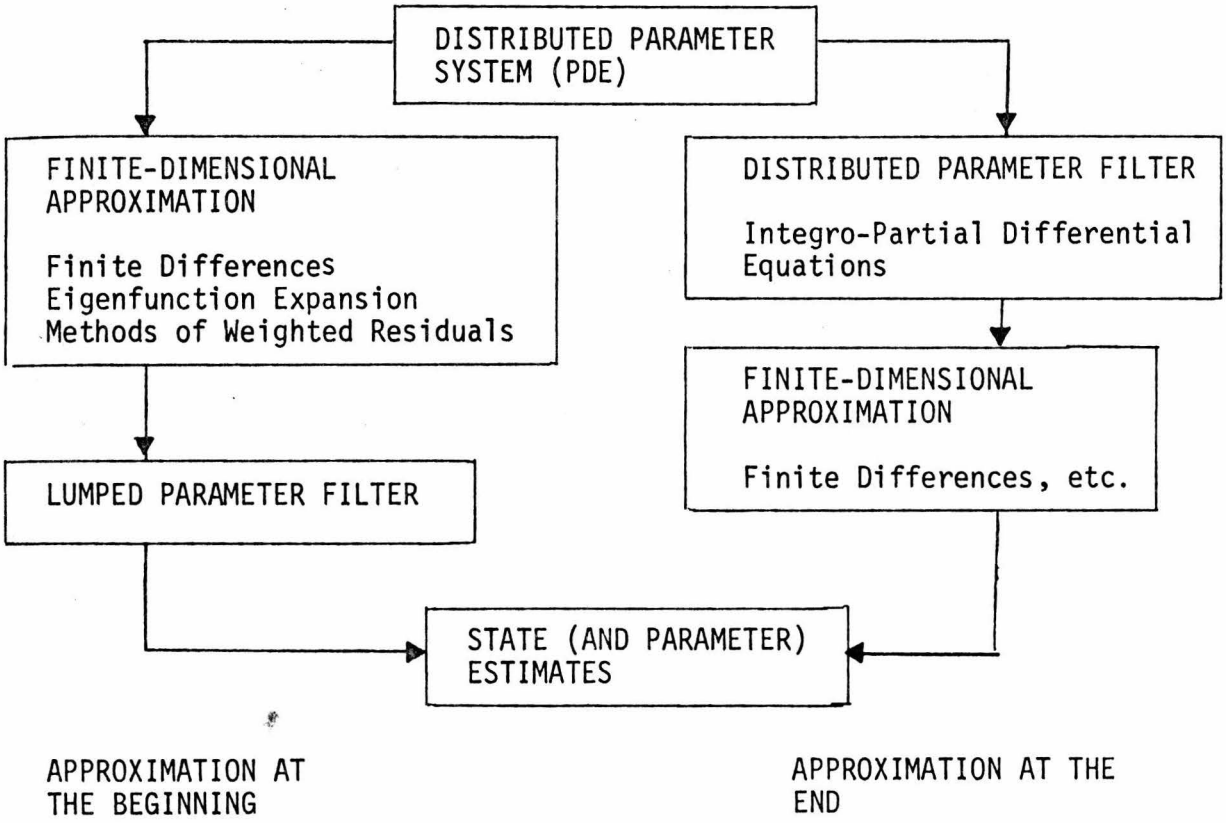

FIGURE 1.2: APPROACHES TO DISTRIBUTED PARAMETER ESTIMATION PROBLEMS

determined by minimizing a scalar measure of this upper bound. The problem requires the solution of a linear partial differential equation rather than the nonlinear Riccati partial differential equation. The linear equation is solved by employing the system Green's function. This approach falls into the category approximation at the end. The optimal sensor locations are obtained by minimizing a function of the variables defining the sensor locations. An example involving one dimensional diffusion system is considered. The effect of process dynamics and varying measurement noise covariance on optimal sensor locations is studied. The results are compared to those obtained from the conventional approach of minimizing a measure of the filter covariance matrix.

In Chapter 3, we consider the optimal sensor location problem for non-adiabatic tubular reactors. The system state is described by two variables, namely concentration and temperature. This is apparently the first time that an optimal sensor location problem for a system with more than one state variable has been attempted. An alternate approach involving approximation at the beginning is developed. The system equations are discretized by orthogonal collocation and the resulting nonlinear equations are linearized around the steady state. The finite-dimensional optimal filter is used, and the optimal sensor locations are determined by employing the matrix minimum principle (Athans, 1968) and an algorithm similar to the one used by Chen and Seinfeld (1975). The effect of process dynamics on the optimal sensor locations is studied. Variations in the optimal sensor locations with different process and measurement noise statistics is also studied. The feasibility of estimating both concentration and temperature profiles based on only temperature

measurements is clearly demonstrated. The question of number of sensors to estimate both concentration and temperature profiles is also investigated. A summary of the work done and recommendations for further work are given in Chapter 4.

CHAPTER 2

OPTIMAL LOCATION OF MEASUREMENTS FOR DISTRIBUTED PARAMETER ESTIMATION

The general optimal measurement design problem for linear systems can be approached with the objective of obtaining the best possible state estimates, in which case the problem becomes one of minimizing a functional depending on the covariance of the optimal filter. The specific problem of optimal measurement locations for linear distributed parameter systems is considered. Bensoussan (1972) and Chen and Seinfeld (1975) have shown that the optimal sensor location problem for distributed systems can be posed as an optimal control problem for a system described by the infinite-dimensional matrix Riccati equation for the filter covariance. In this chapter, a more efficient approach based on an upper bound of the filter covariance is developed. The optimal sensor locations are determined by minimizing a nonlinear function of the variables defining the sensor locations. The relationship between the present approach and that of minimizing a measure of the filter covariance is studied. A detailed example is considered, and the results of the two approaches are compared.

2.1 Introduction

Measurement system design for a physical process generally involves the choice of the states to be measured and the frequency and location of measurements. In this chapter, we consider the problem of the determination of optimal sensor locations for linear distributed parameter systems with continuous time measurements. Measurements at

certain points in the spatial domain of the system may yield more information about the system than the measurements at other points and, therefore, the accuracy of the state estimate depends on the number and locations of sensors. Since the number of sensors is generally governed by economic considerations, it is desirable to locate the given number of measurement sensors at points that lead to a best estimate of the system state. These optimal sensor locations are a function of the process dynamics and boundary conditions under consideration, and of the spatial dependence of measurement and system model uncertainties.

The problem of dynamic measurement system design has been of particular interest. Johnson (1969), Muller and Weber (1972), and Mehra (1976) considered the problem for lumped parameter systems in which various structural parameters in the observability matrix are chosen so that a given measure of the observability matrix is optimized. Athans (1972) considered the problem of selecting one measurement provided by one out of many sensors, at each instant of time, during the observation. Herring and Melsa (1974) generalized Athans' results to selecting the best combination of measurements at each instant of time. Bensoussan (1972) considered the problem of optimal sensor location in distributed parameter systems. He posed an optimal control problem for the system described by the infinite-dimensional matrix Riccati equation governing the filter covariance with the sensor locations considered as control variables. Yu and Seinfeld (1973) considered a modal approach to a general linear distributed parameter

system and developed an algorithm for determining suboptimal sensor locations. Following Bensoussan (1972), Chen and Seinfeld (1975) derived necessary conditions for optimality based on the Riccati equation governing the estimate error covariance, and developed an algorithm for determining the optimal sensor locations. Aidarous (1976) considered a discrete-time measurement distributed parameter filter and determined sensor locations such that a scalar measure of the error variance over one time increment is minimized. The dual problem of optimal pointwise control for distributed systems has also received attention (Amouroux and Babary, 1975).

In previous work (Aidarous, 1976; Chen and Seinfeld, 1975), it has been necessary to solve nonlinear matrix Riccati differential equations to determine optimal sensor locations. In this work, we develop an approach which requires the solution of a linear matrix differential equation, thus making it computationally more attractive. We derive an upper bound for the error covariance matrix of a general stochastic linear distributed parameter system. The upper bound is a sum of two terms, only one of which is a function of the sensor locations. The optimal locations are determined by minimizing a scalar measure of this term with respect to sensor locations. For lumped parameter systems, Mehra (1976) has used a similar approach to select measurement schedules and sensor designs.

In Section 2.2, we define the general linear distributed parameter system under consideration. Section 2.3 describes the general forms of the optimal distributed parameter filter. In Section 2.4,

we develop the integral form for the linear dynamical system described in Section 2.2. Section 2.5 is concerned with the optimality index for defining the optimal sensor locations. In Section 2.6, we develop an upper bound for the error covariance matrix P, involving the error covariance matrix $\bar{P}$ for the optimal filter for the system in the absence of dynamic noise. In order to work with the solution of $\bar{P}$, in Section 2.7 we develop an approximation to the matrix $\bar{P}$ in a finite-dimensional subspace of the original infinite-dimensional space. When expressed in the final form, it is possible to obtain the optimal sensor locations by optimizing a nonlinear function of the variables defining these sensor locations. In Section 2.8, we consider an example involving one-dimensional heat transfer. The effect of boundary conditions, varying measurement noise, and varying initial covariance on the optimal sensor locations is studied. The full nonlinear Riccati equation for the covariance matrix is also solved, and it is shown that the sensor locations obtained by the method developed here are approximately the same as those based on the full nonlinear Riccati equation.

2.2 System Description

In this work, we consider linear systems which can be described by an equation of the form

$$\frac{\partial u(x,t)}{\partial t} = A_x\, u(x,t) + B(x,t)\, w(x,t) \tag{2.1}$$

on a connected open domain D of a d-dimensional Euclidean space E^d, with

boundary ∂D. The d-dimensional spatial coordinate vector is denoted by x. The state u(x,t) is an n-dimensional vector, and A_x is an n x n matrix linear, spatial differential, or integro-differential operator. It is assumed that the operator A_x is well posed. B(x,t) is an n x s dimensional matrix and the process noise w(x,t) is an s-dimensional zero-mean white Gaussian process with covariance

$$E[w(x,t)w^T(y,\tau)] = Q(x,y,t)\delta(t-\tau) \tag{2.2}$$

where Q(x,y,t) is a symmetric positive semi-definite matrix. The initial and boundary conditions for the system are

$$E[u(x,t_0)] = \bar{u}_0(x) \tag{2.3}$$

$$E[\{u(x,t_0)-\bar{u}_0(x)\}\{u(y,t_0) - \bar{u}_0(y)\}^T] = P_0(x,y)$$

and

$$\alpha_x\, u(x,t) = 0 \qquad x \in \partial D \tag{2.4}$$

The initial state $u(x,t_0)$ is an n-dimensional white Gaussian process with mean $\bar{u}_0(x)$ and covariance matrix $P_0(x,y)$. α_x is an n x n matrix, linear, spatial differential operator of suitable order over ∂D. The boundary conditions have been assumed to be homogeneous, although the case of inhomogeneous boundary conditions poses no difficulties. It is well known (Courant and Hilbert, 1966) that a homogeneous differential equation with nonhomogeneous boundary conditions is essentially equivalent to a nonhomogeneous differential equation with homogeneous boundary

conditions. Brogan (1968) considers several examples and establishes in detail the above equivalence through a general approach. For convenience we may express the system equation (2.1) as the stochastic evolution equation on a real Hilbert space v

$$\frac{du(t)}{dt} = A\ u(t) + B(t)\ \omega(t) \tag{2.5}$$

where A is a linear closed operator on V , and is the infinitesimal generator of a strongly continuous semigroup. $B(t)$ denotes a bounded linear transformation, and $\omega(t)$ denotes a white noise process. The system output, in general, is the result of a continuous transformation of the state functions. It is important to note that in a distributed parameter system, the measured variable can either be spatially dependent or spatially independent. The most important case is that in which measurements are made at a finite number of points in the spatial domain. It is possible to represent formally both of these cases by representing the measurements as

$$z(t) = H(t)\ u(t) + v(t) \tag{2.6}$$

where $z(t)$ is an r-dimensional vector and $H(t)$ is a bounded linear operator that may transform the state into spatially dependent or independent outputs. The measurement noise $v(t)$ is assumed to be zero-mean white Gaussian process with covariance $R(t)$. We note that the measurement noise covariance $R(t)$ is spatially dependent or independent based on the type of measurements. We wish to obtain an estimate of the state $u(t)$ based on all the past measurements $z(t')$ $0 \leq t' \leq t$. An

estimate u(t) which minimizes

$$E\{\langle h, u(t) - \hat{u}(t)\rangle^2\} \ , \quad h \in V \tag{2.7}$$

is called the optimate estimate. The estimate error

$$\tilde{u}(x,t) = u(x,t) - \hat{u}(x,t) \tag{2.8}$$

has the covariance P(x,y,t) defined by

$$P(x,y,t) = E[\tilde{u}(x,t)\tilde{u}^T(y,t)] \tag{2.9}$$

The covariance matrix P(x,y,t) is symmetric and positive semi-definite.

2.3 Optimal Filters for Linear Distributed Systems

Let us define the operators $P(t)$ and $Q(t)$ to be integral operators with kernels P(x,y,t) and Q(x,y,t) respectively. The equation defining the optimal estimate is (Balakrishnan, 1976)

$$\frac{d\hat{u}(t)}{dt} = A\,\hat{u}(t) + P(t)H^*(t)R^{-1}(t)\,[z(t) - H(t)\,\hat{u}(t)] \tag{2.10}$$

with the initial condition

$$\hat{u}(t_o) = \bar{u}_o \tag{2.11}$$

The kernel matrix of the operator $P(t)H^*(t)R^{-1}(t)$ is called the gain matrix for the filter. The covariance matrix P(x,y,t) obeys the kernel form of the operator equation

$$\dot{P}(t) = AP(t) + P(t)A^* + B(t)Q(t)B^*(t) - P(t)H^*(t)R^{-1}(t)H(t)P(t) \tag{2.12}$$

where * denotes the adjoint operator. The operator $P(t)$ in (2.12) is a bounded integral operator with kernel $P(x,y,t)$, and is defined as

$$P(t)f = \int_D P(x,y,t)\ f(y)\ dy \tag{2.13}$$

for $f \in L_2(D;R^n)$, where $L_2(D;R^n)$ denotes the vector space of all real-valued functions, square-integrable over the domain D. The covariance operator is trace class and nonnegative definite (Balakrishnan, 1976). Symbolically, we express the nonnegative definiteness as $P(t) \geq 0$, which implies that for any $f \in L_2(D;R^n)$,

$$\int_D \int_D f^T(x)P(x,y,t)f(y)\ dydx \geq 0 \tag{2.14}$$

The initial conditions and the boundary conditions for the covariance $P(x,y,t)$ are

$$P(x,y,t_o) = P_o(x,y) \tag{2.15}$$

$$\begin{aligned} \alpha_x \quad & P(x,y,t) = 0 \qquad x \in \partial D \qquad y \in D \times \partial D \\ & P(x,y,t)\alpha_y^T = 0 \qquad y \in \partial D \qquad x \in D \times \partial D \end{aligned} \tag{2.16}$$

where the transpose of a matrix differential operator $\alpha_y[\cdot]$ is defined by the relation $(\alpha_y P)^T = P^T \alpha_y^T$, and is an operator to the left. For example, if

$$\alpha_y[\cdot] = \alpha_o[\cdot] + \alpha_1 \frac{\partial}{\partial y}[\cdot] + \alpha_2 \frac{\partial^2}{\partial y^2}[\cdot]$$

then

$$[\cdot]\ \alpha_y^T = [\cdot]\ \alpha_o^T + \frac{\partial[\cdot]}{\partial y}\ \alpha_1^T + \frac{\partial^2[\cdot]}{\partial y^2}\ \alpha_2^T$$

where α_o, α_1, and α_2 are assumed to be square matrices.

For spatially dependent measurements, the measurement noise covariance is given by

$$E[v(x,t)v^T(y,\tau)] = R(x,y,t)\ \delta(t-\tau) \tag{2.17}$$

while for spatially independent measurements, we have

$$E[v(t)v^T(\tau)] = R(t)\ \delta(t-\tau) \tag{2.18}$$

The operator $R(t)$ occurring in (2.10) and (2.12) is, therefore, an integral operator with kernel $R(x,y,t)$ in the first case, and simply the matrix $R(t)$ in the second case. For spatially dependent measurements, therefore, we have

$$R(t)(\cdot) = \int_D R(x,y,t)(\cdot)\ dy \tag{2.19}$$

The inverse operator $R^{-1}(t)$ is an integral operator, with the property

$$R^{-1}(t)[R(t)f] = f \tag{2.20}$$

for all functions f in the domain of $R(t)$. In expanded form, this gives

$$\int_D R^{\dagger}(x,y,t) \int_D R(y,z,t)\ f(z)\ dzdy = f(x) \tag{2.21}$$

where $R^{\dagger}(x,y,t)$ is the kernel of the integral operator $R^{-1}(t)$. From equation (2.21), it follows then, that $R^{\dagger}(x,y,t)$, the generalized

inverse of R(x,y,t), must obey the integral equation

$$\int_D R^{\dagger}(x,y,t)\, R(y,z,t)\, dy = I\, \delta(x-z) \tag{2.22}$$

$R^{-1}(t)$ is thus an integral operator with kernel $R^{\dagger}(x,y,t)$ satisfying the integral equation (2.22). For spatially independent measurements, the inverse operator $R^{-1}(t)$ is the ordinary inverse of matrix R(t).

We now proceed to obtain the explicit equations for the optimal estimate $\hat{u}(x,t)$ and the estimate error covariance matrix P(x,y,t) for various kinds of measurement systems. The measurement systems are specified for four cases and corresponding optimal filters are presented in Table2.1. For all the cases, the initial condition and boundary conditions on the optimal estimate u(x,t) are

$$\hat{u}(x,t_o) = \bar{u}_o(x) \tag{2.23}$$

$$\alpha_x\, \hat{u}(x,t) = 0 \qquad x \in \partial D \tag{2.24}$$

The covariance matrix P(x,y,t) has the initial condition

$$P(x,y,t_o) = P_o(x,y) \tag{2.25}$$

and boundary conditions

$$\begin{aligned} \alpha_x\, P(x,y,t) &= 0 \qquad x \in \partial D\,, \quad y \in D x \partial D \\ P(x,y,t)\alpha_y^T &= 0 \qquad y \in \partial D\,, \quad x \in D x \partial D \end{aligned} \tag{2.26}$$

Case 1: Continuous Measurements over the Entire Spatial Domain

The measurement process is defined by

$$z(x,t) = H(x,t)\, u(x,t) + v(x,t) \tag{2.27}$$

where $v(x,t)$ is a white Gaussian process with properties

$$E[v(x,t)] = 0$$

$$E[v(x,t)v^T(y,t)] = R(x,y,t)\, \delta(t-\tau) \tag{2.28}$$

Therefore, the operator $R(t)$ in the optimal filter is given by

$$R(t)(\cdot) = \int_D R(x,y,t)(\cdot)\, dy \tag{2.29}$$

$$R^{-1}(t)(\cdot) = \int_D R^{\dagger}(x,y,t)(\cdot)\, dy \tag{2.30}$$

where $R^{\dagger}(x,y,t)$ is defined by the relation (2.22).

Case 2: Continuous Integral Measurements over the Entire Spatial Domain

The measurement process is defined by

$$z(x,t) = \int_D H(x,y,t)\, u(y,t)\, dy + v(x,t) \tag{2.31}$$

where the measurement noise $v(x,t)$ has the same properties as in Case 1. Consequently $R(t)$ and $R^{-1}(t)$ are also defined as in equations (2.29) and (2.30).

Table 2.1 Optimal Filters for Various Measurement Models

Case 1

$$\frac{\partial \hat{u}(x,t)}{\partial t} = A_x\, \hat{u}(x,t) + \iint_{DD} P(x,x',t)H^T(x',t)R^{\dagger}(x',y',t)\,[z(y',t) - H(y',t)\hat{u}(y',t)]\,dy'dx'$$

$$\frac{\partial P(x,y,t)}{\partial t} = A_x\, P(x,y,t) + P(x,y,t)A_y^T + B(x,t)Q(x,y,t)B^T(y,t) - \iint_{DD} P(x,x',t)H^T(x',t)R^{\dagger}(x',y',t)H(y',t) \cdot P(y',y,t)\,dy'dx'$$

Case 2

$$\frac{\partial \hat{u}(x,t)}{\partial t} = A_x\, \hat{u}(x,t) + \iiint_{DDD} P(x,x',t)H^T(x',x'',t)R^{\dagger}(x'',y'',t)\,[z(y'',t) - \int_D H(y'',y',t)\hat{u}(y',t)dy']\,dy''dx''dx'$$

$$\frac{\partial P(x,y,t)}{\partial t} = A_x\, P(x,y,t) + P(x,y,t)A_y^T + B(x,t)Q(x,y,t)B^T(y,t) - \iiiint_{DDDD} P(x,x',t)H^T(x',x'',t)R^{\dagger}(x'',y'',t)H(y'',y',t)P(y',y,t)\,dy'dy''dx''dx'$$

Case 3

$$\frac{\partial \hat{u}(x,t)}{\partial t} = A_x\, \hat{u}(x,t) + \left[\int_D P(x,x',t)H^T(x',t)dx'\right] R^{-1}(t)\left[z(t) - \int_D H(y',t)\hat{u}(y',t)\,dy'\right]$$

$$\frac{\partial P(x,y,t)}{\partial t} = A_x\, P(x,y,t) + P(x,y,t)A_y^T + B(x,t)Q(x,y,t)B^T(y,t) - \left[\int_D P(x,x',t)H^T(x',t)\,dx'\right] R^{-1}(t)\left[\int_D H(y',t)P(y',y,t)\,dy'\right]$$

Table 2.1 (continued)

Case 4

$$\frac{\partial \hat{u}(x,t)}{\partial t} = A_x\, \hat{u}(x,t) + \sum_{i,j=1}^{m} P(x,\eta_i,t) H_i^T(t) \left[R^{-1}(t) \right]_{ij} \left[z_j(t) - H_j(t)\hat{u}(x_j,t) \right]$$

$$\frac{\partial P(x,y,t)}{\partial t} = A_x\, P(x,y,t) + P(x,y,t)A_y^T + B(x,t)Q(x,y,t)B^T(y,t)$$

$$- \sum_{i,j=1}^{m} P(x,\eta_i,t) H_i^T(t) \left[R^{-1}(t) \right]_{ij} H_j(t) P(\eta_j,y,t)$$

Case 3: Spatially-Independent Integral Measurements

The measurement equation takes the form

$$z(t) = \int_D H(x,t)\, u(x,t)\, dx + v(t) \tag{2.32}$$

where $v(t)$ is a white Gaussian process with properties

$$E[v(t)] = 0$$

$$E[v(t)v^T(\tau)] = R(t)\, \delta(t-\tau) \tag{2.33}$$

The operator $\mathcal{R}(t)$ in this case is the matrix $R(t)$ and $\mathcal{R}^{-1}(t)$ is the ordinary inverse of matrix $R(t)$.

Case 4: Continuous Measurements at m Discrete Points in Space

The measurements are represented as

$$z_i(t) = H_i(t)\, u(x_i,t) + v_i(t) \qquad i = 1,2,\cdots,m \tag{2.34}$$

where $v_i(t)$ is a white Gaussian process with properties

$$\begin{aligned} &E[v_i(t)] = 0 && i = 1,2,\cdots,m \\ &E[v_i(t)\, v_j^T(\tau)] = C_{ij}(t)\, \delta(t-\tau) && i \le i,j \le m \end{aligned} \tag{2.35}$$

The measurements given by (2.34) can be represented in the form (2.32) by considering the mr-dimensional vectors $z(t)$ and $v(t)$ defined by

$$z(t) = \left[z_1^T(t)\ z_2^T(t) \cdot \cdot \cdot \cdot \cdot z_m^T(t) \right]^T \tag{2.36}$$

and

$$v(t) = \left[v_1^T(t)\ v_2^T(t) \cdot \cdot \cdot \cdot \cdot v_m^T(t) \right]^T \tag{2.37}$$

The kernel matrix H(x,t) in equation (30) takes the form

$$H(x,t) = \left[H_1^T(t)\ \delta(x_1-x) \cdot \cdot \cdot \cdot \cdot H_m^T(t)\ \delta(x_m-x) \right]^T \tag{2.38}$$

The operator R(t) is the mr x mr matrix R(t) with $C_{ij}(t)$ as the (i,j)th submatrix. In the filter equations $[R^{-1}(t)]_{ij}$ is the (i,j)th submatrix of dimensions r x r in the matrix $R^{-1}(t)$. It may be pointed out that $C_{ij}(t)$, the covariance matrix of the measurement errors at locations x_i and x_j may be obtained by evaluating a given function C(x,x',t) at $x = x_i$ and $x' = x_j$. The matrix function C(x,x',t) specifies the measurement error covariance as a continuous function of any two points x and x' in the spatial domain D.

2.4 Integral Form for the Linear Dynamical System

The general solution of equation (2.1) with homogeneous boundary conditions can be expressed (Courant and Hilbert, 1966) in the form

$$u(x,t) = \int_D G(x,t;x',t_o)\ u(x',t_o)\ dx' + \int_{t_o}^{t} \int_D G(x,t;x',t')\ B(x',t')\ w(x',t')\ dx'dt' \tag{2.39}$$

where G(x,t; x',t') is the Green's function matrix, and satisfies the equation

$$\frac{\partial G(x,t;x',t')}{\partial t} = A_x\ G(x,t;x't') \tag{2.40}$$

with the terminal condition

$$G(x,t';x',t') = I\ \delta(x-x') \tag{2.41}$$

and boundary condition

$$\alpha_x\ G(x,t;x',t') = 0 \qquad x \in \partial D \tag{2.42}$$

If the operator A_x is time and space-invariant, it is sufficient to consider $G(x,t;0,0)$ and then use the relation

$$G(x,t;x',t') = G(x-x',t-t';0,0) \tag{2.43}$$

For convenience, we can express (24) as

$$u(t) = \Phi(t,t_o)u(t_o) + \int_{t_o}^{t} \Phi(t,t')B(t')\omega(t')\ dt' \tag{2.44}$$

where $\Phi(t,t_o)$ and $\Phi(t,t')$ define linear transformations, the domain of which is the set of bounded functions of x and the range of which is a subset of the domain. The transformation $\Phi(t,t')$ is defined by the relation

$$[\Phi(t,t')f] = \int_D G(x,t;x',t')f(x')\ dx'$$

for any $f \in L_2(D;R^n)$, and obeys the relations

$$\frac{\partial\Phi(t,t')}{\partial t} = A\Phi(t,t') \tag{2.45}$$

$$\lim_{t\to t'} \Phi(t,t') = I \tag{2.46}$$

The equivalent concept of a transition matrix in lumped systems has the important property of invertibility. However, in distributed parameter

systems, the operator $\Phi(t,t')$ may or may not be invertible, depending on the system under consideration. The transformations that have the property of invertibility are termed group operators, whereas the transformations lacking this property are called semi-group operators. Parabolic systems, for example the diffusion equation, give rise to semi-group operators. (As a consequence of this property, solving the heat equation backwards in time is not a well-posed problem).

However, if the operator $\Phi(t,t')$ has the properties of a group, the complete past history of the system can be determined. For example, in wave processes, a complete knowledge of the state at a given time t, and of the inputs applied to the system is sufficient to reconstruct all future and past states. We now list some important properties of semigroup operators (Hille and Phillips, 1957; Yosida, 1966).

$$
\begin{aligned}
&(1)\quad \Phi(t,t') \text{ is a bounded operator} \\
&(2)\quad \lim_{t\to t'} \Phi(t,t') = I \\
&(3)\quad \Phi(t,t'')\Phi(t'',t') = \Phi(t,t') \qquad t > t'' > t' \geq 0 \\
&(4)\quad \Phi(t,t') \text{ is strongly continuous, i.e.,}
\end{aligned}
\tag{2.47}
$$

$$\lim_{\delta\to 0} \|(\Phi(t+\delta,t') - \Phi(t,t'))u(t)\| = 0 \quad \text{for all } u \text{ in the domain}$$

An abstract approach for the development of Green's functions has been developed (Hille and Phillips, 1957; Yosida, 1966) in relation to semi-group theory and parallels the development of transition matrices in lumped systems. However, we shall not dwell here on this abstract approach but will concentrate on the problem of constructing Green's

function for the well-posed physical problem, assuming existence and uniqueness properties. Green's functions for distributed parameter dynamical systems can be constructed in a variety of ways. Often it is possible to use analytical methods, such as integral transforms, to obtain the Green's function for linear systems. Expansion in spatial eigenfunctions and constructing the Green's function from eigenvalues and eigenfunctions is a very powerful method for linear systems (Morse and Feshbach, 1953; Stakgold, 1968). For these systems, one can find the eigenvalues and eigenfunctions if the spatial domain is a well defined geometrical region like a rectangle, a circle, or an ellipse, and the boundary conditions are specified in the corresponding principal coordinate directions. Two- and three-dimensional problems can also be treated and the eigenfunctions are generally obtained as separable products of functions of the coordinate variables. For systems in which it is not possible to find analytical expressions for the Green's functions, one can construct Green's functions by numerical methods.

2.5 Optimality Index

The covariance matrix $P(x,y,t)$ is a function of the measurement locations x_i, $i = 1,2,\cdots,m$. In order to define optimal locations, we must choose an optimality index that is a suitable measure of the covariance matrix $P(x,y,t)$. For the case of a scalar state, a robust criterion is to minimize the spatial integral of the estimate error variance, i.e.

$$J(t) = \int_D P(x,x,t)\, dx \tag{2.48}$$

For finite-dimensional systems, the analogue is to minimize the trace of the covariance matrix. For n-dimensional state vectors in distributed parameter systems, a natural extension is to

$$J(t) = \int_D \text{Tr } P(x,x,t)\, dx \tag{2.49}$$

The indices (2.48) and (2.49) arise naturally because using Mercer's theorem (Stakgold, 1968; Balakrishnan, 1976) they can be proved to be the sum of all the eigenvalues of the corresponding covariance operators.

2.6 Upper Bound for the Covariance Matrix

Because of the nonlinearity and dimensions of the partial differential Riccati equation governing the covariance matrix P(x,y,t), it is difficult to obtain results for the optimal sensor location problem without going into extensive numerical computations (Chen and Seinfeld, 1975). In order to develop a computationally tractable approach, we prove a theorem relating to an upper bound on the covariance matrix of the optimal linear distributed filter. We now state and prove the basic theorem, based in part on the work of Sorenson (1968) in which a similar upper bound is derived for a discrete-time finite dimensional system. We prove the theorem for the case of spatially independent integral measurements from which the case of measurements at discrete points in space is readily derived, as shown in Section 2.3. It may be pointed out that the result derived here holds for all types of measurement models which can be described by the equation (2.6). Before stating the theorem,

let us define the inequality notation to be used.

If $\Gamma_1(x,y)$ and $\Gamma_2(x,y)$ are two nxn nonnegative definite matrices, then

$$\Gamma_1(x,y) \leq \Gamma_2(x,y) \tag{2.50}$$

implies that for any n-dimensional vector f(x),

$$\int_D \int_D f^T(x)\Gamma_1(x,y)f(y)\, dydx \leq \int_D \int_D f^T(x)\Gamma_2(x,y)f(y)\, dydx \tag{2.51}$$

From the above definition, it follows that

$$\int_D \text{Tr}\, \Gamma_1(x,x)\, dx \leq \int_D \text{Tr}\, \Gamma_2(x,x)\, dx \tag{2.52}$$

Now we state the theorem for the upper bound for the covariance matrix P(x,y,t). A proof of this theorem is given in Appendix A.

Theorem: The covariance matrix for the optimal filter has an upper bound described by

$$P(x,y,t) \leq \bar{P}(x,y,t) + W(x,y,t) \tag{2.53}$$

where $\bar{P}(x,y,t)$ is the optimal filter covariance matrix for the system (2.1) in the absence of dynamic noise, and W(x,y,t) is the matrix defined by

$$W(x,y,t) = \int_{t_o}^{t} \iint_{DD} G(x,t;x',\tau)B(x',\tau)Q(x',y',\tau)B^T(y',\tau)G^T(y,t;y',\tau)\, dy'dx'd\tau \tag{2.54}$$

Proof: See Appendix A.

The solution of the optimal filter covariance equation $\bar{P}(x,y,t)$ for the process in the absence of dynamic noise can be written in a closed form in terms of the system Green's function matrix. The equation for $\bar{P}(x,y,t)$ for the case of point measurements can be obtained by setting $Q(x,y,t) = 0$ for the covariance equation in case 4. Thus, we have

$$\frac{\partial \bar{P}(x,y,t)}{\partial t} = A_x \bar{P}(x,y,t) + \bar{P}(x,y,t) A_y^T - \sum_{i,j=1}^{m} \bar{P}(x,\eta_i,t) H_i^T(t) (R^{-1}(t))_{ij} H_j(t) \bar{P}(\eta_j,y,t) \quad (2.55)$$

I.C. $\bar{P}(x,y,t_o) = P_o(x,y)$

B.C. $\alpha_x \bar{P}(x,y,t) = 0 \qquad x \in \partial D \qquad y \in D \times \partial D \quad (2.56)$

$\bar{P}(x,y,t)\alpha_y^T = 0 \qquad y \in \partial D \qquad x \in D \times \partial D \quad (2.57)$

The solution of equations (39)-(41) can be written in the form

$$\bar{P}(x,y,t) = \int_D \int_D G(x,t;x',t_o) [P_o^{+}(x',y') + M(x',y',t)]^{+} G^T(y,t;y',t_o) \, dy'dx' \quad (2.58)$$

where $G(x,t;x',t')$ is the system Green's function matrix, and

$$M(x,y,t) = \int_{t_o}^{t} \sum_{i,j=1}^{m} G^T(\eta_i,\tau;x,t_o) H_i^T(\tau) [R^{-1}(\tau)]_{ij} H_j(\tau) G(\eta_j,\tau;y,t_o) \, d\tau \quad (2.59)$$

The matrix $M(x,y,t)$ defined above is closely related to the concept of observability. The system (2.1)-(2.6) is observable in the sense of

Wang (1964), if and only if $M(x,y,t)$ has a bounded generalized inverse for some finite $t \geq t_o$. However, for (2.58) to be valid we need not assume the existence of a generalized inverse for $M(x,y,t)$. Indeed, for $M(x,y,t) \equiv 0$, (2.58) is still a valid solution of (2.55)-(2.57) because in this case $[P_o^\dagger(x',y') + M(x',y',t)]^\dagger = P_o(x',y')$. The validity of (2.58) as a solution of (2.55)-(2.57) is verified in Appendix B.

2.7 Approximation of $\overline{P}$ in Finite-Dimensional Subspace

The expression (2.58) for $\overline{P}(x,y,t)$ involves generalized inverses. Since the generalized inverse is defined by the integral equation (2.22), it is convenient to approximate it in a finite-dimensional subspace of the original infinite-dimensional space. Let us consider a real scalar valued symmetric function $k(x,y)$ whose generalized inverse is denoted by $k^\dagger(x,y)$. We can represent $k(x,y)$ as a doubled series (Courant and Hilbert, 1966; Stakgold, 1968)

$$k(x,y) = \sum_{i,j=1}^{\infty} k_{ij}\, \phi_i(x)\, \phi_j(y)$$

where the basis functions $\{\phi_i\}$ form a complete orthonormal set. The expansion coefficients k_{ij} are given by

$$k_{ij} = \iint_{DD} k(x,y)\phi_i(x)\phi_j(y)\, dydx \tag{2.60}$$

The function $k(x,y)$ can be approximated in the norm by a finite double series

$$k(x,y) = \sum_{i,j=1}^{N} k_{ij}\, \phi_i(x)\phi_j(y) \tag{2.61}$$

We can also write equation (2.61) as $k(x,y) = \Phi^T(x)\, K\Phi(y)$, where $\Phi(x)$ is the N-dimensional column vector of elements $\phi_i(x)$ $1 \leq 1 \leq N$, and K is the N x N matrix with elements k_{ij}. The generalized inverse $k^\dagger(x,y)$ can then be approximated by

$$k^\dagger(x,y) = \Phi^T(x)\, K^{-1}\Phi(y) \tag{2.62}$$

To verify this we may consider $k(x,y)$ to be the kernel of the integral operator K, and $k^\dagger(x,y)$ to be the kernel of the integral operator K^{-1}. Let us also consider an arbitrary function $f(x)$ which can be approximated as

$$f(x) = \sum_{i=1}^{N} a_i\, \phi_i(x) = \Phi^T(x)\, a \tag{2.63}$$

where a is the N-dimensional column vector of elements a_i. Then by the definition of inverse operator

$$K^{-1}(Kf) = \int_D k^\dagger(x,y) \int_D k(y.z)f(z)\, dzdy = f(x) \tag{2.64}$$

Substituting the expressions for $k^\dagger(x,y)$, $k(x,y)$, and $f(x)$, we find that the definition (2.62) is, indeed, satisfied[‡]. We may also note that if $k(x,y)$ is time-dependent, the elements of the matrix K will be time-dependent. For the case of an n x n dimensional matrix-valued function $k(x,y)$, the approximation can again be written as $k(x,y) = \Phi^T(x)\, K\Phi(y)$; however, in this case $\Phi(x)$ is an nN x n matrix given by

---

[‡]The basis functions $\{\phi_i\}$ are not necessarily the eigenfunctions of the operator K

$$\Phi(x) = \begin{bmatrix} \phi_1(x) & \cdots & \phi_N(x) & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \vdots & & \vdots \\ \vdots & & \vdots & \vdots & & \vdots \\ \vdots & & \vdots & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \phi_1(x) & \cdots & \phi_N(x) \end{bmatrix}^T$$

and K is nNxnN composite matrix made of NxN submatrices K^{ij} $1 \leq i,j \leq n$, where K^{ij} is the NxN matrix of expansion coefficients for the (i,j)th element in k(x,y). We may note that the orthonormality of $\{\phi_i\}$ gives

$$\int_D \Phi(x)\, \Phi^T(x)\, dx = I \tag{2.65}$$

for both the scalar and matrix cases. We now consider the case of scalar $\bar{P}(x,y,t)$ but the results can be interpreted for matrix case with the above definitions in mind.

In order to obtain an approximate solution to $\bar{P}(x,y,t)$ for a scalar case, we consider the complete orthonormal set $\phi_i(x)$ $i = 1,2,\cdots,\infty$. In the N-dimensional subspace, the basis functions considered are $\phi_i(x)$, $i = 1,2,\cdots,N$. Denoting the N-dimensional column vector of the basis functions $\phi_i(x)$ by $\Phi(x)$, we can approximate the scalar Green's function G(x,t;x',t') as

$$G(x,t;x',t') = \Phi^T(x)A(t,t')\Phi(x') \tag{2.66}$$

where A(t,t') is the N x N symmetric matrix of time dependent coefficients. We shall also approximate the initial covariance $P_0(x,y)$ as

$$P_o(x,y) = \Phi^T(x)\ \psi_o\ \Phi(y) \tag{2.67}$$

so that $P_o^{\dagger}(x,y) = \Phi^T(x)\ \psi_o^{-1}\ \Phi(y)$. The expression (2.59) for $M(x,y,t)$ can then be written as

$$M(x,y,t) = \int_{t_o}^{t} \sum_{i,j=1}^{m} \Phi^T(x)A(\tau,t_o)\Phi(\eta_i)(R^{-1}(\tau))_{ij}\ \Phi^T(\eta_j)A(\tau,t_o)\Phi(y)\ d\tau \tag{2.68}$$

or,

$$M(x,y,t) = \Phi^T(x)\ S(\eta_i;t)\ \Phi(y) \tag{2.69}$$

where $S(\eta_i;t)$ depends on the sensor locations η_i, $i = 1,2,\ldots, m$ and is given by

$$S(\eta_i;t) = \int_{t_o}^{t} \sum_{i,j=1}^{m} A(\tau,t_o)\Phi(\eta_i)(R^{-1}(\tau))_{ij}\ \Phi^T(\eta_j)A(\tau,t_o)\ d\tau \tag{2.70}$$

Therefore,

$$P_o^{\dagger}(x,y) + M(x,y,t) = \Phi^T(x)\ [\psi_o^{-1} + S(\eta_i;t)]\ \Phi(y) \tag{2.71}$$

and,

$$[P_o^{\dagger}(x,y) + M(x,y,t)]^{\dagger} = \Phi^T(x)\ [\psi_o^{-1} + S(\eta_i;t)]^{-1}\ \Phi(y) \tag{2.72}$$

With the help of this expression, we can express $\bar{P}(x,y,t)$ given in (2.58) as

$$\bar{P}(x,y,t) = \iint_{DD} \Phi^T(x)A(t,t_o)\Phi(x')\Phi^T(x')\ [\psi_o^{-1} + S(\eta_i;t)]^{-1}\ \Phi(y')\Phi^T(y') \cdot A(t,t_o)\Phi(y)\ dy'dx'$$

Using the orthonormality property, we get

$$\bar{P}(x,y,t) = \Phi^T(x)A(t,t_o)\ [\psi_o^{-1} + S(\eta_i;t)]^{-1}\ A(t,t_o)\ \Phi(y) \qquad (2.73)$$

Thus, we have obtained an expression for $\bar{P}(x,y,t)$ in terms of the N basis functions and the expansion coefficients of Green's function. The dependence on sensor locations η_i, $i = 1,2,\cdots,m$ is through the dependence of matrix S on these sensor locations. As proved in Section 2.6, $P(x,y,t) \leq \bar{P}(x,y,t) + W(x,y,t)$. It then follows that

$$\int_D P(x,x,t)\ dx \leq \int_D \bar{P}(x,x,t)\ dx + \int_D W(x,x,t)\ dx$$

or,

$$J(t) \leq \int_D \bar{P}(x,x,t)\ dx + \Gamma(t) \qquad (2.74)$$

where $$\Gamma(t) = \int_D W(x,x,t)\ dx$$

Of the two terms in the upper bound, $\Gamma(t)$ is independent of the sensor locations. Therefore to minimize this upper bound of $J(t)$ we need only to minimize $\int_D \bar{P}(x,x,t)\ dx$ with respect to sensor locations. From equation (2.73)

$$\int_D \bar{P}(x,x,t)\ dx = \int_D \Phi^T(x)A(t,t_o)\ \left[\psi_o^{-1} + S(\eta_i;t)\right]^{-1} A(t,t_o)\Phi(x)\ dx \qquad (2.75)$$

The right hand side is a nonlinear function of the sensor locations η_i, $i = 1,2,\cdots,m$. The optimal sensor locations are the values η_i that minimize this nonlinear function, and can be determined by using a

suitable gradient method. A slightly modified version of the Fletcher-Powell method (Fletcher and Powell, 1963) was used to obtain the optimal sensor locations for the example considered in this work.

The optimality index (2.49) neglects the cross-correlation of estimate errors at different points in space. If the cross-correlation at different spatial points is important, a suitable optimality index is

$$J_1(t) = \int_D \int_D \text{Tr } P(x,y,t)\, dydx \tag{2.76}$$

Then utilizing the upper bound

$$\int_D \int_D \text{Tr } P(x,y,t)\, dydx \leq \int_D \int_D \text{Tr } \bar{P}(x,y,t)\, dydx + \int_D \int_D \text{Tr } W(x,y,t)\, dydx \tag{2.77}$$

and (2.73) for $\bar{P}(x,y,t)$, optimal sensor locations for minimum $J_1(t)$ can be readily determined.

2.8 Optimal Location of Sensors in a One-Dimensional Diffusion System

We consider heat conduction through a long bar of uniform cross-section, along which heat is lost to the surroundings. The unsteady state temperature $u(x,t)$ is described by

$$\frac{\partial u(x,t)}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} - \beta u \tag{2.78}$$

Assume that the initial temperature is not known exactly, and we have

$$E[u(x,0)] = 0$$

$$E[u(x,0)u^T(y,0)] = P_0(x,y) \tag{2.79}$$

(Equation (2.78) also describes the process of diffusion of a species A in a liquid medium B where A reacts homogeneously with B. In some cases, neutron transport can also be described by the same equation.) Let us suppose that equation (2.78) does not model the process exactly, and we introduce a random dynamic error w(x,t), a Gaussian process with properties

$$\begin{aligned} E[w(x,t)] &= 0 \\ E[w(x,t)w^T(y,\tau)] &= Q(x,y,t)\ \delta(t-\tau) \end{aligned} \tag{2.80}$$

where Q(x,y,t) is a symmetric non-negative scalar-valued function. Assume that the temperature u(x,t) is measured continuously at a finite number of points, x_i $i = 1,2,\cdots,m$, and the measurements $z_i(t)$ are described by

$$z_i(t) = u(x_i,t) + v_i(t) \qquad i = 1,2,\cdots,m \tag{2.81}$$

where the measurement noise $v_i(t)$ is a Gaussian process with properties

$$\begin{aligned} E[v_i(t)] &= 0 \\ E[v_i(t)v_j(\tau)] &= \begin{cases} 0 & i \neq j \\ r_i(t)\ \delta(t-\tau) & i = j \end{cases} \end{aligned} \tag{2.82}$$

The variance of the measurement noise can be evaluated from a continuous function R(x) of the measurement location x, i.e., $r_i = R(x)\big|_{x=x_i}$. It is desired to select optimal sensor locations x_i, $i = 1,2,\cdots,m$.

As outlined before, we minimize an upper bound of $J(t)$ by minimizing $\overline{J}(t)$ given by

$$\overline{J}(t) = \int_D \overline{P}(x,x,t)\, dx \tag{2.83}$$

We have studied the case of two sensor locations for the parameter values $\kappa = 0.1$, and $\beta = 0.25$. For studying the effect of different boundary conditions, measurement noise covariance functions, and initial covariances, sensor locations for minimizing $\overline{J}(t)$ at $t = 1$ were considered.

2.8.1 Effect of Boundary Conditions

Three different boundary conditions are considered. The boundary conditions and corresponding eigenfunctions and Green's functions are given in Table 2.2. The eigenfunctions were employed as the basis functions $\{\phi_i(x)\}$. Two sensor locations were determined for a bar of unit length. For ease of computation, the initial covariance $P_0(x,y)$ was chosen to be $2\delta(x-y)$. Although this choice of P_0 is not trace class, it can be viewed as the limiting case of the covariance matrix of a random process that is correlated over a small interval. Moreover, for computations we must use a finite dimensional representation of $P_0(x,y)$, which is always trace class. Therefore, the difficulties associated with P_0 not being trace class do not arise. The measurement noise covariance was taken to be unity independent of the sensor location, i.e., $R(x) = 1$. The results are summarized in Table 2.3.

Table 2.2 Eigenfunctions and Green's Functions for Different Boundary Conditions

	Boundary Conditions	Eigenfunctions	Green's Function $G(x,t;x',t')$
(A)	$u(0,t) = 0$ $\left.\frac{\partial u(x,t)}{\partial x}\right\|_{x=1} = 0$	$\sqrt{2}\sin(n-1/2)\pi x$ $n = 1,2,\ldots$	$2\sum_{n=1}^{\infty} \exp[-((n-1/2)^2\pi^2\kappa+\beta)(t-t')]\sin[(n-1/2)\pi x]$ $\cdot\sin[(n-1/2)\pi x']$
(B)	$u(0,t) = 0$ $u(1,t) = 0$	$\sqrt{2}\sin n\pi x$ $n = 1,2,\ldots.$	$2\sum_{n=1}^{\infty} \exp[-(n^2\pi^2\kappa+\beta)(t-t')]\sin(n\pi x)\sin(n\pi x')$
(C)	$\left.\frac{\partial u(x,t)}{\partial x}\right\|_{x=o} = 0$ $\left.\frac{\partial u(x,t)}{\partial x}\right\|_{x=1} = 0$	$1;\ \sqrt{2}\cos n\pi x$ $n = 1,2,\ldots$	$e^{-\beta(t-t')} + 2\sum_{n=1}^{\infty} \exp[-(n^2\pi^2\kappa+\beta)(t-t')]\cos(n\pi x)\cos(n\pi x')$

Table 2.3 Optimal Sensor Locations for Different Boundary Conditions

Initial Covariance $P_0(x,y) = 2\delta(x-y)$

Measurement Noise Covariance $R(x) = 1$

Boundary Conditions	Sensor Locations
(A) $u(0,t) = 0, \quad \left.\frac{u(x,t)}{x}\right\|_{x=1} = 0$	0.57 , 0.87
(B) $u(0,t) = 0, \quad u(1,t) = 0$	0.43 , 0.57
(C) $\left.\frac{\partial u(x,t)}{\partial x}\right\|_{x=0} = \left.\frac{\partial u(x,t)}{\partial X}\right\|_{x=1} = 0$	0.21 , 0.79

It is observed that the optimal sensor locations are, in general, removed from the boundaries when the boundaries are kept at fixed temperature, but are close to the boundary when the boundary condition is of zero flux. When the boundaries are held at specified temperature, we do not expect to gain much information about the system by making measurements near the boundary. On the other hand, if the boundary condition is specified to be zero flux, the temperature near the boundary is constantly adjusting because of the heat flow through the bar. Consequently, measurements near the boundary convey more information about the dynamics of the heat transfer process.

2.8.2 Effect of R(x)

For the boundary conditions of case A, the effect of varying R(x) on the optimal sensor locations was studied. In these experiments, the initial covariance $P_0(x,y)$ was maintained at $2\delta(x-y)$. The results are given in Table 2.4.

For constant R, the optimal locations are found to be 0.57 and 0.87. For cases (b) and (d), R(x) decreases as we move towards the end $x = 1$; therefore the second sensor location moves to $x = 1$, where R(x) is minimum. In case (d), R(x) is relatively high at the point $x = 0.57$, and therefore the optimal location for the first sensor changes to $x = 0.37$ where R(x) has a lower value. In cases (c) and (e), the end $x = 1$ has very high value of R(x) and therefore the second sensor moves to positions of lower R(x). The first sensor moves to the position $x = 0.50$ where R(x) achieves its minimum for case (e) and is quite low

Table 2.4 Effect of Measurement Noise Covariance R(x) on Optimal Sensor Locations

Boundary Conditions: $u(0,t) = 0$

$$\left.\frac{\partial u(x,t)}{\partial x}\right|_{x=1} = 0$$

Initial Covariance: $P_0(x,y) = 2\delta(x-y)$

R(x)	Sensor Locations
(A) 1.0	0.57 , 0.87
(B) 0.8 exp[-2x]	0.50 , 1.0
(C) 0.8 exp[-2(1-x)]	0.50 , 0.85
(D) 0.8 exp[-4|x-0.5|]	0.37 , 1.0
(E) 0.8 exp[+4|x-0.5|]	0.50 , 0.71

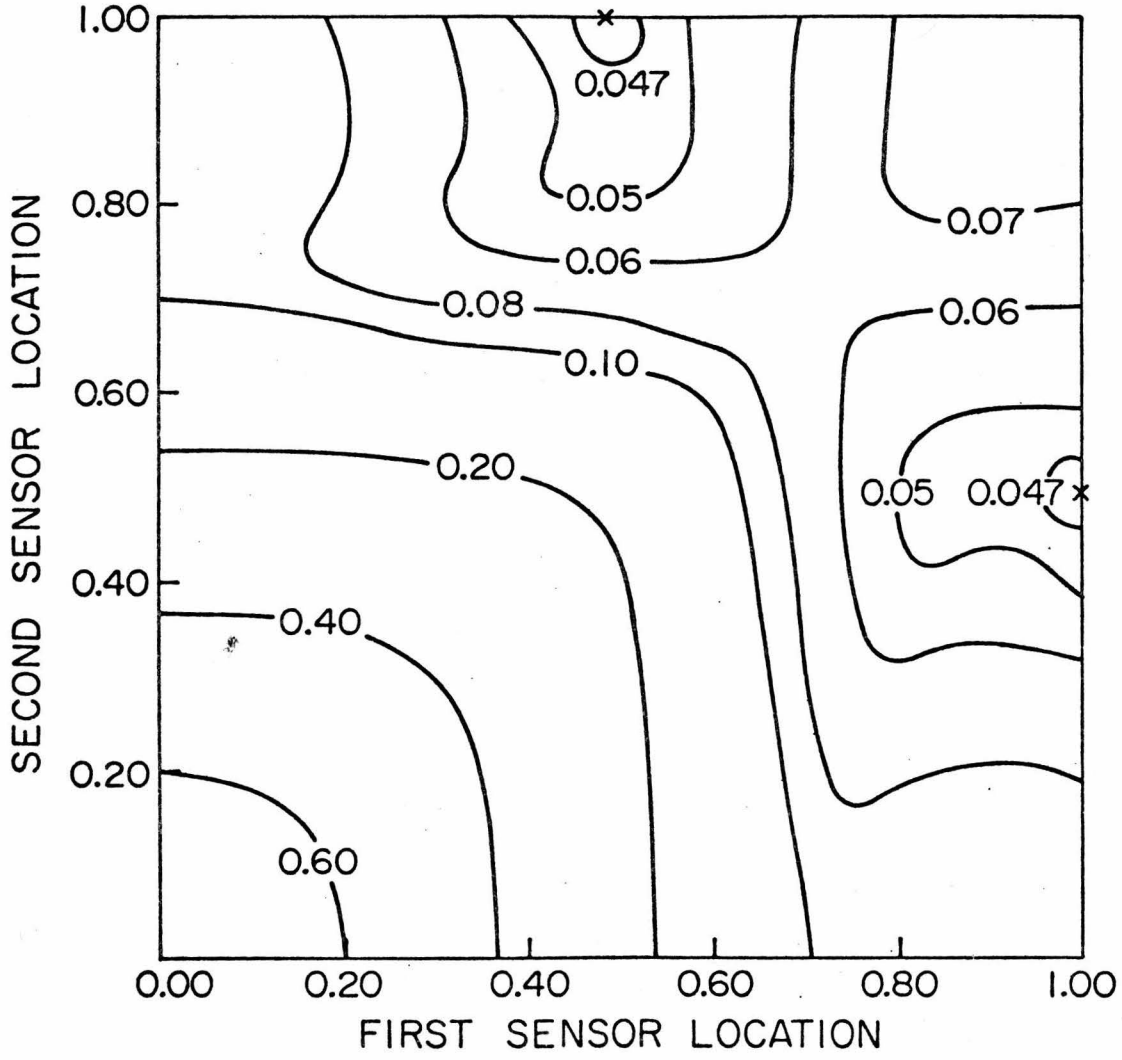

FIGURE 2.1: CONTOUR PLOT OF $\bar{J}$ FOR R(x) = 0.8 EXP (-2x)

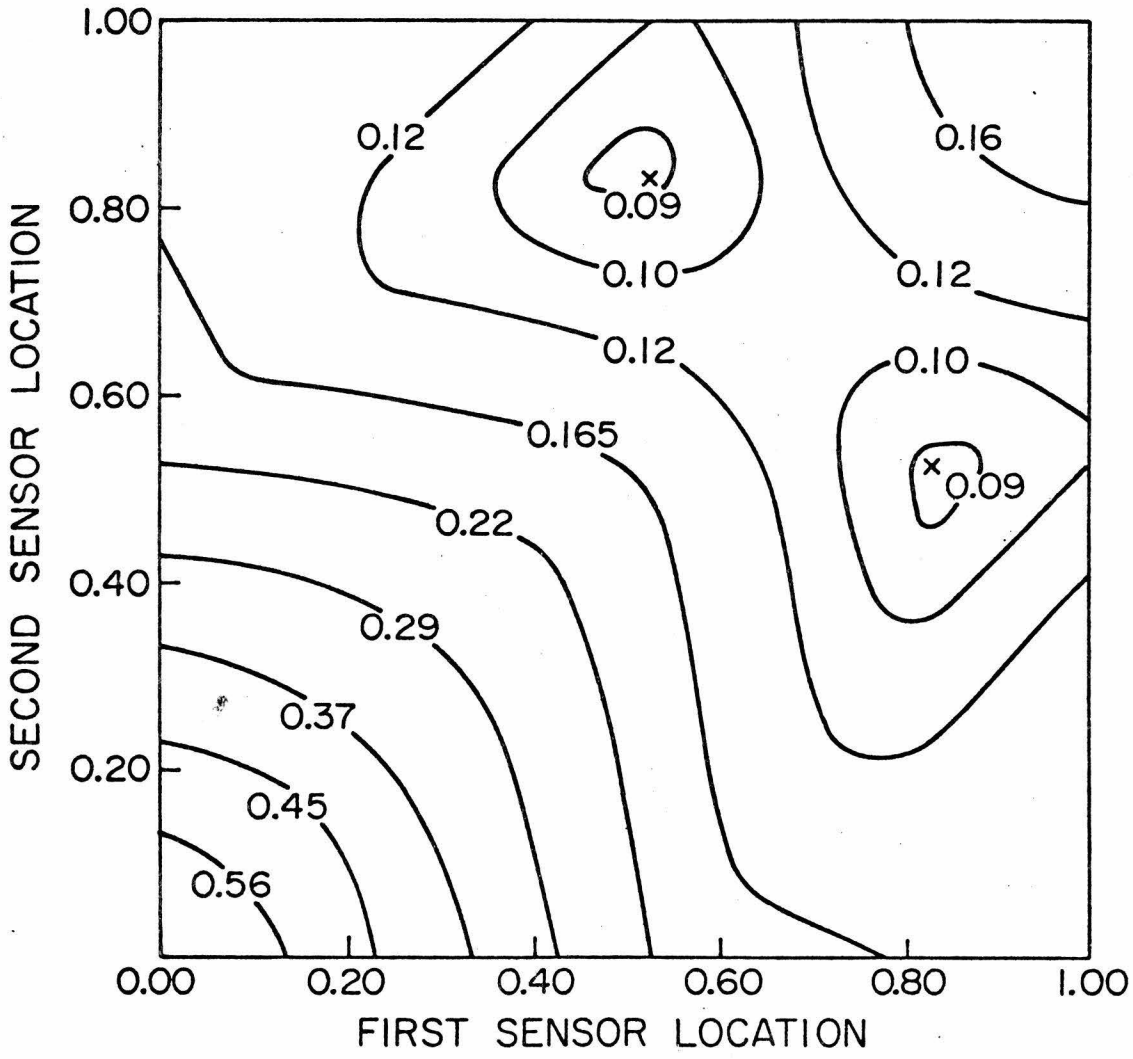

FIGURE 2.2: CONTOUR PLOT OF $\bar{J}$ FOR $R(x) = 0.8 \exp[-2(1-x)]$

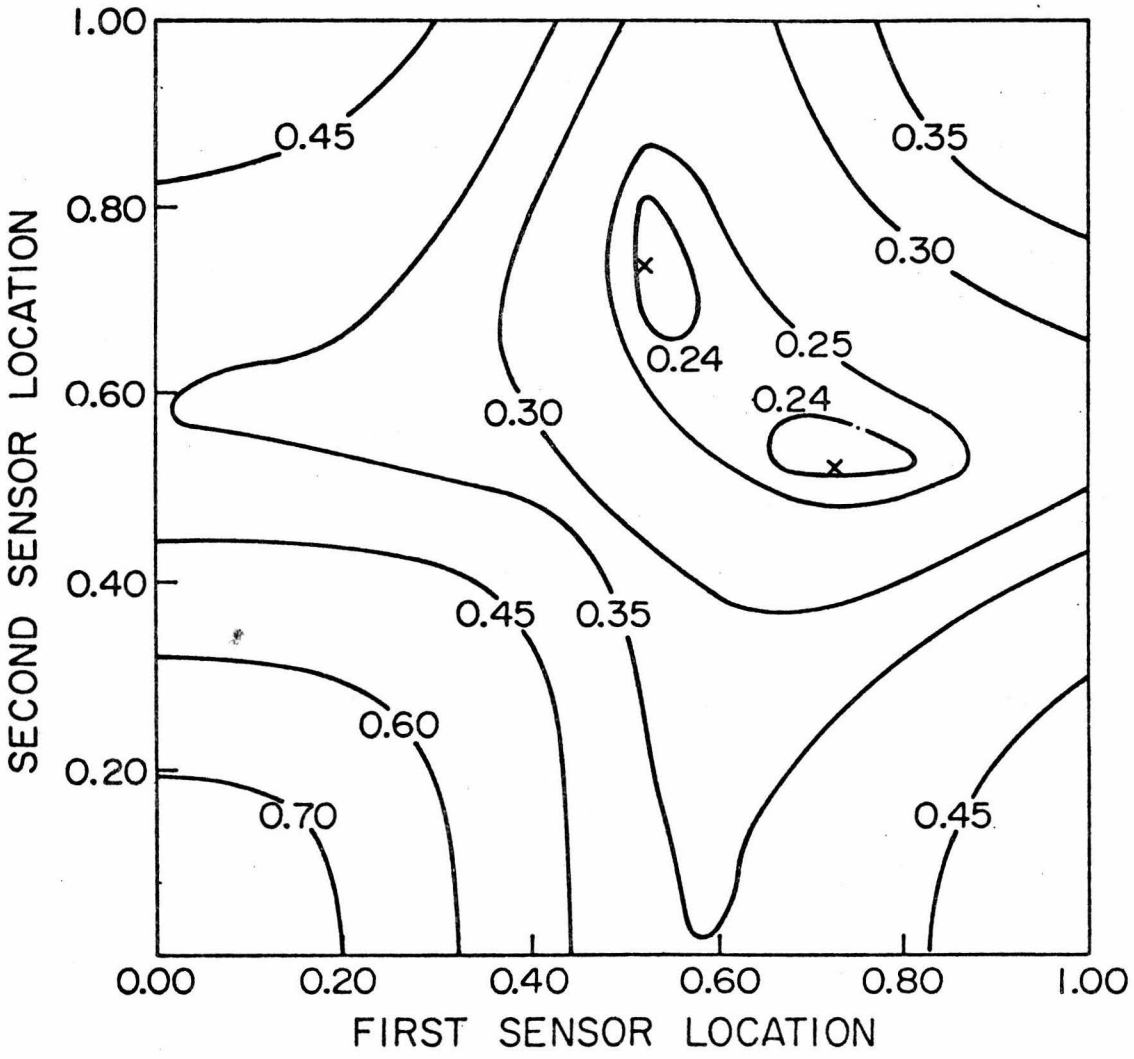

FIGURE 2.3: CONTOUR PLOT OF $\bar{J}$ FOR $R(x) = 0.8\ \mathrm{EXP}[+4|x-0.5|]$

for case (c). Although it is difficult to separate out the effects of the dynamics of the process, and the measurement noise covariance, the sensor locations, in general, move towards points of lower measurement error variance.

Contours of constant $\bar{J}(t)$ are shown in Figures 2.1, 2.2, and 2.3 for cases (b), (c), and (e). The plots are symmetric about the 45° line as the two sensors are equivalent. The optimal locations are indicated by crosses.

2.8.3 Effect of $P_o(x,y)$

To study the effect of initial covariance $P_0(x,y)$, the boundary conditions of case A were considered, and R(x) was specified as $R(x) = 0.8 \exp[-2(1-x)]$. Different values of $P_0(x,y)$ were assumed and sensor locations were obtained. The results are given in Table 2.5.

2.8.4 Comparison of the Results to Solution of the Riccati Equation

Now we consider the full equation for the covariance matrix P(x,y,t) and study the effect on the sensor locations of considering the upper bound of P(x,y,t) rather than P(x,y,t) itself. The full nonlinear Riccati equation governing the covariance matrix P(x,y,t) was solved using an alternating-direction implicit method. The values for the optimality index

$$J(t) = \int_D P(x,x,t)\, dx \tag{2.84}$$

were evaluated at $t = 0.10$ for varying Q(x,y,t). Initial covariance

Table 2.5 Effect of Initial Covariance $P_0(x,y)$ on Optimal Sensor Locations

Boundary Conditions: $u(0,t) = 0$

$$\left.\frac{\partial u(x,t)}{\partial x}\right|_{x=1} = 0$$

Measurement Noise Covariance: $R(x) = 0.8 \exp[-2(1-x)]$

	$P_0(x,y)$	Sensor Locations
(A)	$0.2\,\delta(x-y)$	0.60 , 0.75
(B)	$2\delta(x-y)$	0.50 , 0.85
(C)	$20\delta(x-y)$	0.48 , 0.84

Table 2.6 Values of J(t) Obtained by Solving the Full Riccati Equation for Various Combinations of Sensor Locations

$Q(x,y,t) = 0$

x_1/x_2	0.1	0.3	0.5	0.7	0.9
0.1	--	2.817	2.698	2.758	2.714
0.3	2.817	--	2.460	2.364	2.310*
0.5	2.698	2.460	--	2.544	2.370
0.7	2.758	2.364	2.544	--	2.558
0.9	2.714	2.310*	2.370	2.558	--

$Q(x,y,t) = 0.6 \exp [-10(x-y)]$

x_1/x_2	0.1	0.3	0.5	0.7	0.9
0.1	--	2.839	2.719	2.780	2.736
0.3	2.839	--	2.481	2.384	2.330*
0.5	2.719	2.481	--	2.566	2.391
0.7	2.780	2.384	2.566	--	2.580
0.9	2.736	2.330*	2.391	2.580	--

$Q(x,y,t) = 0.5\ \delta(x-y)$

x_1/x_2	0.1	0.3	0.5	0.7	0.9
0.1	--	2.986	2.864	2.926	2.881
0.3	2.986	--	2.622	2.524	2.469*
0.5	2.864	2.622	--	2.709	2.530
0.7	2.926	2.524	2.709	--	2.723
0.9	2.881	2.469*	2.530	2.723	--

$P_0(x,y)$ was maintained at $2\delta(x-y)$, and $R(x) = 0.8 \exp[-2(1-x)]$ was used. The sensor locations x_1 and x_2 were restricted to five points 0.1, 0.3, 0.5, 0.7, and 0.9. The values of J(t) for different combinations of sensor locations, and different Q(x,y,t) are given in Table 2.6. For the three cases considered, J(t) for the optimal sensor locations is indicated by * . In all three cases, optimal sensor locations are seen to be 0.3 and 0.9 based on the prespecified locations. The optimal sensor locations determined by using the method developed in this chapter are 0.296 and 0.866. Thus, we see that the method works quite well for reasonable covariance functions Q(x,y,t) and provides considerable savings in computation time.

2.9 Conclusions

In this chapter we propose a computationally attractive approach for the optimal sensor location problem in distributed parameter systems. An upper bound to the filter covariance matrix for linear distributed parameter systems is developed. When the optimal sensor location problem is posed as a minimization problem for a suitable measure of this upper bound, the computational effort involved is significantly smaller compared with the effort necessary for minimizing a measure of the filter covariance matrix (Aidarous, 1976; Chen and Seinfeld, 1975). An example involving one-dimensional heat conduction is considered and the results obtained by the two approaches are compared. The upper bound in (2.53) may indeed be a weak one for certain cases. However, the term $\overline{P}(x,y,t)$ in the upper bound takes into account the effect of both the

system dynamics and the measurement noise covariance on the sensor locations. The numerical results of the example show that for spatially independent $Q(x,y,t)$, the optimal sensor locations obtained by considering the full matrix Riccati equation are not different from those obtained by using the upper bound approach developed here.

CHAPTER 3

OPTIMAL LOCATION OF MEASUREMENTS IN TUBULAR REACTORS

3.1 Introduction

In this Chapter, we consider the problem of determining optimal sensor locations for a meaningful chemical engineering system. Most systems of interest are described by more than one state variable . In practice, it may be difficult to obtain continuous measurements of some of the state variables while measurements of other variables may be disturbed by noise. Often, for control purposes, it is desired that the state variables be estimated accurately from a knowledge of the system model and some measurements on the system. In a situation where we wish to estimate the system state using only a limited number of measurements, an important question is the selection of sensor locations. It may also be desirable to determine the number of sensors required in order to estimate the state to a given accuracy.

The particular system considered in this Chapter is a non-adiabatic tubular reactor in which a first order exothermic chemical reaction is taking place. The reaction term introduces nonlinearity in the mass and energy balance equations and makes the system very interesting. The non-adiabatic reactor model was chosen because it is more realistic than the isothermal or adiabatic models. The steady state profiles in non-adiabatic reactors are often characterized by hot spots and the random input disturbances may cause considerable deviations away from the steady state concentration and temperature profiles. It is, therefore, desirable to obtain good estimates of the concentration and temperature profiles. In this work, we deal with the problem of determining optimal sensor locations with the objective of estimating concentration and temperature profiles as accurately as possible.

Keeping in mind the random nature of input disturbances and inherent uncertainties in the system parameters and the measurements, the sensor location problem is approached from a stochastic point of view. We use the framework of estimation theory and consider the location of sensors so that a best estimate of the concentration and temperature profiles is obtained. Since the tubular reactor is a nonlinear system with two state variables, it is difficult to directly apply the theories available (Aidarous, 1976; Chen and Seinfeld, 1975). The approach developed in Chapter 2 will require the numerical computation of Green's function matrix for the linearized problem which can be very time consuming. An alternate approach based on discretization of the reactor equations is developed and the optimal sensor locations are selected from a specified set of locations.

In Section 3.2, we introduce the equations describing the tubular reactor and nondimensionalize them by introducing appropriate dimensionless variables. The steady state equations are obtained and the reactor equations are linearized around the steady state. In Section 3.3, we give a brief outline of the method of orthogonal collocation, and following Georgakis et al. (1975), the reactor equations are discretized using the orthogonal collocation method. The nonlinear discrete equations are linearized around the steady state. Equations for the optimal state estimate and the corresponding covariance matrix are obtained in Section 3.4 using the familiar Kalman filter (Jazwinski, 1970). The optimality index for sensor locations is defined in Section 3.5 and an iterative algorithm for determining optimal sensor locations is developed based on Pontryagin's minimum principle. In Section 3.6 we describe in detail the results of a numerical example. The parameters in the model are chosen so that a unique

stable steady state is guaranteed (Varma and Amundson, 1973b). The effect of process dynamics, process noise, and the measurement noise on the optimal sensor locations is studied.

3.2 Reactor Model

The system under consideration is a non-adiabatic tubular reactor in which a single first order chemical reaction is taking place. We have chosen to deal with a non-adiabatic reactor model as against the isothermal or adiabatic models because it is more representative of the practical situation. Varma and Amundson (1972, 1973a, 1973b) have considered the question of uniqueness and stability of the steady state of non-adiabatic tubular reactors. Georgakis et al. (1975, 1976) have studied the problem of stabilization of unstable tubular chemical reactors by modal control and observer design.

Fluid consisting of species A_1 enters the tubular reactor of radius R and length L at concentration c'_{in} and temperature T'_{in}, and undergoes a first order chemical reaction

$$A_1 \rightarrow A_2$$

with reation rate r'(c',T') and heat of reaction ΔH. The concentration of species A_1 is denoted by c', and T' denotes the temperature of the reaction mixture at any point along the reactor length. The reactor is cooled by a heat exchanger in which the coolant is maintained at an essentially constant temperature T'_a. The over-all heat transfer coefficient U is assumed constant. The density, heat capacity, and thermal conductivity of the reacting mixture are denoted by ρ, C_p, and k respectively. In order to

write down the transient heat and mass balance equations, we assume that the fluid density, heat capacity, thermal conductivity and heat of reaction all remain constant. The axial diffusivity is denoted by D and radial gradients are assumed to be negligible. Under these assumptions, the transient equations governing the mass balance for species A_1 and the overall energy balance are

$$\frac{\partial c'}{\partial t'} = D \frac{\partial^2 c'}{\partial s'^2} - V \frac{\partial c'}{\partial s'} - r'(c',T') \tag{3.1}$$

$$\rho C_p \frac{\partial T'}{\partial t'} = k \frac{\partial^2 T'}{\partial s'^2} - \rho V C_p \frac{\partial T'}{\partial s'} + (-\Delta H) r'(c',T') + \frac{2U}{R} (T_a' - T') \tag{3.2}$$

where t' is the time, s' is the distance along the reactor length, and V is the velocity of the reaction mixture. The boundary conditions for (3.1) and (3.2) are

at s' = 0

$$Vc_{in}' = \left(Vc' - D \frac{\partial c'}{\partial s'} \right)_{s'=0^+} \qquad t' > 0 \tag{3.3}$$

$$\rho V C_p T_{in}' = \left(\rho V C_p T' - k \frac{\partial T'}{\partial s'} \right)_{s'=0^+} \qquad t' > 0 \tag{3.4}$$

at s' = L

$$\frac{\partial c'}{\partial s'} = 0 \qquad t' > 0 \tag{3.5}$$

$$\frac{\partial T'}{\partial s'} = 0 \qquad t' > 0 \tag{3.6}$$

Equations (3.1)-(3.6) can be non-dimensionalized by introducing

$$c = \frac{c'}{c_{in}'} \qquad T = \frac{T'}{T_{in}'}$$

$$s = \frac{s'}{L} \qquad t = \frac{t'D}{L^2} \tag{3.7}$$

The dimensionless reactor equations are

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial s^2} - P_{e_m} \frac{\partial c}{\partial s} - \alpha r \tag{3.8}$$

$$Le \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial s^2} - P_{e_h} \frac{\partial T}{\partial s} + \alpha\beta r + \gamma(T_a - T) \tag{3.9}$$

where P_{e_h} and P_{e_m} are the heat and mass transfer Peclet numbers, Le is the Lewis number, and β, γ and r are the dimensionless heat of reaction, heat transfer coefficient, and reaction rate respectively. The dimensionless parameters are defined as follows

$$P_{e_h} = \frac{\rho V C_p L}{k} \qquad P_{e_m} = \frac{VL}{D}$$

$$Le = \frac{\rho C_p D}{k} = \frac{P_{e_h}}{P_{e_m}} \qquad \alpha = \frac{L^2 r'(c'_{in}, T'_{in})}{D\, c'_{in}} \tag{3.10}$$

$$\beta = \frac{(-\Delta H)\, D\, c'_{in}}{k\, T'_{in}} \qquad \gamma = \frac{2UL^2}{kR}$$

$$r = \frac{r'(c', T')}{r'(c'_{in}, T'_{in})} \qquad T_a = \frac{T'_a}{T'_{in}}$$

For a first order reaction, the dimensionless reaction rate r(c,T) takes the form

$$r(c,T) = c \exp[\delta(1 - 1/T)] \tag{3.11}$$

where $\delta(= E'/R_g T'_{in})$, the dimensionless activation energy, is defined in terms of the activation energy E', the gas constant R_g, and the inlet temperature T'_{in} of the reactant stream. The boundary conditions for (3.8)

and (3.9) are

at s = 0,

$$\frac{\partial c}{\partial s} = P_{e_m}(c - 1) \tag{3.12}$$

$$\frac{\partial T}{\partial s} = P_{e_h}(T - 1) \tag{3.13}$$

at s = 1,

$$\frac{\partial c}{\partial s} = 0 \tag{3.14}$$

$$\frac{\partial T}{\partial s} = 0 \tag{3.15}$$

The steady state concentration $\bar{c}$ and temperature $\bar{T}$ are governed by

$$\frac{d^2\bar{c}}{ds^2} - P_{e_m}\frac{d\bar{c}}{ds} - \alpha r = 0 \tag{3.16}$$

$$\frac{d^2\bar{T}}{ds^2} - P_{e_h}\frac{d\bar{T}}{ds} + \alpha\beta r + \gamma(T_a - T) = 0 \tag{3.17}$$

with boundary conditions

at s = 0,

$$\frac{d\bar{c}}{ds} = P_{e_m}(\bar{c} - 1)$$

$$\frac{d\bar{T}}{ds} = P_{e_h}(\bar{T} - 1) \tag{3.18}$$

at s = 1,

$$\frac{d\bar{c}}{ds} = 0$$

$$\frac{d\bar{T}}{ds} = 0 \tag{3.19}$$

The dimensionless reactor equations (3.8) and (3.9) are now modified to account for the random inputs to the system. We assume that these random disturbances can be modeled as additive white Gaussian processes $w_c(s,t)$ and $w_T(s,t)$ with properties

$$E[w(s,t)] = 0$$
$$E[w(s,t)w^T(s',\tau)] = Q^+(s,s',t)\delta(t-\tau) \tag{3.20}$$

where $E[\cdot]$ is the expectation operator and $w(s,t)$ is the two dimensional column vector $[w_c(s,t)\ w_T(s,t)]^T$. The white noise assumption implies that the disturbances at two different times t and τ are uncorrelated. The 2x2 covariance matrix $Q^+(s,s',t)$ is symmetric in s and s', and is non-negative definite. The modified equations describing the reactor dynamics are

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial s^2} - P_{e_m}\frac{\partial c}{\partial s} - \alpha r + w_c(s,t) \tag{3.21}$$

$$Le\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial s^2} - P_{e_h}\frac{\partial T}{\partial s} + \alpha\beta r + \gamma(Ta-T) + w_T(s,t) \tag{3.22}$$

with boundary conditions (3.12)-(3.15). Let $\psi(s,t)$ and $\theta(s,t)$ define the random deviations in concentration and temperature away from the steady state profiles $\bar{c}(s)$ and $\bar{T}(s)$,

$$\psi(s,t) = c(s,t) - \bar{c}(s)$$
$$\theta(s,t) = T(s,t) - \bar{T}(s) \tag{3.23}$$

where $c(s,t)$ and $T(s,t)$ are the concentration and temperature values in equations (3.21) and (3.22). The equations for $\psi(s,t)$ and $\theta(s,t)$ can be

linearized around the steady state for small deviations. These linearized equations are

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial s^2} - P_{e_m} \frac{\partial \psi}{\partial s} - \alpha \left[\psi \left(\frac{\partial r}{\partial c} \right)_{\bar{c},\bar{T}} + \theta \left(\frac{\partial r}{\partial T} \right)_{\bar{c},\bar{T}} \right] + w_c(s,t) \tag{3.24}$$

$$Le \frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial s^2} - P_{e_h} \frac{\partial \theta}{\partial s} + \alpha\beta \left[\psi \left(\frac{\partial r}{\partial c} \right)_{\bar{c},\bar{T}} + \theta \left(\frac{\partial r}{\partial T} \right)_{\bar{c},\bar{T}} \right] + w_T(s,t) \tag{3.25}$$

with boundary conditions

at $s = 0$

$$\frac{\partial \psi}{\partial s} = P_{e_m} \psi$$

$$\frac{\partial \theta}{\partial s} = P_{e_h} \theta \tag{3.26}$$

at $s = 1$

$$\frac{\partial \psi}{\partial s} = 0$$

$$\frac{\partial \theta}{\partial s} = 0 \tag{3.27}$$

The initial values for ψ and θ are assumed to be white Gaussian processes with properties

$$E \begin{bmatrix} \psi(s,0) \\ \theta(s,0) \end{bmatrix} = 0 \tag{3.28}$$

$$E\left[\begin{Bmatrix}\psi(s,0)\\ \theta(s,0)\end{Bmatrix}\begin{Bmatrix}\psi(s',0) & \theta(s',0)\end{Bmatrix}\right] = P_o^+(s,s') \qquad (3.29)$$

The initial covariance matrix $P_o^+(s,s')$ is a 2x2 symmetric positive definite matrix.

3.3 Discretization by Orthogonal Collocation

The non-adiabatic tubular reactor has been described by a set of nonlinear partial differential equations. These equations need to be discretized to enable their solution. In conventional finite difference methods, the partial differential equations need to be discretized on a relatively fine mesh. The high dimensionality of the resulting lumped parameter system makes the computations time consuming. Thus, a discretization method which results in a lower order system is highly desirable. The method of orthogonal collocation is one such method and can be advantageously used to reduce the dimensionality of the problem. We shall now give a brief outline of the method of orthogonal collocation for solving the transient concentration and temperature profiles governed by the deterministic equations (3.8) and (3.9). The supporting theory and mathematical justification are treated in detail by Villadsen (1970) and Finlayson (1972).

The orthogonal collocation method is a special case of the method of weighted residuals. The unknown exact solution is approximated by a trial solution consisting of a series of known functions of the spatial variable(s). These known functions are chosen to be a family of suitable

orthogonal polynomials. The trial solution is substituted into the partial differential equation and the unknown time-dependent coefficients are determined so that the partial differential equation is satisfied at a set of grid points called the collocation points. The number of terms in the trial solution can be increased arbitrarily, and the unknown time-dependent coefficients are determined by requiring that the partial differential equation be satisfied at more and more collocation points. The orthogonal collocation method utilizes a continuous representation of the approximate solution over the whole region of space. Therefore, the spatial derivative at any point is expressed in terms of the values at all other collocation points, rather than in terms of just the neighboring points as is the case in finite difference methods. Thus, the orthogonal collocation method requires fewer equations, although the advantages of dealing with a tridiagonal matrix are lost. However, as the number of collocation points is increased, the rate of convergence increases very fast for the orthogonal collocation method. The rate of convergence for the usual second order finite difference methods is $1/(N-1)^2$ where N is the number of grid points. On the other hand, for orthogonal collocation method the rate of convergence is $(1/N)^N$ (Ciarlet et al., 1967), where N is the number of interior collocation points. The choice of trial function depends on the particular problem under consideration. For problems in which the solution is symmetric about a central axis, the solution can be expanded in terms of powers of s^2. However, for problems whose solutions do not possess symmetry properties, we must include both odd and even powers of s. Since for the tubular reactor, we do not expect the profiles to be symmetric with respect to s, we choose a trial function of

the form

$$c(s,t) = d(t) + e(t)s + s(1-s) \sum_{i=1}^{N} g_i(t)\, Y_{i-1}^{(p,q)}(s) \tag{3.30}$$

where $Y_{i-1}^{(p,q)}(s)$ are the first N orthogonal Jacobi polynomials over the interval (0,1) with weight function $s^q(1-s)^p$. The trial function (3.30) includes both odd and even powers of s, and has N+2 constants. The requirement that the solution satisfy the partial differential equation (3.8) at N interior collocation points provides N conditions, and the other two are provided by the boundary conditions at s = 0 and s = 1.

The mth polynomial $Y_m^{(p,q)}(s)$ in the family of orthogonal Jacobi polynomials is a linear combination of powers of s with highest power m

$$Y_m^{(p,q)}(s) = \sum_{j=0}^{m} b_j\, s^j$$

starting with $Y_0^{(p,q)}(s) = 1$, the coefficients in the successive polynomials are determined by requiring $Y_m^{(p,q)}(s)$ to be orthogonal to all the polynomials of order less than m. The Jacobi polynomials $Y_m^{(p,q)}(s)$ are determined by solving the equation

$$\int_0^1 s^q(1-s)^p\, Y_n^{(p,q)}(s)\, Y_m^{(p,q)}(s)\, ds = 0 \qquad n = 0, 1, 2, \ldots, m-1 \tag{3.31}$$

The polynomials $Y_m^{(p,q)}(s)$ are determined to a multiplicative constant, which is determined by requiring the first coefficient to be 1. For

p=q=0, these polynomials are the shifted Legendre polynomials. In the trial functions, we have chosen p=q=0 and the polynomials $Y_i(s)$ are written without any superscript. The trial function (3.30) is a polynomial of degree N+1 in s. We rewrite (3.30) as a polynomial in s with time dependent coefficients $f_j(t)$

$$c(s,t) = \sum_{j=1}^{N+2} f_j(t)s^{j-1} \tag{3.32}$$

At the N collocation points s_i; i = 2,3,..., N+1 and the two boundary points $s_1 = 0$ and $s_{N+2} = 1$, we can write the concentration c(s,t) and its first two spatial derivatives as

$$c(s_i,t) = \sum_{j=1}^{N+2} f_j(t)s_i^{j-1}$$

$$\left.\frac{\partial c}{\partial s}\right|_{s_i} = \sum_{j=2}^{N+2} (j-1)f_j(t)s_i^{j-2} \tag{3.33}$$

$$\left.\frac{\partial^2 c}{\partial s^2}\right|_{s_i} = \sum_{j=3}^{N+2} (j-1)(j-2)f_j(t)s_i^{j-3}$$

In terms of the matrix elements G_{ij}, K_{ij}, and L_{ij}, (3.33) can be written as

$$c(s_i,t) = \sum_{j=1}^{N+2} G_{ij}f_j(t) \quad ; \quad G_{ij} = \left.s^{j-1}\right|_{s_i}$$

$$\left.\frac{\partial c}{\partial s}\right|_{s_i} = \sum_{j=1}^{N+2} K_{ij} f_j(t) \quad ; \quad K_{ij} = \left.\frac{ds^{j-1}}{ds}\right|_{s_i}$$

$$\left.\frac{\partial^2 c}{\partial s^2}\right|_{s_i} = \sum_{j=1}^{N+2} L_{ij} f_j(t) \quad ; \quad L_{ij} = \left.\frac{d^2 s^{j-1}}{ds^2}\right|_{s_i} \tag{3.34}$$

One can write a similar trial solution for T(s,t) and substitute the two trial solutions into (3.8) and (3.9). The coefficients d(t), e(t), and $g_i(t)$ are then determined by satisfying the partial differential equations (3.8) and (3.9) at the N interior collocation points, chosen to be the zeros of the Nth order polynomial $Y_N(s)$. However, for computational purposes it is more convenient to solve for the concentrations and temperatures at the collocation points. The first and second derivatives in (3.34) can be expressed in terms of $c_i(t) = c(s_i,t)$ as follows,

$$\left.\frac{\partial c}{\partial s}\right|_{s_i} = \sum_{j=1}^{N+2} A_{ij}\, c_j(t), \qquad i = 1,2,\ldots, N+2$$

$$\left.\frac{\partial^2 c}{\partial s^2}\right|_{s_i} = \sum_{j=1}^{N+2} B_{ij}\, c_j(t), \qquad i = 1,2,\ldots, N+2 \tag{3.35}$$

The (N+2) x (N+2) dimensional matrices A, B with elements A_{ij}, B_{ij}, are given by

$$A = K\, G^{-1}$$

$$B = L\, G^{-1} \tag{3.36}$$

where K, L, and G are the (N+2)x(N+2) matrices with elements K_{ij}, L_{ij}, and G_{ij} in (3.34)

The boundary conditions at s=0 and s=1 can also be approximated and their linearity allows the concentrations and temperatures at the two ends to be eliminated. Georgakis et al. (1975) give the detailed equations. Because of different non-dimensionalization, our equations are slightly different and, for the sake of completeness, are given in Appendix C. The discrete equations, for the case Le = 1, are

$$\frac{dc_j}{dt} = \sum_{k=2}^{N+1} D_{jk}c_k - \alpha r(c_j,T_j) + p_j \qquad (3.37)$$

$$(j = 2,3,\ldots, N+1)$$

$$\frac{dT_j}{dt} = \sum_{k=2}^{N+1} S_{jk}T_k + \alpha\beta r(c_j,T_j) + \gamma(T_a-T_j) + q_j \qquad (3.38)$$

$$(j = 2,3,\ldots, N+1)$$

where D_{jk}, S_{jk}, p_j, and q_j are defined in the Appendix C and are functions of the elements of matrices A and B and P_{e_h} and P_{e_m}. The solution of (3.37)-(3.38) with proper initial conditions gives us the concentration and temperature values at the interior collocation points. The boundary values are determined by equations (C.4) and (C.5). Once the concentration values at collocation points are known, one can evaluate the coefficients f_j's in the polynomials approximating the concentration profile. The concentration at any other point can be determining readily by using (3.32). The temperature at any point can also be determined in a similar way.

The steady state profiles can be determined by solving (3.37)-(3.38) with arbitrary initial conditions over a sufficiently long period of time so that the left hand sides reach an arbitrarily small constant. The steady state values $\bar{c}_j$ and $\bar{T}_j$ can also be determined by solving the algebraic equations,

$$\sum_{k=2}^{N+1} D_{jk}\bar{c}_k - \alpha r(\bar{c}_j,\bar{T}_j) + p_j = 0 \tag{3.39}$$

$$\sum_{k=2}^{N+1} S_{jk}\bar{T}_k + \alpha\beta r(\bar{c}_j,\bar{T}_j) + \gamma(T_a-\bar{T}_j) + q_j = 0 \tag{3.40}$$

The solution of (3.39) and (3.40) gives the steady state concentrations $\bar{c}_j$ and temperatures $\bar{T}_j$ at the N interior collocations points s_j, $j = 2,\ldots,$ N+1. The steady state concentration at any other point can then be determined by evaluating the coefficients f_j's in (3.33) and using (3.32). The steady state temperature profile can be determined in a similar way.

Let us now consider the random deviations $\psi(s,t)$ and $\theta(s,t)$ of (3.23). At the collocation points s_j, these deviations are denoted by $x_j(t)$ and $y_j(t)$

$$x_j(t) = \psi(s_j,t)$$

$$j = 2,\ldots, N+1 \tag{3.41}$$

$$y_j(t) = \theta(s_j,t)$$

The dynamical equations governing x_j and y_j, $j = 2,\ldots,$ N+1 can be written as

$$\frac{dx_j}{dt} = \sum_{k=2}^{N+1} D_{jk}x_k - \alpha\left[x_j\left(\frac{\partial r}{\partial c}\right)_{\bar{c}_j,\bar{T}_j} + y_j\left(\frac{\partial r}{\partial T}\right)_{\bar{c}_j,\bar{T}_j}\right] + w_c(s_j,t) \quad (3.42)$$

$$\frac{dy_j}{dt} = \sum_{k=2}^{N+1} S_{jk}y_k + \alpha\beta\left[x_j\left(\frac{\partial r}{\partial c}\right)_{\bar{c}_j,\bar{T}_j} + y_j\left(\frac{\partial r}{\partial T}\right)_{\bar{c}_j,\bar{T}_j}\right] + w_T(s_j,t) \quad (3.43)$$

Equations (3.42) and (3.43) can also be obtained by linearizing (3.37) and (3.38) around the steady state values $\bar{c}_j$ and $\bar{T}_j$, and introducing the random disturbances $w_c(s_j,t)$ and $w_T(s_j,t)$. The initial values for x_j and y_j are white Gaussian processes with properties.

$$E\begin{bmatrix} x_j(0) \\ y_j(0) \end{bmatrix} = 0 \quad (3.44)$$

$$E\left[\begin{Bmatrix} x_j(0) \\ y_j(0) \end{Bmatrix}\begin{Bmatrix} x_k(0) & y_k(0) \end{Bmatrix}\right] = P_o^+(s_j,s_k) \quad (3.45)$$

where $P_o^+(s_j,s_k)$ is the covariance matrix $P_o^+(s,s')$ evaluated at $s=s_j$ and $s'=s_k$.

3.4 State Space Formulation and Optimal Estimate

In conventional state space notation, the state vector u is the 2N-dimensional column vector, $[x_2\ y_2\ x_3\ y_3\ \ldots\ldots x_{N+1}\ y_{N+1}]^T$. The transient equations (3.42)-(3.43) can be written as

$$\frac{du}{dt} = F\,u(t) + \xi(t) \quad (3.46)$$

$$u(0) = u_0 \tag{3.47}$$

where the 2N x 2N matrix F is a matrix the $(\hat{i},\hat{j})$th element of which is the 2x2 matrix $F_{\hat{i}\hat{j}}$, $\hat{i},\hat{j} = 1,2,\ldots, N$ given by

$$F_{\hat{i}\hat{j}} = \begin{cases} \begin{bmatrix} D_{ij} & 0 \\ 0 & S_{ij} \end{bmatrix} & ; \hat{i} \neq \hat{j} \\ \begin{bmatrix} D_{ii} - \alpha \left(\frac{\partial r}{\partial c}\right)_{\bar{c}_i,\bar{T}_i} & -\alpha \left(\frac{\partial r}{\partial T}\right)_{\bar{c}_i,\bar{T}_i} \\ \alpha\beta \left(\frac{\partial r}{\partial c}\right)_{\bar{c}_i,\bar{T}_i} & S_{ii} + \alpha\beta \left(\frac{\partial r}{\partial T}\right)_{\bar{c}_i,\bar{T}_i} \end{bmatrix} & ; \hat{i} = \hat{j} \end{cases} \tag{3.48}$$

where $i = \hat{i}+1$ and $j = \hat{j}+1$. The process noise $\xi(t)$ is the 2N-dimensional vector

$$[w_c(s_2,t)\ w_T(s_2t)\ w_c(s_3,t)\ w_T(s_3,t)\ \ldots\ldots\ w_c(s_{N+1},t)\ w_T(s_{N+1},t)]^T \tag{3.49}$$

The properties of w(s,t) assumed in Section (3.2) imply that $\xi(t)$ is a zero-mean white Gaussian process with 2N x 2N covariance matrix Q(t). The (i,j)th element of Q(t), i, j = 1,2,..., N is the 2x2 matrix $Q^+(s_{i+1},s_{j+1},t)$. Thus we have

$$\begin{aligned} E[\xi(t)] &= 0 \\ E[\xi(t)\xi^T(\tau)] &= Q(t)\delta(t-\tau) \end{aligned} \tag{3.50}$$

where

$$Q(t) = \begin{bmatrix} Q^+(s_2,s_2,t) & \cdots & Q^+(s_2,s_{N+1},t) \\ Q^+(s_3,s_2,t) & \cdots & Q^+(s_3,s_{N+1},t) \\ \vdots & & \vdots \\ Q^+(s_{N+1},s_2,t) & \cdots & Q^+(s_{N+1},s_{N+1},t) \end{bmatrix} \tag{3.51}$$

The initial state u_o is also a zero-mean white Gaussian process with 2N x 2N covariance matrix $P_o(t)$. The (i,j)th element of $P_o(t)$, i,j = 1, 2,..., N is the 2x2 matrix $P_o^+(s_{i+1},s_{j+1},t)$.

We assume that point measurements of concentration and temperature can be made in principle at any given point along the reactor length. Let us consider the case when both concentration and temperature measurements are made at the N interior collocation points. The measurement vector is described by

$$z_i(t) = H_i\, u_i(t) + v_i(t) \qquad i = 1,2,3,\ldots, N \tag{3.52}$$

where $z_i(t)$ is the vector of concentration and temperature measurements at s_{i+1}, and $u_i(t)$ is the two dimensional column vector with elements x_{i+1} and y_{i+1}. The measurement matrix H_i can be chosen to specify the type of measurements — concentration or temperature or both. For measuring both concentration and temperature at the collocation points, H_i is a 2x2 matrix and is assumed to be time invariant without loss of generality. The measurement noise vector $v_i(t)$ is a zero-mean white Gaussian process with covariance

$$E[v_i(t)v_j(\tau)] = \begin{cases} R_{ii}(t)\delta(t-\tau) & , \ i = j \\ 0 & , \ i \neq j \end{cases} \tag{3.53}$$

The above assumption implies that the measurement noise at two different locations s_i and s_j is not correlated. The 2N-dimensional total measurement vector $z(t)$ can be written as

$$z(t) = Hu(t) + v(t) \tag{3.54}$$

where H is a 2N x 2N matrix and $v(t)$ is a 2N dimensional vector. In detailed form, (3.54) is

$$\begin{bmatrix} z_1(t) \\ \\ \\ z_N(t) \end{bmatrix} = \begin{bmatrix} H_1E_1 \\ H_2E_2 \\ \cdot \\ \cdot \\ H_NE_N \end{bmatrix} \begin{bmatrix} u_1(t) \\ u_2(t) \\ \cdot \\ \cdot \\ u_N(t) \end{bmatrix} + \begin{bmatrix} v_1(t) \\ v_2(t) \\ \cdot \\ \cdot \\ v_N(t) \end{bmatrix} \tag{3.55}$$

where E_i is a 2x2N matrix composed of N 2x2 submatrices, of which the $\underline{i}$th submatrix is the identity matrix and all the rest are zero. The measurement noise vector $v(t)$ is a zero-mean white Gaussian process with positive definite covariance matrix $R(t)$. The 2N x 2N matrix $R(t)$ is a quasi-diagonal matrix with the $\underline{i}$th diagonal block $R_{ii}(t)$, $i = 1,2,\ldots, N$. We now wish to obtain the best estimate of the state $u(t)$, given the measurements $z(\tau)$, $0 \leq \tau \leq t$.

Let us denote an estimate of the system state by $u_e(t)$. The estimate error covariance matrix is defined by

$$E[\{u(t) - u_e(t)\}\{u(t) - u_e(t)\}^T]$$

This error covariance matrix is nonnegative definite. For a given system and measurement scheme, the estimate $u_e(t)$ for which the covariance matrix is minimum is called the optimal estimate. Let us denote this optimal estimate by $\hat{u}(t)$ and corresponding covariance matrix by $P(t)$. Thus

$$P(t) = E[\{u(t) - \hat{u}(t)\}\{u(t) - \hat{u}(t)\}^T] \tag{3.56}$$

It has been shown by Kalman that the optimal estimate $\hat{u}(t)$ for the system (3.46)-(3.54) is governed by the differential equation (Jazwinski, 1970)

$$\begin{aligned} \frac{d\hat{u}(t)}{dt} &= F\hat{u}(t) + P(t)H^T R^{-1}(t)[z(t) - H\hat{u}(t)] \\ \hat{u}(0) &= E[u_o] = 0 \end{aligned} \tag{3.57}$$

The covariance matrix $P(t)$ is governed by the nonlinear Riccati equation

$$\begin{aligned} \frac{dP(t)}{dt} &= FP(t) + P(t)F^T + Q(t) - P(t)H^T R^{-1}(t)HP(t) \\ P(0) &= P_o \end{aligned} \tag{3.58}$$

The equations governing $\hat{u}(t)$ and $P(t)$ are also known as the Kalman filter or the optimal filter equations. Using the notation of (3.55), the equations defining the optimal filter can be written as

$$\begin{aligned} \frac{d\hat{u}(t)}{dt} &= F\hat{u}(t) + \sum_{i=1}^{N} P(t)E_i^T H_i^T R_{ii}^{-1}(t)[z_i(t) - H_i E_i \hat{u}(t)] \\ \hat{u}(0) &= 0 \end{aligned} \tag{3.59}$$

and,

$$\frac{dP(t)}{dt} = FP(t) + P(t)F^T + Q(t) - \sum_{i=1}^{N} P(t)E_i^T H_i^T R_{ii}^{-1}(t) H_i E_i P(t)$$

$$P(0) = P_0 \tag{3.60}$$

It should be noted here that the equation for P(t) is independent of the measurements z(t) but depends on the system matrix F, the measurement matrix H_i, and the noise covariances Q(t) and R(t). Consequently, we can evaluate the error covariance P(t) off-line.

Let us assume that the concentration and temperature measurements can be made only at the interior collocation points and the optimal sensor locations are to be chosen from this set of N points. This may seem to be an unnecessary restriction, but the number of interior collocation points can be increased arbitrarily. Let us introduce the parameters $a_i(t)$, i = 1,2,..., N such that

$$a_i(t) = \begin{cases} 1 & \text{, if a measurement is made at } s_{i+1} \text{ at time t} \\ 0 & \text{, otherwise} \end{cases} \tag{3.61}$$

If the number of sensors is specified to be m, only m of the $a_i(t)$ values will be 1. Thus the equations for u(t) and P(t) for measurements at only m locations can be written as

$$\frac{d\hat{u}}{dt} = F\hat{u}(t) + \sum_{i=1}^{N} a_i(t)P(t)E_i^T H_i^T R_{ii}^{-1}(t)[z_i(t) - H_i E_i \hat{u}(t)]$$

$$\hat{u}(0) = 0 \tag{3.62}$$

and

$$\frac{dP(t)}{dt} = FP(t) + P(t)F^T + Q(t) - \sum_{i=1}^{N} a_i(t)P(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i P(t) \tag{3.63}$$

$$P(0) = P_0$$

3.5 Optimality Index and The Minimum Principle

The measurement locations are specified through the parameters $a_i(t)$, $i = 1,2,\ldots, N$. Different measurement policies will lead to different estimates $\hat{u}(t)$ and covariance matrices $P(t)$. Since the covariance matrix $P(t)$ indicates the accuracy of the estimate, it is natural that an optimal measurement policy be defined as one that minimizes a specified scalar measure of $P(t)$. This scalar measure will be called the optimality index. Since $P(t)$ is a nonnegative definite matrix, its trace is a good measure of its magnitude, and we can choose the optimality index J to be

$$J = \alpha_1 \mathrm{Tr}\ P(t_f) + \beta_1 \int_0^{t_f} \mathrm{Tr}\ P(t)\, dt \tag{3.64}$$

where t_f is the specified final time and α_1 and β_1 are two positive constants specifying the relative weights of the two terms. The optimal sensor location problem can now be viewed as a deterministic control problem in which the state matrix $P(t)$ is governed by the matrix Riccati equation (3.62) and the optimality index J is to be minimized with respect to the parameters $a_i(t)$; $i = 1,2,\ldots, N$ regarded as control variables. A matrix minimum principle corresponding to Pontryagin's minimum principle

has been formulated by Athans (1968) for optimal control problems in which the state is governed by a matrix differential equation. We shall now develop the necessary conditions for minimizing J by employing this matrix minimum principle. The algorithm used for determining the optimal sensor locations is based on the work of Chen and Seinfeld (1975).

Let $\Phi(t)$ denote the 2N x 2N adjoint variable matrix associated with the state matrix P(t). Then the Hamiltonian $H(t)$ is defined as

$$H(t) = \beta_1 \mathrm{Tr}P(t) + \mathrm{Tr}[\dot{P}(t)\,\Phi^T(t)] \tag{3.65}$$

or

$$H(t) = \beta_1 \mathrm{Tr}P(t) + \mathrm{Tr}\Bigg[\Big\{FP(t) + P(t)F^T + Q(t) - P(t)\left(\sum_{i=1}^{N} a_i(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i\right)P(t)\Big\}\Phi^T(t)\Bigg]$$

The adjoint matrix $\Phi(t)$ is governed by the matrix differential equation

$$\dot{\Phi}(t) = -\frac{\partial H(t)}{\partial P(t)} \tag{3.66}$$

$$\dot{\Phi}(t) = -\beta_1 I - F^T\Phi(t) - \Phi(t)F + \Phi(t)P(t)\left[\sum_{i=1}^{N} a_i(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i\right] + \left[\sum_{i=1}^{N} a_i(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i\right]P(t)\Phi(t) \tag{3.67}$$

with the terminal condition

$$\Phi(t_f) = \alpha_1 I \tag{3.68}$$

The optimal values for the a_i are then determined by the application of minimum principle which states that

$$H(P^*(t),\Phi^*(t),a_i^*(t),t) \leq H(P^*(t),\Phi^*(t), a_i(t),t) \tag{3.69}$$

where $a_i^*(t)$ is the set of optimal parameters $a_i(t)$, $P^*(t)$ and $\Phi^*(t)$ are the corresponding state and adjoint variable matrices. By using the definition of the Hamiltonian, the inequality (3.69) simplifies to

$$\sum_{i=1}^{N} a_i^*(t)\mathrm{Tr}\left[P^*(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i P^*(t)\Phi^{*T}\right]$$
$$\geq \sum_{i=1}^{N} a_i(t)\mathrm{Tr}\left[P^*(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i P^*(t)\Phi^{*T}(t)\right] \tag{3.70}$$

This inequality forms the basis of the numerical algorithm used here for determination of optimal set of parameters $a_i^*(t)$. It should be noted here that in the inequalities (3.69) and (3.70) the parameters $a_i(t)$ have been assumed to be time dependent and therefore will lead to the time dependent optimal sensor locations. In most situations however, one is interested in obtaining time-independent sensor locations. For fixed sensor locations the parameters a_i are independent of time and the inequality corresponding to (3.70) is

$$\sum_{i=1}^{N} a_i^* \int_0^{t_f} \mathrm{Tr}\left[P^*(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i P^*(t)\Phi^{*T}(t)\right] dt$$
$$\geq \sum_{i=1}^{N} a_i \int_0^{t_f} \mathrm{Tr}\left[P^*(t)E_i^T H_i^T R_{ii}^{-1}(t)H_i E_i P^*(t)\Phi^*(t)\right] dt \tag{3.71}$$

Let us define the switching functions σ_i; i = 1,2,..., N as

$$\sigma_i = \int_0^{t_f} \mathrm{Tr}\left[P(t)H_i^T E_i^T R_{ii}^{-1}(t) H_i E_i P(t)\Phi(t) \right] dt \qquad (3.72)$$

In order to minimize J, we must choose the m a_i's corresponding to m largest σ_i's as equal to 1 and rest zero. Therefore, a simple iterative algorithm for determining optimal sensor locations is

(1) Choose m a_i's corresponding to the initial guess of sensor locations as 1 and rest zero.

(2) Evaluate the covariance matrix P(t), the adjoint variable matrix $\Phi(t)$, and the switching functions σ_i; i = 1,2,..., N

(3) Choose the m a_i's corresponding to m largest σ_i's as 1 and rest zero

(4) If there is no change in the values of a_i's, stop; otherwise go to step 2.

The set of a_i's determined by this iterative procedure gives us the optimal sensor locations.

3.6 Numerical Example and Results

In this Section, we present the results for a numerical example. In Section 3.4, we have formulated the problem for the case where both concentration and temperature measurements are made simultaneously. However, in practice it is costly and difficult to make continuous concentration measurements. Therefore, we consider the case in which only point measurements of temperatures are made, and it is desired to estimate both concentration and temperature profiles from these measurements.

3.6.1 Steady State Solution

The determination of optimal sensor locations requires the knowledge of the steady state values of concentration and temperature at the collocation points. Varma and Amundson (1972, 1973a, 1973b) have explored in detail the steady state multiplicity and stability aspects of nonadiabatic tubular reactors. In this example, the parameters for the reactor model were chosen to guarantee a unique stable steady state. The parameter values are

$$P_{e_m} = P_{e_h} = 5$$

$$\alpha = 0.875$$

$$\beta = 0.5$$

$$\gamma = 12.5$$

$$\delta = 25$$

$$T_a = 1$$

The number of interior collocation points N was chosen to be 7. The collocation points are the zeros of the polynomial $Y_7(s)$. Table 3.1 gives the polynomials $Y_i(s)$, $i = 0,1, \ldots, 7$ and the interior collocation points s_i, $i = 2,\ldots, 8$. The steady state values of concentration and temperature at the collocation points were determined by solving the 14 nonlinear algebraic equations (3.39)-(3.40). These algebraic equations were solved by using a combination of Powell's method (Powell, 1970) and the Newton-Raphson method. Powell's method worked well for initial guesses far away from the true values but did not converge to the true solution. At this point, the Newton-Raphson method worked very well. The concentration and temperature values at other points were determined by interpolation. The steady state concentration and temperature profiles are plotted in Figures 3.1 and 3.2. The steady state

Table 3.1. Orthogonal Polynomials and the Interior Collocation Points

$$Y_0(s) = 1$$

$$Y_1(s) = 2s - 1$$

$$Y_2(s) = 6s^2 - 6s + 1$$

$$Y_3(s) = 20s^3 - 30s^2 + 12s - 1$$

$$Y_4(s) = 70s^4 - 140s^3 + 90s^2 - 20s + 1$$

$$Y_5(s) = 252s^5 - 630s^4 + 560s^3 - 210s^2 + 30s - 1$$

$$Y_6(s) = 924s^6 - 2772s^5 + 3150s^4 - 1680s^3 + 420s^2 - 42s + 1$$

$$Y_7(s) = 3432s^7 - 12012s^6 + 16632s^5 - 11550s^4 + 4200s^3 - 756s^2 + 56s - 1$$

The interior collocation points $s_2, s_3, \ldots, s_8$ are the zeros of $Y_7(s)$ given below:

$$s_2 = 0.0254$$

$$s_3 = 0.1292$$

$$s_4 = 0.2971$$

$$s_5 = 0.5000$$

$$s_6 = 0.7029$$

$$s_7 = 0.8708$$

$$s_8 = 0.9746$$

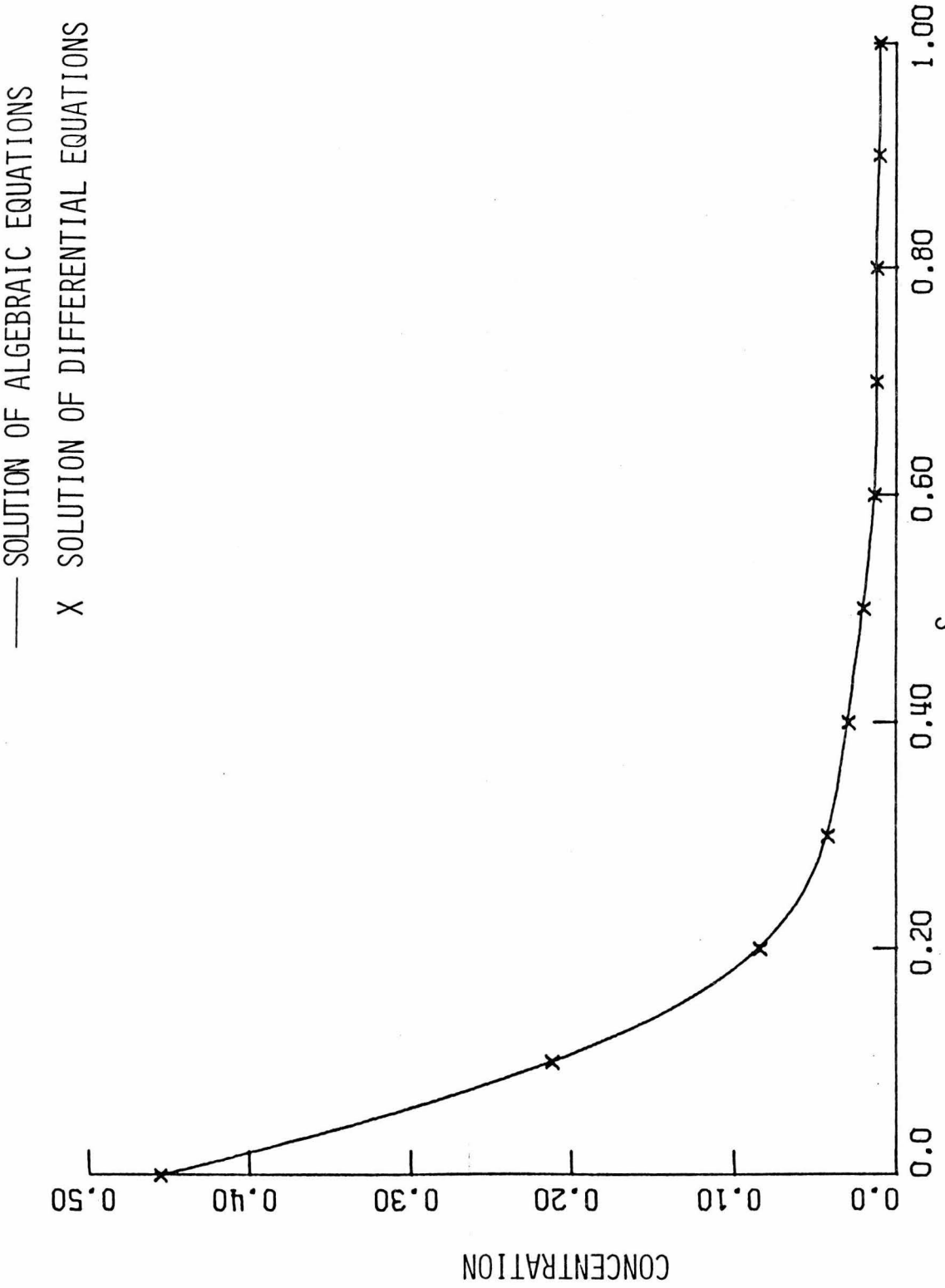

FIGURE 3.1: STEADY STATE CONCENTRATION AS A FUNCTION OF S

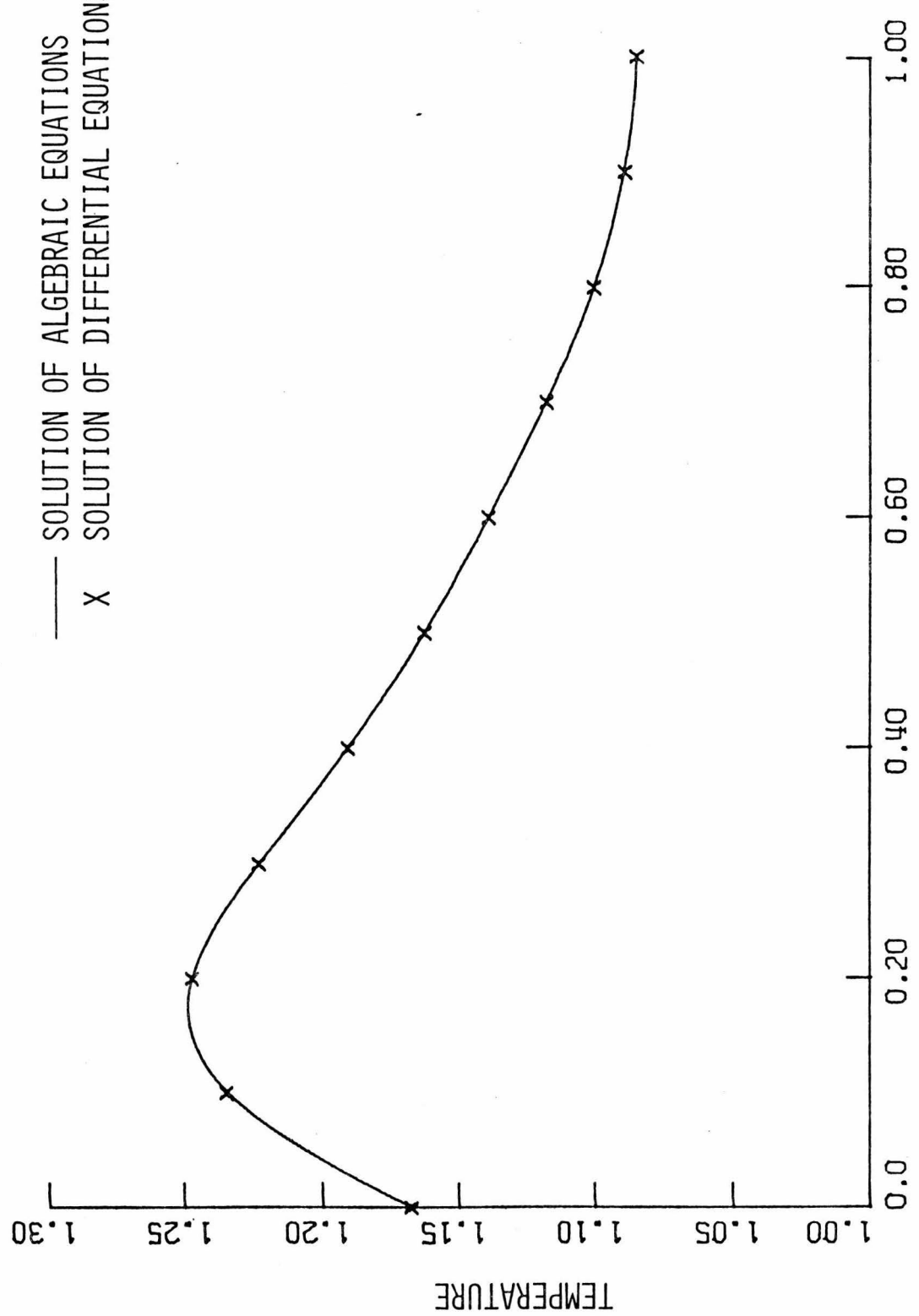

FIGURE 3.2: STEADY STATE TEMPERATURE AS A FUNCTION OF S

concentration decreases monotonically along the reactor length while the temperature profile shows the existence of a hot spot near the entrance. The steady state temperature is greater than the inlet temperature at all points along the reactor length.

As mentioned in Section 3.3, the steady state profiles can also be determined by solving the 2N differential equations (3.37)-(3.38) over a sufficiently long period of time. These equations were solved with proper initial conditions, and the resulting concentration and temperature values at a finite number of points are shown in Figures 3.1 and 3.2. The results obtained by the two methods are in good agreement. For the initial conditions $c_j(0) = 0.20$, $T_j(0) = 1.10$ $j = 2,3,\ldots,$ N+1, the steady state was reached approximately at $t = 1.4$.

3.6.2 Determination of Optimal Locations

The initial covariance $P_0^+(s,s')$ and the process noise covariance $Q^+(s,s',t)$ are assumed to be diagonal matrix functions of the form

$$P_0^+(s,s') = \begin{bmatrix} k_1 \exp(-|s-s'|/\ell_1) & 0 \\ 0 & k_1 \exp(-|s-s'|/\ell_2) \end{bmatrix} \tag{3.73}$$

$$Q^+(s,s',t) = \begin{bmatrix} k_2 \exp(-|s-s'|/\ell_3) & 0 \\ 0 & k_2 \exp(-|s-s'|/\ell_4) \end{bmatrix} \tag{3.74}$$

where k_1 and k_2 are constants and ℓ_i, $i = 1,\ldots, 4$ are the characteristic lengths for correlation between differential spatial points. The matrix $Q^+(s,s',t)$ is assumed to be time invariant. Let us further assume, for simplicity, that the largest characteristic length ℓ is much smaller

compared to the distance between any two collocation points

$$\ell << |s_j - s_k| \qquad j,k = 2,3,\ldots, N+1 \quad j \neq k$$

In this case, the 2N x 2N covariance matrices P_o and Q are approximated by

$$P_o = k_1 I$$
$$Q = k_2 I \tag{3.75}$$

This choice of P_o implies that any correlation between the uncertainties in the initial state at different collocation points is negligible. Similarly the choice of Q assumes that the correlation between system model uncertainties at various collocation points is negligible. The time invariant measurement noise variance at point s_i is given by the scalar R_{ii}. In practice, one can evaluate R_{ii} from a continuous function R(s) of the variable s, i.e. $R_{ii} = R(s)\big|_{s=s_i}$. For all cases the constant k_1 in P_o was chosen to be 0.04 thus giving trace $P_o = 0.56$. The constants α_1 and β_1 in the optimality index were both chosen to be unity. The adjoint variable matrix $\chi(t)$ is governed by a differential equation with final value specified. In order to change it to an initial value problem, we define

$$\tau = t_f - t$$

and (3.76)

$$\chi(\tau) = \Phi(t)$$

The matrix $\chi(\tau)$ is governed by

$$\frac{d\chi(\tau)}{d\tau} = \beta_1 \, I + F^T\chi(\tau) + \chi(\tau) \, F$$

$$- \chi(\tau)P(t_f-\tau)\left[\sum_{i=1}^{N} a_i(t_f-\tau)E_i^T H_i^T R_{ii}^{-1} H_i E_i\right]$$

$$-\left[\sum_{i=1}^{N} a_i(t_f-\tau)E_i^T H_i^T R_{ii}^{-1} H_i E_i\right] P(t_f-\tau)\chi(\tau) \qquad (3.77)$$

with the initial condition

$$\chi(0) = \alpha_1 \, I \qquad (3.78)$$

The switching functions σ_i of (3.72) are

$$\sigma_i = \int_0^{t_f} Tr\left[P(t_f-\tau)H_i^T E_i^T R_{ii}^{-1} H_i E_i P(t_f-\tau)\chi(\tau)\right] d\tau \qquad (3.79)$$

The advantage of expressing σ_i in the form (3.79) is that one need not store the matrix $\chi(\tau)$. The covariance matrix P(t) is calculated and stored. The adjoint variable matrix $\chi(\tau)$ is calculated but only the scalar integrand in the expression for σ_i need be stored for use in integration.

For seven interior collocation points, the matrices P(t) and $\chi(t)$ are governed by 14x14 matrix differential equations. Taking the advantage of the symmetry property of these matrices, one needs to solve 105 nonlinear differential equations in each case. A variety of computer programs are available for solving large systems of differential equations. The implementation of the Gear technique by Hindmarsh and Byrne (1975) was chosen because of the ability of the program to handle stiff differential

equations. This program uses a variable step, variable order method and employs linear multistep backward difference formulae. The optimal sensor locations are determined by using the algorithm of Section 3.5.

3.6.3 Effect of Varying Measurement Noise

The effect of varying measurement noise was studied by determining optimal locations for a fixed Q and varying R(s). The process noise covariance Q was taken to be 0.01 I. In the first two cases, R(s) was kept constant at 0.0004 and 0.004 respectively. In the third case R(s) was taken to be a function of s, namely

$$R(s) = 10^{-4} \exp(+10|s-0.5|)$$

The results for the optimal sensor location problem for these three cases are summarized in Table 3.2 which gives the initial and the optimal locations and corresponding values of the optimality index J. For the case of constant R(s), the optimal locations are governed mainly by the dynamics of the system and remain same in the two cases although the magnitude of R(s) is ten times higher in the second case. The magnitude of J is higher for the second case because of the larger uncertainty in measurements. In both cases, the optimal value of J is smaller compared to the initial value by a factor of 2 to 4. It is observed that the optimal locations for the temperature sensors are near the hot spot in the steady state temperature profile. This would seem to be quite natural because the uncertainty in temperature resulting from the process noise is expected to be high near this hot spot.

Table 3.2 Effect of Measurement Noise

$P_o = 0.04\ I$

$Q = 0.01\ I$

	R(s)	Initial Locations	Optimal Locations	No. of Iterations	Initial J	Optimal J
1	0.0004	s_4, s_6	s_2, s_3	1	11.78×10^{-2}	3.42×10^{-2}
2	0.004	s_4,s6	s_2, s_3	1	27.46×10^{-2}	10.55×10^{-2}
3	.0001 exp(+10|s-.5|)	s_3, s_6	s_3, s_4	2	14.19×10^{-2}	11.00×10^{-2}

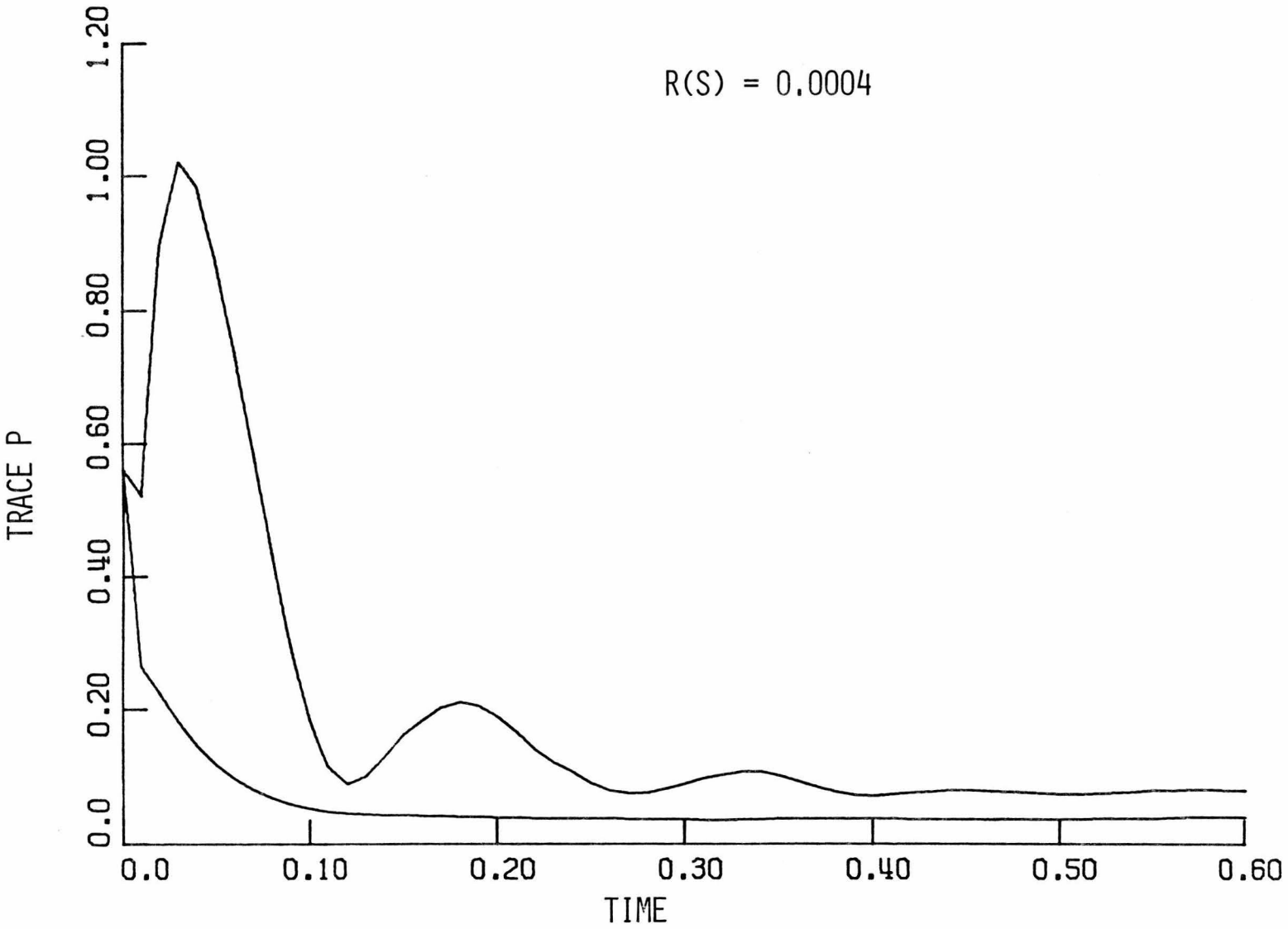

FIGURE 3.3: TRACE P AS A FUNCTION OF TIME FOR TWO SENSORS LOCATED AT (A) POSITIONS S_4 AND S_6 (B) OPTIMAL POSITIONS S_2 AND S_3

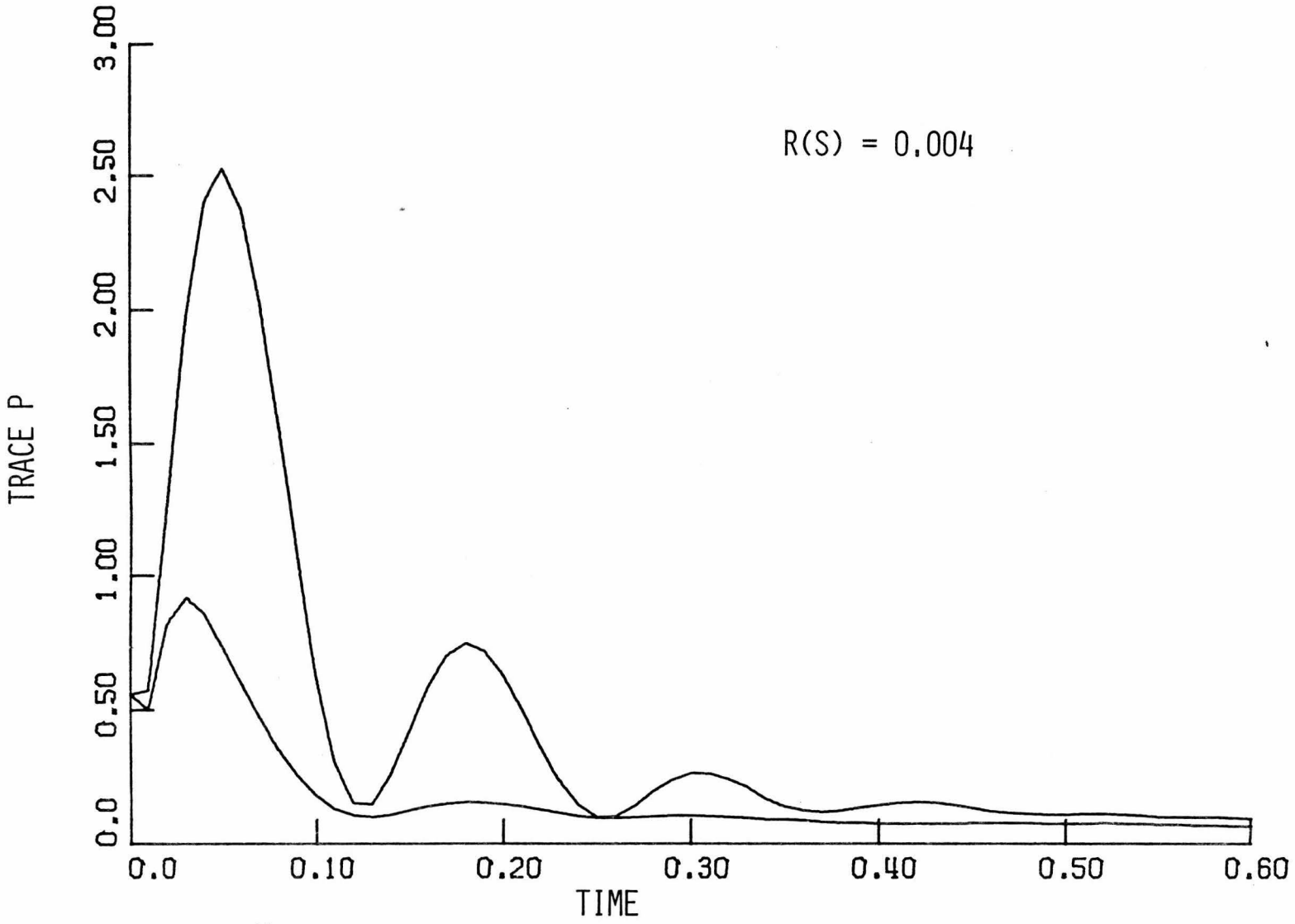

FIGURE 3.4: TRACE P AS A FUNCTION OF TIME FOR TWO SENSORS LOCATED AT (A) POSITIONS S_4 AND S_6 (B) OPTIMAL POSITIONS S_2 AND S_3

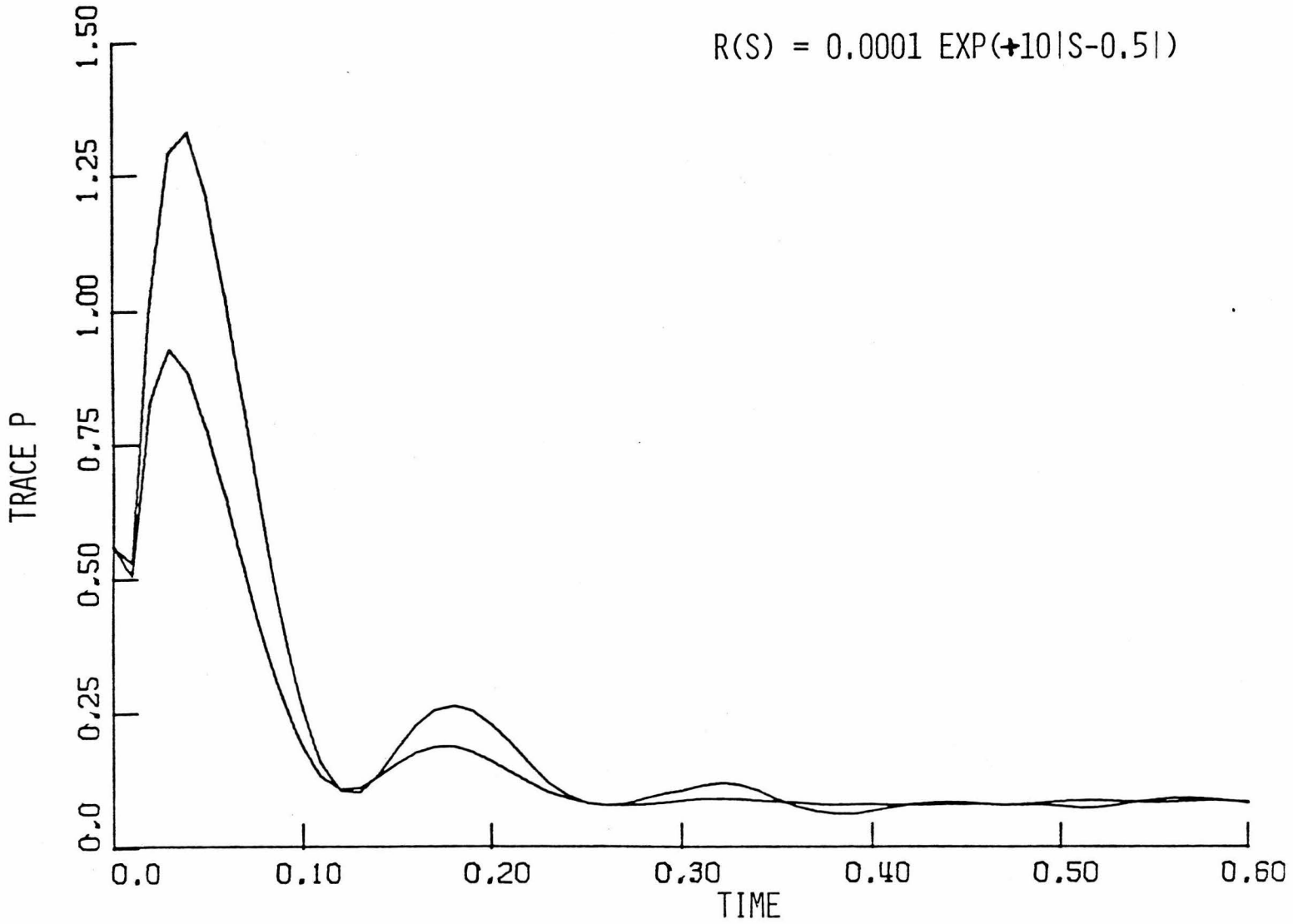

FIGURE 3.5: TRACE P AS A FUNCTION OF TIME FOR TWO SENSORS LOCATED AT (A) POSITIONS S_3 AND S_6 (B) OPTIMAL POSITIONS S_3 AND S_4

For the third case, the measurement noise variance assumes its lowest value near the center point s = 0.5 and increases exponentially as we move towards either end. The optimal sensor locations change. One sensor is still located near the hot spot while the other moves to a position of low measurement uncertainty. The plots of trace P vs. time for the initial locations and the optimal measurement locations are shown in Figures 3.3, 3.4 and 3.5.

3.6.4 Effect of System Noise

The measurement noise variance R(s) was kept fixed and the optimal sensor locations were determined for three covariance matrices Q. In the first two cases Q was taken as 0.01 I and 0.1 I, respectively. As discussed before, these choices of Q assume negligible correlation between the system model errors at different collocation points. In the third case these errors were assumed to be correlated and Q was determined from the matrix $Q^+(s,s')$ given by

$$Q^+(s,s') = \begin{bmatrix} 0.01\ \exp(-10|s-s'|) & 0 \\ 0 & 0.01\ \exp(-10|s-s'|) \end{bmatrix} \qquad (3.80)$$

This choice of Q^+ assumes that there is no correlation between the disturbances $w_c(s,t)$ and $w_T(s,t)$.

The results for the three cases are summarized in Table 3.3. The optimality index J is high in the second case because of high system noise covariance. The optimal locations remain unchanged in the three cases because the system noise Q is not a function of the spatial variable s even though the magnitude of Q is varying. Figures 3.6 and 3.7 show the

Table 3.3. Effect of Process Noise

$P_o = 0.04\ I$

$R(s) = 0.0004$

	Q	Initial Locations	Optimal Locations	No. of Iterations	Initial J	Optimal J
1	0.01 I	s_4, s_6	s_2, s_3	1	11.78×10^{-2}	3.42×10^{-2}
2	0.1 I	s_4, s_6	s_2, s_3	1	27.82×10^{-2}	7.13×10^{-2}
3	Q evaluated from (3.80)	s_4, s_6	s_2, s_3	1	12.85×10^{-2}	3.81×10^{-2}

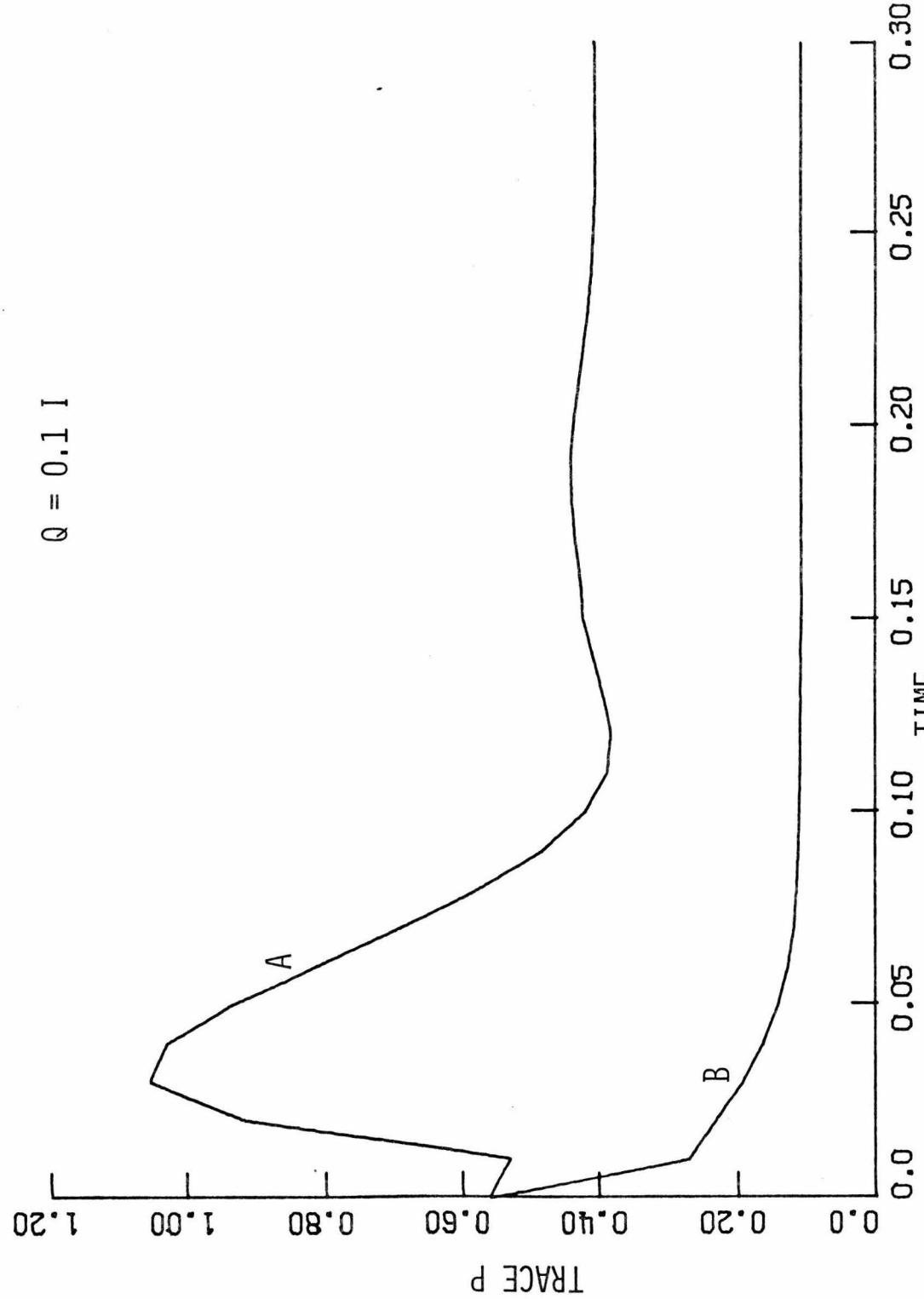

FIGURE 3.6: TRACE P AS A FUNCTION OF TIME FOR TWO SENSORS LOCATED AT (A) POSITIONS S_4 AND S_6 (B) OPTIMAL POSITIONS S_2 AND S_3

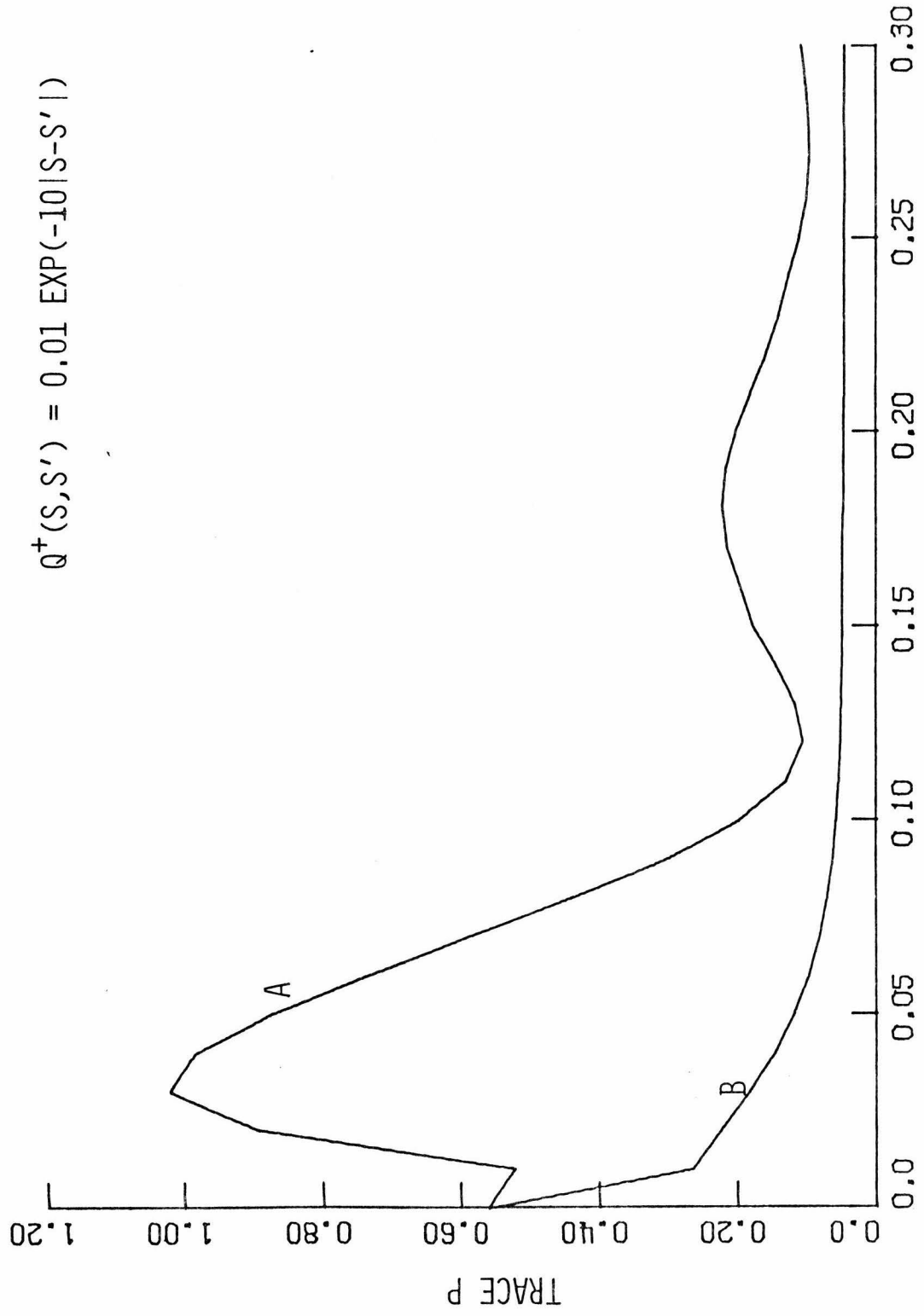

FIGURE 3.7: TRACE P AS A FUNCTION OF TIME FOR TWO SENSORS LOCATED AT (A) POSITIONS S_4 AND S_6 (B) OPTIMAL POSITIONS S_2 AND S_3

plots of trace P vs. time for the second and third case, while the plot for the first case is shown in Figure 3.3

3.6.5 Number of Sensors

Optimal locations for 1, 3, and 5 sensors were determined for the case of constant Q and R. In each case only one iteration was required. The plots of trace P vs. time for the initial and optimal sensor locations are shown in Figures 3.8, 3.9, and 3.10. Table 3.4 shows the results for the case of 1, 2, 3, and 5 sensors. From the plots it is observed that for optimally located sensors, trace P is a monotonically decreasing function of time. This implies that the concentration and temperature estimates become more accurate as more temperature measurements become available for use in estimation. The errors in the state estimate are a function of time and space. The optimally located sensors are near the region where the errors are expected to be highest. However, when the sensors are not optimally located, the measurements cannot give accurate information about the state at points far away,and therefore the total uncertainty, measured by trace P , may increase at a particular time. That is why for nonoptimally located sensors trace P is, in general, not a decreasing function of time.

The question of number of sensors required can be answered from the data in Table 3.4. We plot trace P vs. time t for 1, 2, 3, 5, and 7 optimally located sensors in Figure 3.11. From this Figure, we conclude that for the tubular reactor under consideration, very little improvement in the accuracy of the state estimate is possible by using more than two sensors. One optimally located sensor can also give good state estimates.

Table 3.4. Optimal Locations for One, Two, Three, and Five Sensors

$P_o = 0.04\ I$

$Q = 0.01\ I$

$R(s) = 0.0004$

Number of Sensors	Initial Locations	Optimal Locations	No. of Iterations	Initial J	Optimal J
1	s_8	s_2	1	36.57×10^{-2}	4.72×10^{-2}
2	s_4, s_6	s_2, s_3	1	11.78×10^{-2}	3.42×10^{-2}
3	s_4, s_6, s_7	s_2, s_3, s_4	1	11.28×10^{-2}	3.20×10^{-2}
5	s_4, s_5, s_6 s_7, s_8	s_2, s_3, s_4 s_5, s_6	1	11.10×10^{-2}	3.11×10^{-2}

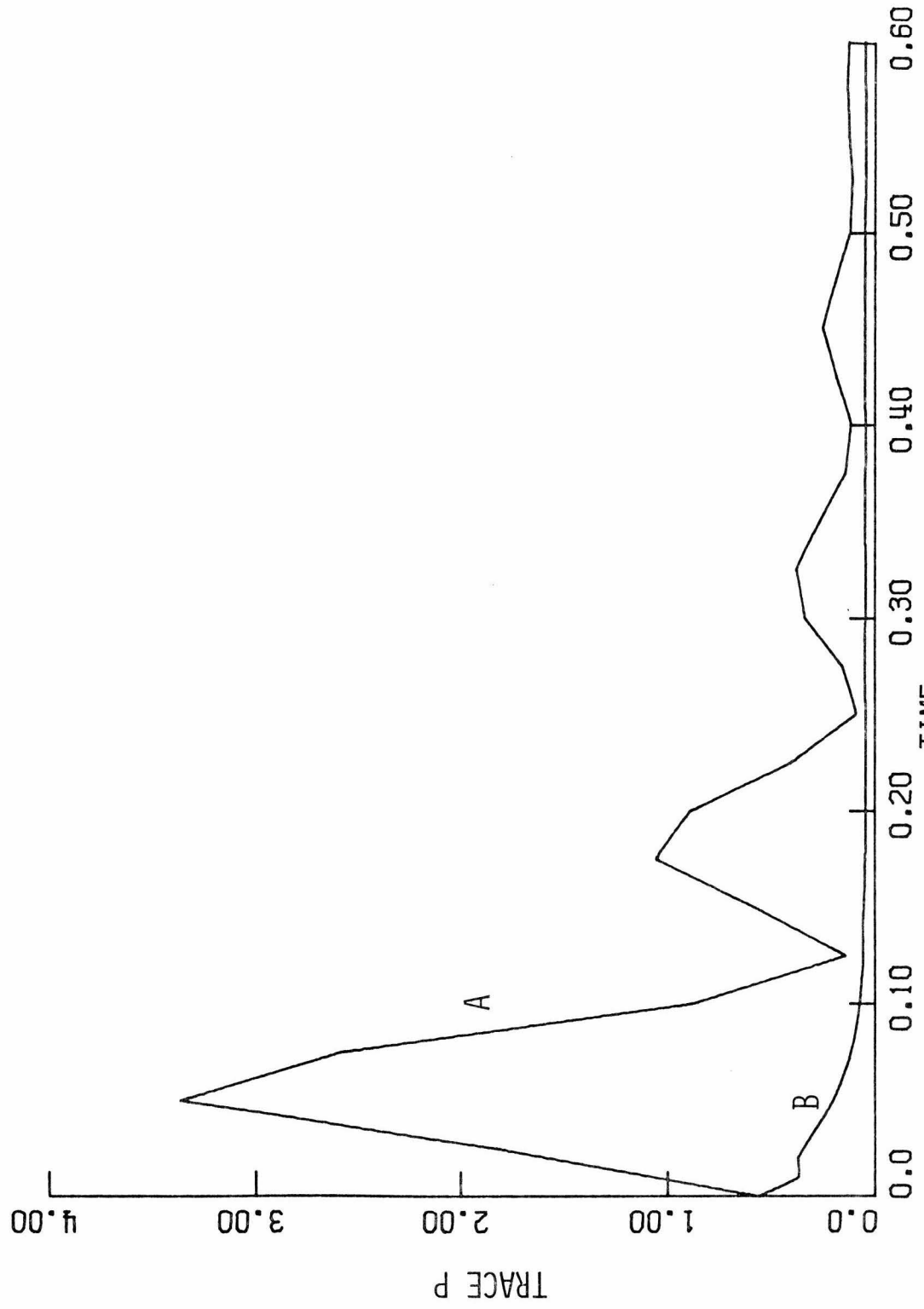

FIGURE 3.8: TRACE P AS A FUNCTION OF TIME FOR ONE SENSOR LOCATED AT (A) POSITION S_8 (B) OPTIMAL POSITION S_2

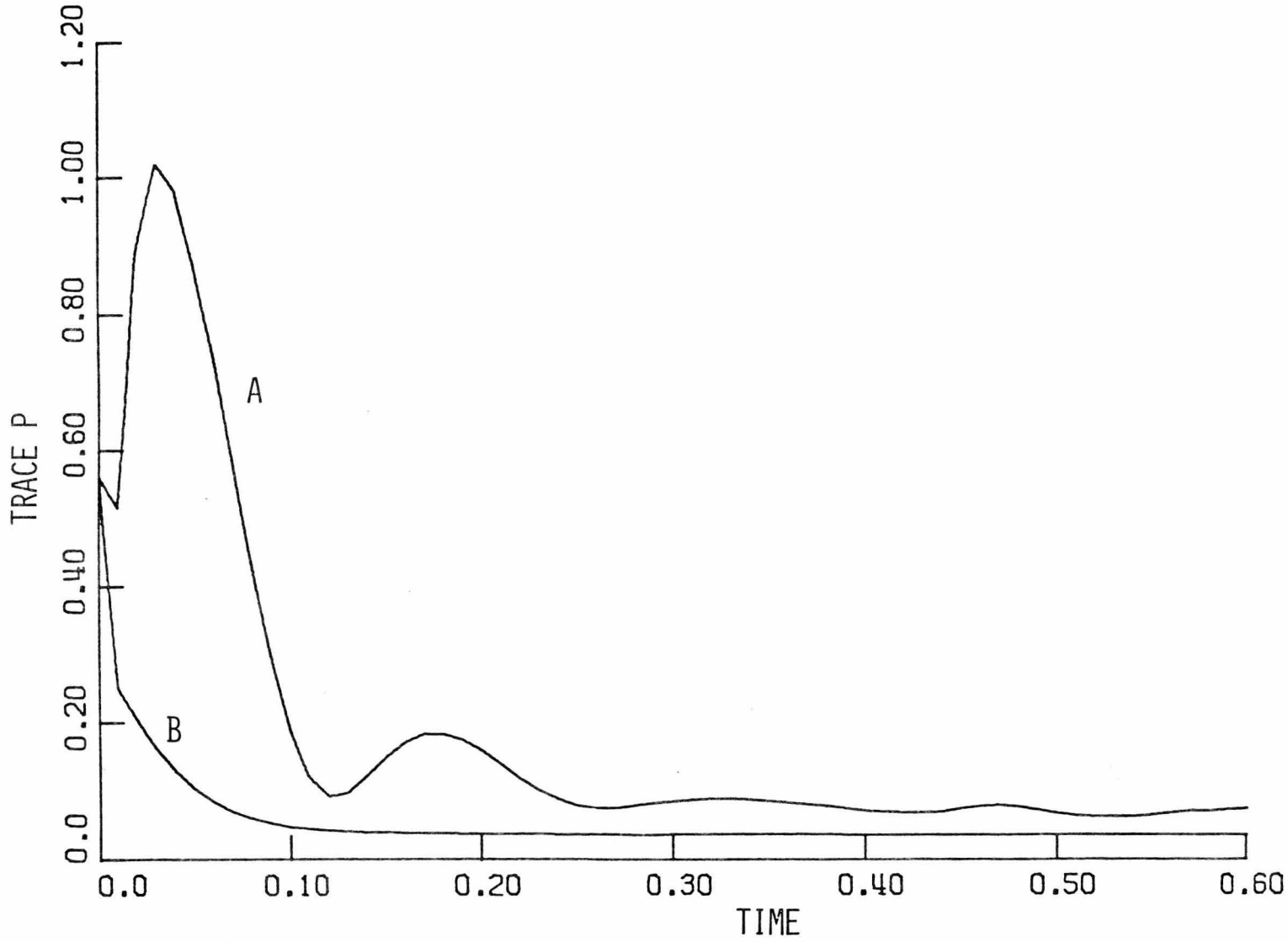

FIGURE 3.9: TRACE P AS A FUNCTION OF TIME FOR THREE SENSORS LOCATED AT (A) POSITIONS S_4, S_6, S_7 (B) OPTIMAL POSITIONS S_2, S_3, S_4

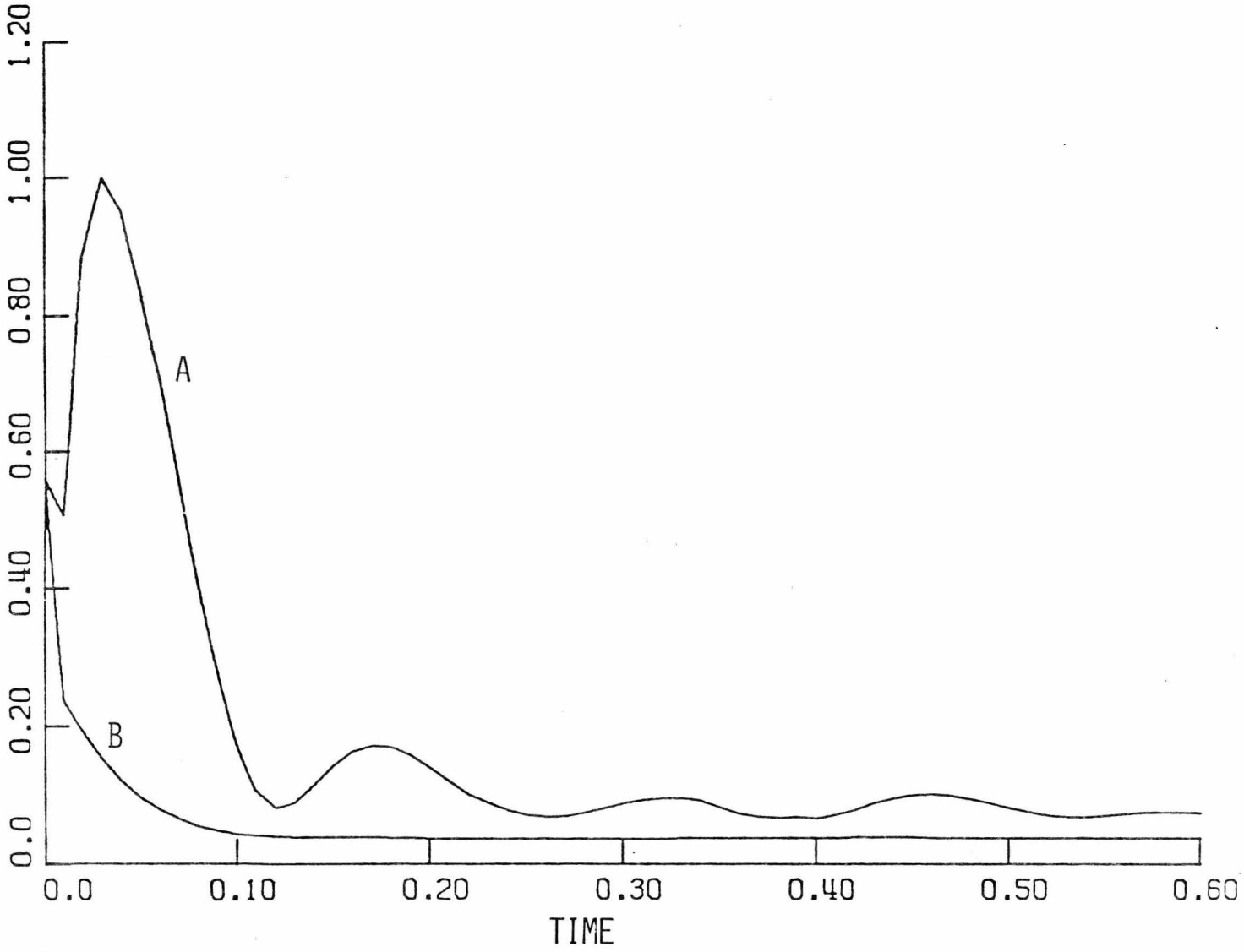

FIGURE 3.10: TRACE P AS A FUNCTION OF TIME FOR FIVE SENSORS LOCATED AT (A) POSITIONS S_4, S_5, S_6, S_7, S_8 (B) OPTIMAL POSITIONS S_2, S_3, S_4, S_5, S_6

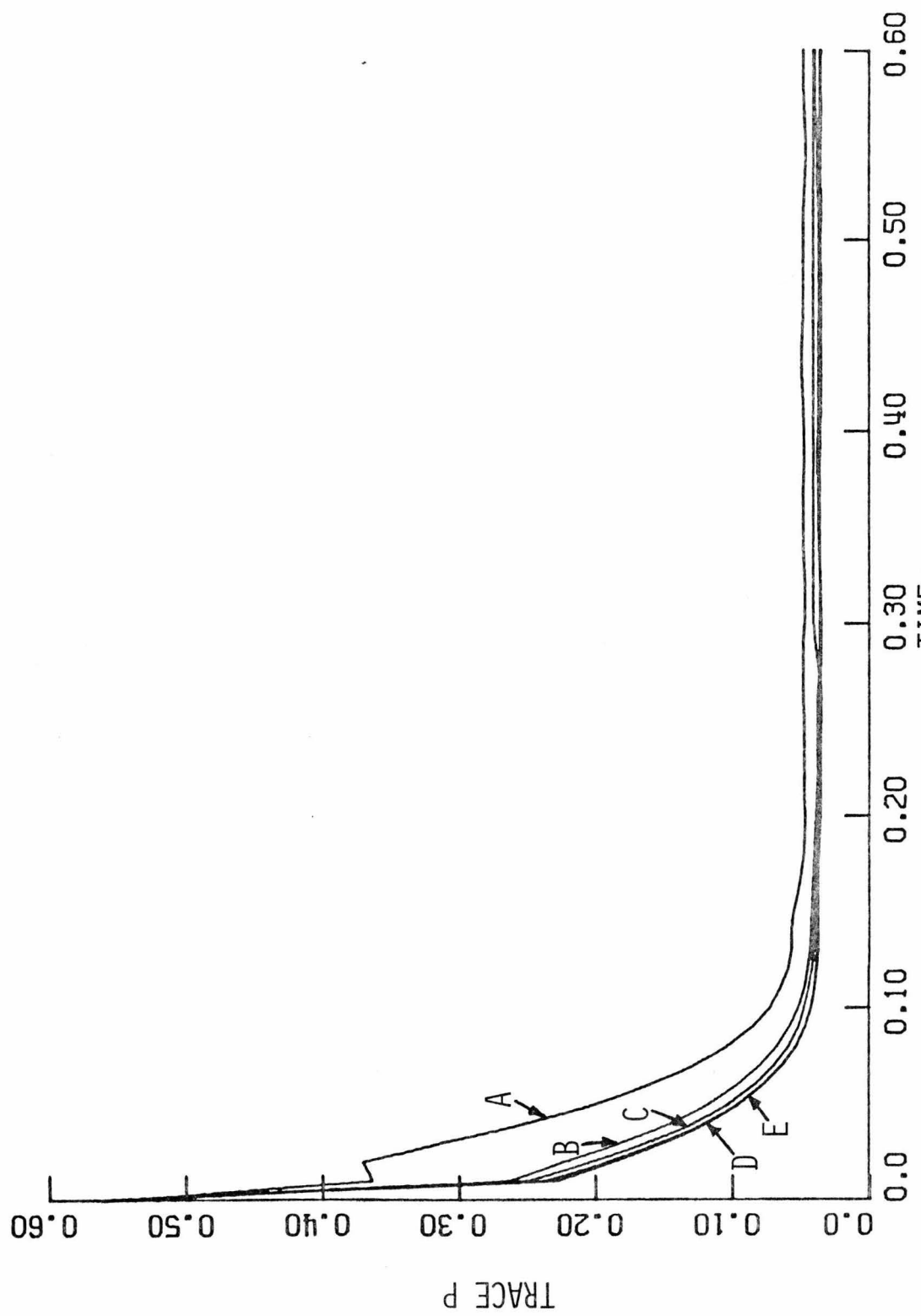

FIGURE 3.11: TRACE P AS A FUNCTION OF TIME FOR (A) ONE (B) TWO (C) THREE (D) FIVE, AND (E) SEVEN OPTIMALLY LOCATED SENSORS

However, as is evident from the results in Table 3.4, even five sensors with arbitrary locations may not give an estimate as accurate as provided by just one optimally located sensor.

3.6.6 Accuracy of Concentration and Temperature Estimates

The tubular reactor is a system with two state variables, concentration and temperature. The trace of the covariance matrix P(t) is a measure of the total uncertainty at time t in the estimates of concentration and temperature profiles. The uncertainties in the concentration and temperature estimates are measured by trace $P_c(t)$ and trace $P_T(t)$ respectively, where

$$\text{Tr } P_c(t) = \sum_{i=1}^{N} P_{2i-1,2i-1}(t)$$

and, (3.81)

$$\text{Tr } P_T(t) = \sum_{i=1}^{N} P_{2i,2i}(t)$$

Since the concentration and temperature equations are coupled, we can obtain good estimates of the concentration profiles even though only temperature is being measured. In Figures 3.12-3.16, we plot trace P, trace P_c and trace P_T vs. time for optimally located 1, 2, 3, 5 and 7 sensors. In each case all the three variables being plotted are decreasing functions of time. The concentration estimates also become better with time as more temperature measurements are made available. At the steady state, trace P_c is larger than trace P_T. This is an expected result

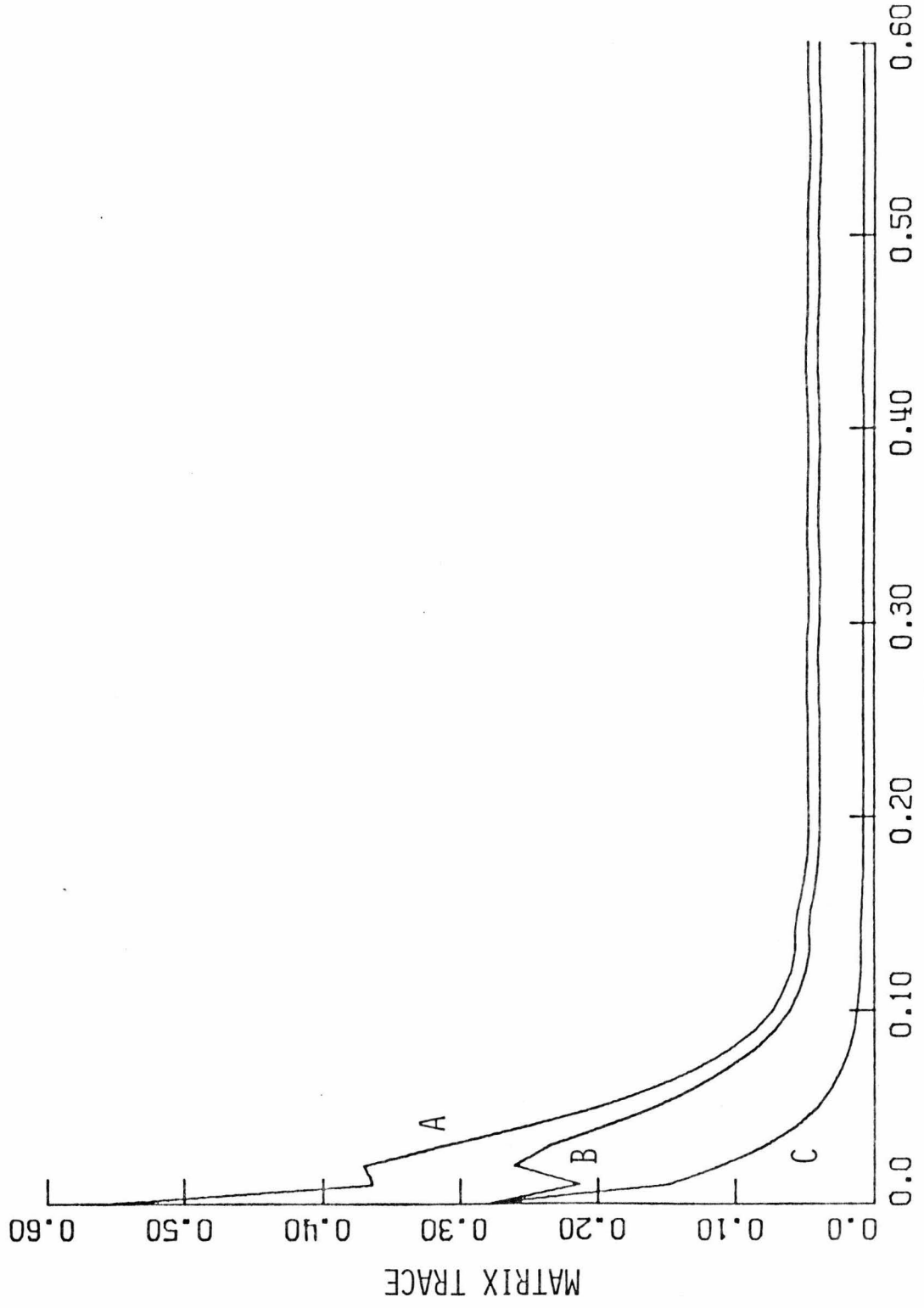

FIGURE 3.12: (A) TRACE P (B) TRACE P_C AND (C) TRACE P_T AS FUNCTIONS OF TIME FOR ONE OPTIMALLY LOCATED SENSOR

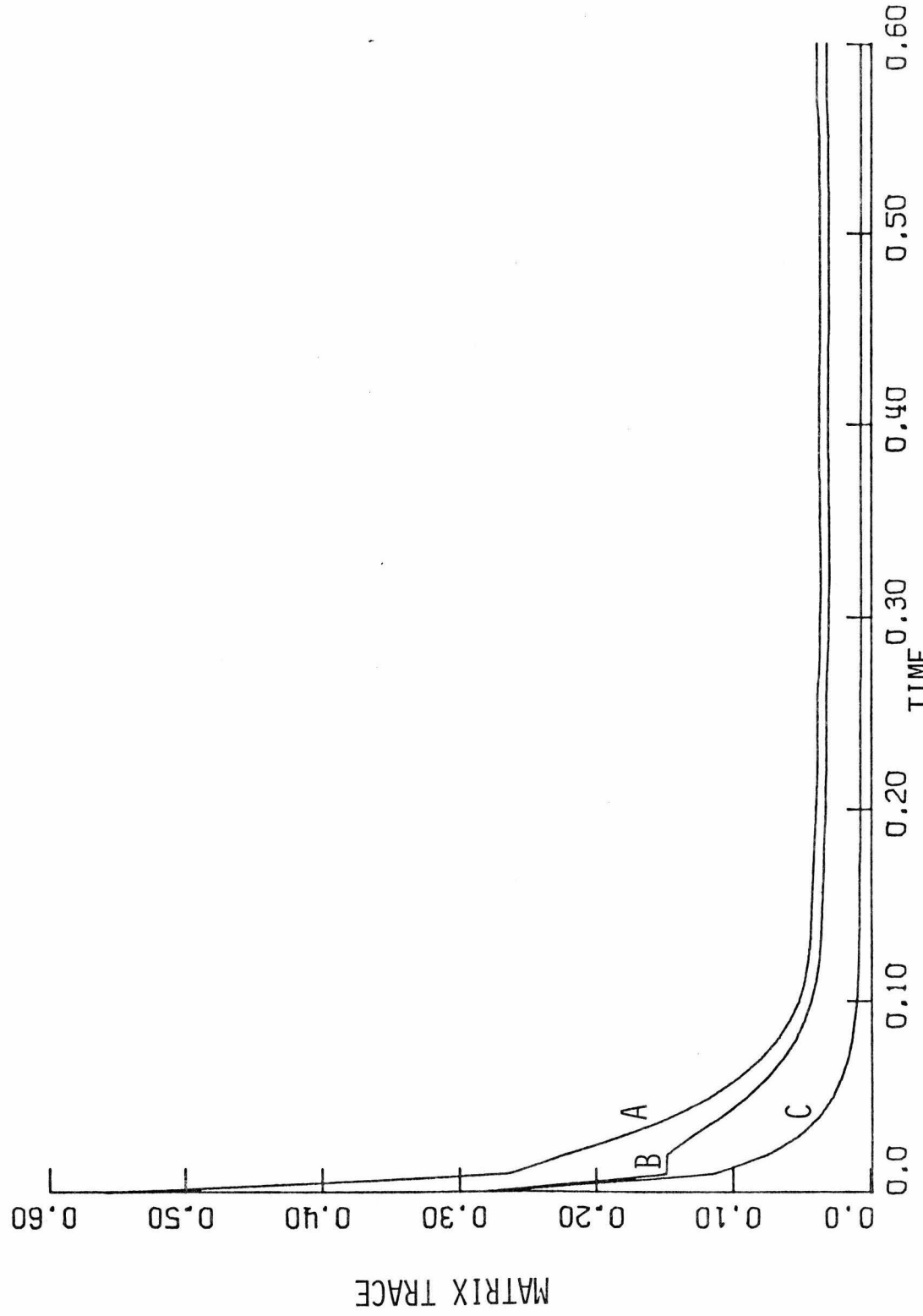

FIGURE 3.13: (A) TRACE P(B) TRACE P_C, AND (C) TRACE P_T AS FUNCTIONS OF TIME FOR TWO OPTIMALLY LOCATED SENSORS

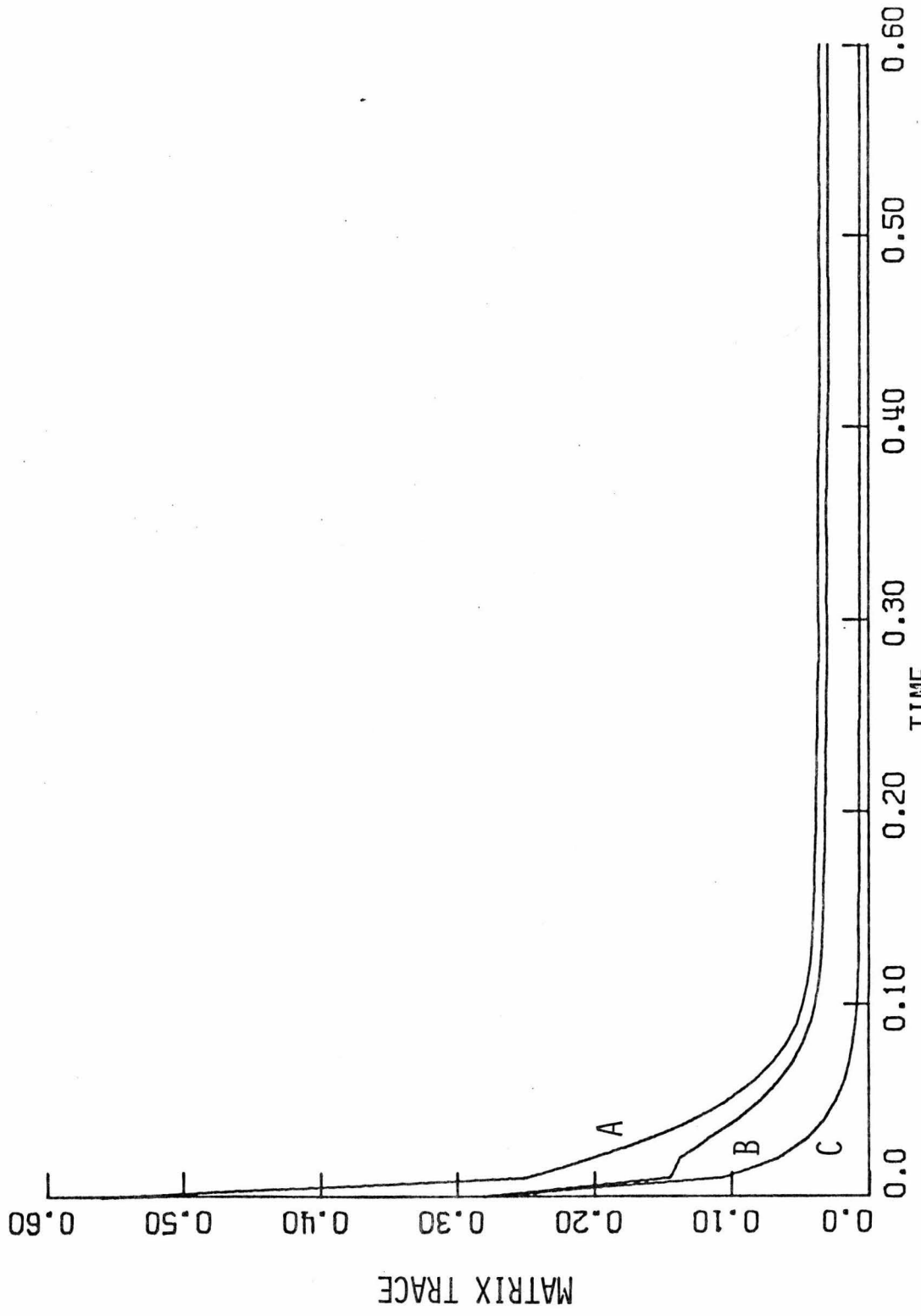

FIGURE 3.14: (A) TRACE P (B) TRACE P_C (C) TRACE P_T AS FUNCTIONS OF TIME FOR THREE OPTIMALLY LOCATED SENSORS

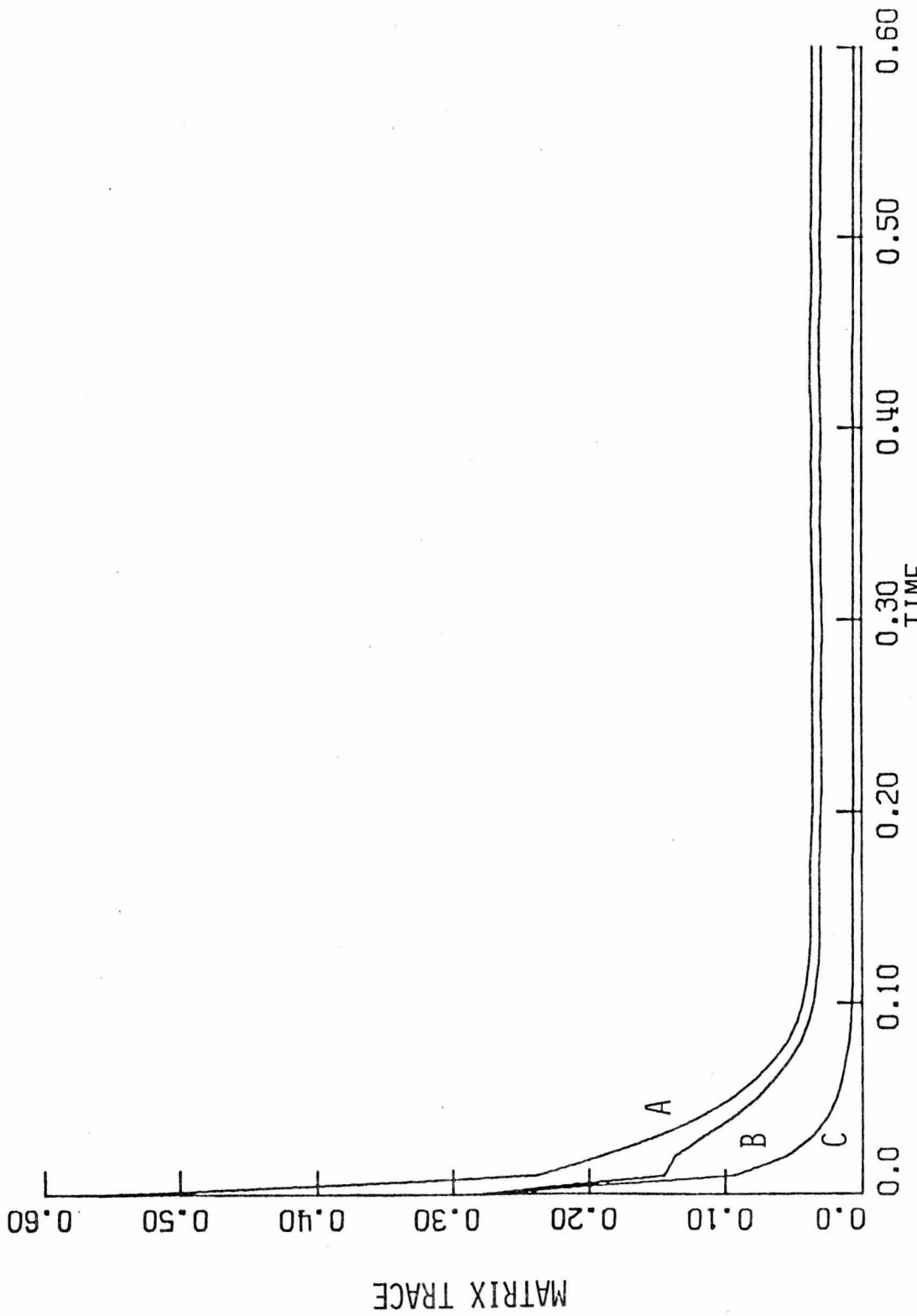

FIGURE 3.15: (A) TRACE P (B) TRACE P_C, AND (C) TRACE P_T AS FUNCTIONS OF TIME FOR FIVE OPTIMALLY LOCATED SENSORS

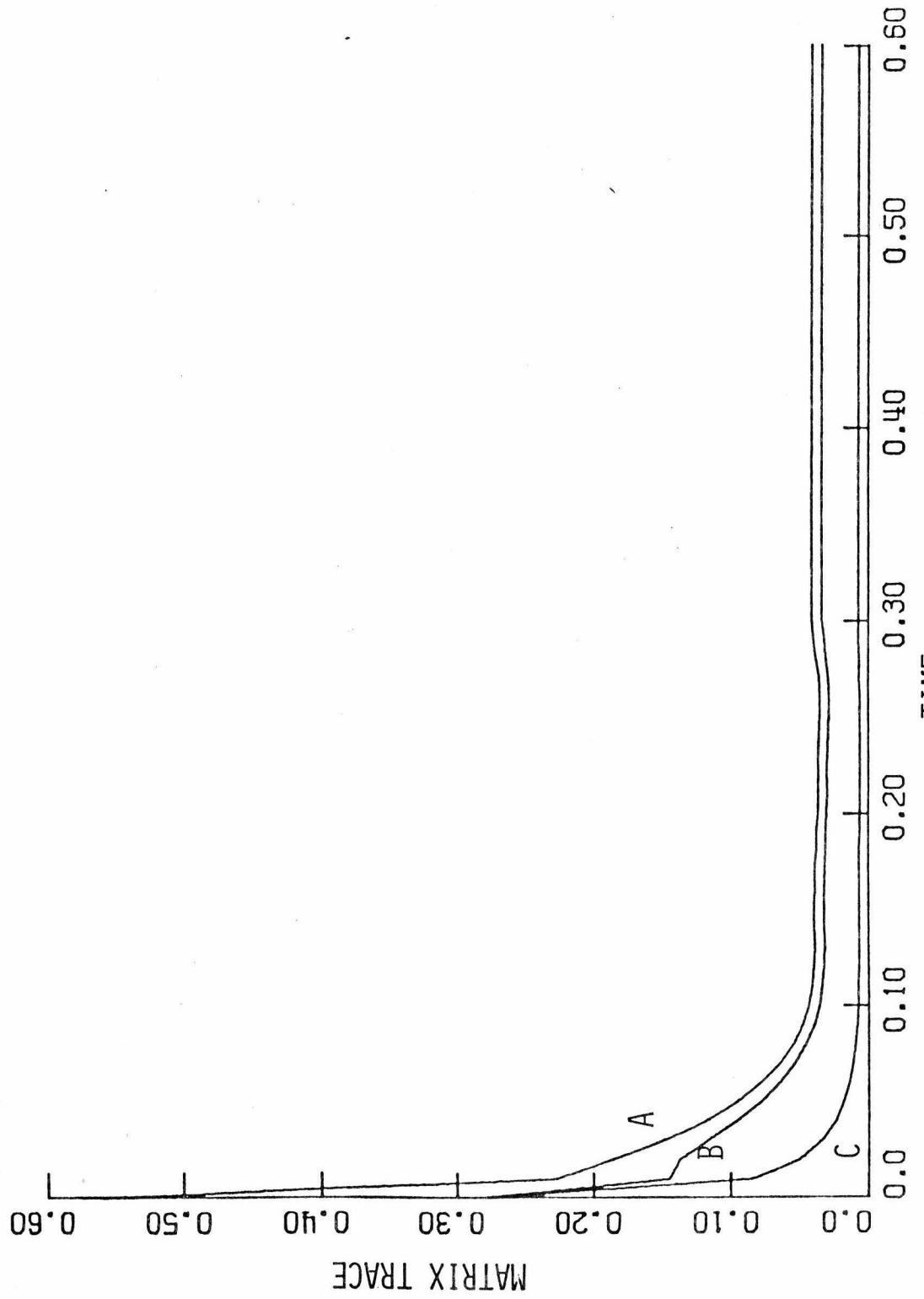

FIGURE 3.16: (A) TRACE P (B) TRACE P_C, AND (C) TRACE P_T AS FUNCTIONS OF TIME FOR SEVEN SENSORS

since we are making only temperature measurements and estimating both temperature and concentration from these measurements. For all the cases in Figures 3.12 - 3.16, the steady state trace P_C is about 4 to 5 times the steady state trace P_T.

3.7 Summary

In this Chapter, we have studied the problem of optimal sensor locations for a non-adiabatic tubular reactor. The concentration and temperature equations are discretized by the orthogonal collocation method and the optimal sensor locations are determined by employing the matrix minimum principle. A detailed example is considered and the effect of process noise and measurement noise on the optimal locations is studied. We have also looked at the question of number of sensors required for estimating the concentration and temperature profiles to a desired accuracy.

CHAPTER 4

SUMMARY AND RECOMMENDATIONS

In this work, we have considered the problem of optimal measurement system design in distributed parameter systems. The measurement system design problem has been treated within the framework of estimation theory with the objective of estimating the system states as accurately as possible.

An upper bound for the error covariance of state estimate has been developed. The optimal sensor location problem is then posed as a minimization problem for a scalar measure of this upper bound. The use of this upper bound enables us to simplify considerably the computational aspects of the problem. This approach has been illustrated by an example involving one-dimensional heat conduction. The effect of process dynamics on optimal sensor locations has been clearly demonstrated, and it is shown that the state estimates can be considerably improved by proper choice of sensor locations.

The optimal sensor location problem for a tubular chemical reactor has also been considered. Chemical reactors are an integral part of the process industry and the knowledge of concentration and temperature profiles is often required. The sensor location problem for this system is very interesting because it has two state variables, concentration and temperature, which are coupled through the mass and energy balance equations. The optimal locations of sensors in this system have been determined based on an initial discretization of the system equations. The accuracy of concentration and temperature estimates depends strongly on the sensor locations. For spatially invariant error statistics, the optimal sensor locations are governed mainly by process dynamics. The

feasibility of estimating both concentration and temperature profiles based on temperature measurements only has been investigated. It has been shown that the concentration profiles can indeed be estimated quite accurately on the basis of temperature measurements. The question of the number of temperature sensors necessary for an accurate estimation of the profiles has also been investigated.

Most systems of interest in the process industry are distributed in nature and are often described by more than one state variable. The optimal sensor locations for these processes can be determined by using the approach developed in Chapter 3. The equations describing the system can be discretized using a low-order discretization method and the sensor locations can be selected using the same approach. The approach developed here can be used for selecting optimal sensor locations in a general process system. The optimal control problem for a dynamic process is the dual of the optimal estimation problem. Therefore, the problem of optimal pointwise controls can be approached in a way similar to the optimal sensor location problem. It is hoped that the approach developed here will find potential applications in the optimal location of pointwise controls.

In addition to the problem of optimal location of pointwise controls, some other interesting areas of research are the following:

- The problem of the number of sensors required for a given accuracy in state estimate should be further investigated. By properly assigning a value to improved estimate accuracy, and comparing it to the cost of adding more sensors, the cost-effective number of sensors can be determined.

— Sensor location problem can be investigated based on other objectives. The location of sensors with the objective of "best" estimating certain spatially varying parameters in the systems is an important area of research.

— In this work, we have dealt with the case of measurements continuous in time. However, in certain situations continuous measurements may be very costly. For such systems, the determination of optimal timing and frequency of measurements should be investigated.

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APPENDIX A

This appendix gives the proof of the inequality (2.53). The optimal filter for the process with spatially independent integral measurements is given by (2.32) and (2.33), where $u(x,t)$ is the optimal estimate of the state $u(x,t)$, and $P(x,y,t)$ is the error covariance matrix. Let us now consider two processes described by the following equations:

$$\frac{\partial u^I(x,t)}{\partial t} = A_x\, u^I(x,t) + B(x,t)w(x,t) \tag{A.1}$$

(Process I)

$$z^I(t) = \int_D H(x,t)u^I(x,t)\, dx \tag{A.2}$$

$$\text{I.C.} \qquad u^I(x,t_o) = 0 \tag{A.3}$$

$$\text{B.C.} \qquad \alpha_x\, u^I(x,t) = 0 \qquad x \in \partial D\ . \tag{A.4}$$

$$\frac{\partial u^{II}(x,t)}{\partial t} = A_x\, u^{II}(x,t) \tag{A.5}$$

(Process II)

$$z^{II}(t) = \int_D H(x,t)u^{II}(x,t)\, dx + v(t) \tag{A.6}$$

$$\text{I.C.} \qquad E[u^{II}(x,t_o)] = \bar{u}_o(x)$$

$$E[\{u^{II}(x,t_o)-\bar{u}_o(x)\}\{u^{II}(y,t_o)-\bar{u}_o(y)\}^T] = P_o(x,y) \tag{A.7}$$

$$\text{B.C.} \qquad \alpha_x\, u^{II}(x,t) = 0 \qquad x \in \partial D \tag{A.8}$$

We note that

$$u(x,t) = u^{I}(x,t) + u^{II}(x,t) \tag{A.9}$$

and process II is simply the original process with no dynamic noise. Let us now define the suboptimal estimates $\hat{u}^{I}(x,t)$ and $\hat{u}^{II}(x,t)$ for the two processes, utilizing the gain matrix for the optimal estimate $\hat{u}(x,t)$ of the original system. The suboptimal estimates for the two processes are governed by

$$\frac{\partial \hat{u}^{I}(x,t)}{\partial t} = A_x\, \hat{u}^{I}(x,t)$$

$$+ \int_D P(x,x',t)H^{T}(x',t)R^{-1}(t)\left[z^{I}(t) - \int_D H(y',t)\hat{u}^{I}(y',t)dy' \right] dx' \tag{A.10}$$

$$\text{I.C.} \qquad \hat{u}^{I}(x,t_o) = 0 \tag{A.11}$$

$$\text{B.C.} \qquad \alpha_x\, \hat{u}^{I}(x,t_o) = 0 \qquad x \in \partial D \tag{A.12}$$

$$\frac{\partial \hat{u}^{II}(x,t)}{\partial t} = A_x\, \hat{u}^{II}(x,t) + \int_D P(x,x',t)H^{T}(x',t)R^{-1}(t)\left[z^{II}(t) - \int_D H(y',t)\hat{u}^{II}(y',t)\, dy' \right] dx' \tag{A.13}$$

$$\text{I.C.} \qquad \hat{u}^{II}(x,t_o) = \bar{u}_o(x) \tag{A.14}$$

$$\text{B.C.} \qquad \alpha_{\cdot}\, \hat{u}^{II}(x,t) = 0 \qquad x \in \partial D \tag{A.15}$$

Note that in equations (A.10) and (A.13), $P(x,x',t)$ is the error covariance for the optimal estimate $\hat{u}(x,t)$ in (2.32). The optimal estimate $\hat{u}(x,t)$ of the original process and the suboptimal estimates $\hat{u}^{I}(x,t)$ and $\hat{u}^{II}(x,t)$ of the processes I and II obey the relationship $\hat{u}(x,t) = \hat{u}^{I}(x,t) + u^{II}(x,t)$. In terms of the estimate errors, we have $\tilde{u}(x,t) = \tilde{u}^{I}(x,t) + \tilde{u}^{II}(x,t)$. The covariance matrix $P(x,y,t)$ is, by definition

$$\begin{aligned} P(x,y,t) &= E[\tilde{u}(x,t)\tilde{u}^{T}(y,t)] \\ &= P^{I}(x,y,t) + P^{II}(x,y,t) + E[\{\tilde{u}^{I}(x,t)\}\{\tilde{u}^{II}(y,t)\}^{T}] \\ &\quad + E[\{\tilde{u}^{II}(x,t)\}\{\tilde{u}^{I}(y,t)\}^{T}] \end{aligned} \tag{A.16}$$

where $P^{I}(x,y,t)$ and $P^{II}(x,y,t)$ are the error covariance matrices for the estimates $\hat{u}^{I}(x,t)$ and $\hat{u}^{II}(x,t)$ of the states $u^{I}(x,t)$ and $u^{II}(x,t)$, respectively. The cross-variance terms, $E[\{\tilde{u}^{I}(x,t)\}\{\tilde{u}^{II}(y,t)\}^{T}]$ and $E[\{\tilde{u}^{II}(x,t)\}\{\tilde{u}^{I}(y,t)\}^{T}]$ are zero each because the two processes are forced by uncorrelated white-noise processes and have uncorrelated initial conditions. Therefore

$$P(x,y,t) = P^{I}(x,y,t) + P^{II}(x,y,t) \tag{A.17}$$

If we use a suboptimal gain to obtain an estimate for the state $u(x,t)$ with corresponding error covariance matrix $P^{S}(x,y,t)$, we must have $P(x,y,t) \leq P^{S}(x,y,t)$. Using the same suboptimal gain for obtaining estimates of the states $u^{I}(x,t)$ and $u^{II}(x,t)$ with error covariances

$P^{Is}(x,y,t)$ and $P^{IIs}(x,y,t)$, we shall have the relation

$$P(x,y,t) \leq P^{Is}(x,y,t) + P^{IIs}(x,y,t) \tag{A.18}$$

We choose the suboptimal gain to be the gain that yields an optimal estimate for the process II, and use the same gain for state estimation in process I. Let us denote the error covariance $P^{IIs}(x,y,t)$ for the optimal estimate of process II by $\overline{P}(x,y,t)$. The error covariance matrix $P^{Is}(x,y,t)$ for process I cannot be larger than the error covariance $W(x,y,t)$ for an estimate obtained by using zero gain. The matrix $W(x,y,t)$ is governed by the equation

$$\frac{\partial W(x,y,t)}{\partial t} = A_x\, W(x,y,t) + W(x,y,t)\, A_y^T + B(x,t)Q(x,y,t)B^T(y,t) \tag{A.19}$$

$$\text{I.C.} \qquad W(x,y,t_o) = 0 \tag{A.20}$$

$$\begin{aligned} &\text{B.C.} && \alpha_x\, W(x,y,t) = 0 && x \in \partial D && y \in D \times \partial D \\ &&& W(x,y,t)\, \alpha_y^T = 0 && y \in \partial D && x \in D \times \partial D \end{aligned} \tag{A.21}$$

It can be easily verified that the solution to (A.19)-(A.21) is given by (2.54). The inequality (2.53) is thus proved.

APPENDIX B

In this appendix we verify the validity of (2.58) as a solution of the equations (2.55)-(2.57). From equation (2.58)

$$\bar{P}(x,y,t_o) = \iint_{DD} G(x,t_o;x',t_o)[P_o^{\dagger}(x',y') + M(x',y',t_o)]^{\dagger}G^{T}(y,t_o;y',t_o)\, dy'dx' \tag{B.1}$$

Using the fact that $M(x,y,t_o) = 0$, and $G(x,t_o;x',t_o) = I\,\delta(x-x')$, we get $\bar{P}(x,y,t_o) = P_o(x,y)$. The initial condition (2.56) is thus verified. Boundary conditions (2.57) can be easily verified by using the properties of the Green's function matrix $G(x,t;x',t')$. To verify that the $\bar{P}(x,y,t)$ given by (2.58) obeys the partial differential equation (2.55) we shall need, in addition to the properties of the Green's function matrix, the following identity

$$\frac{\partial A^{\dagger}(x,y,t)}{\partial t} = -\iint_{DD} A^{\dagger}(x,x',t)\,\frac{\partial A(x',y',t)}{\partial t}\,A^{\dagger}(y',y,t)\, dy'dx' \tag{B.2}$$

Differentiating (2.58) with respect to t, and using the properties of the Green's function matrix, we have

$$\frac{\partial \bar{P}(x,y,t)}{\partial t} = A_x\,\bar{P}(x,y,t) + \bar{P}(x,y,t)\,A_y^{T}$$

$$+ \iint_{DD} G(x,t;x',t_o)\,\frac{\partial}{\partial t}\left[P_o^{\dagger}(x',y') + M(x',y',t)\right]^{\dagger} G^{T}(y,t;y',t_o)\, dy'dz' \tag{B.3}$$

Using the identity (B.2), the last term on the r.h.s. of (B.3) is

$$- \iint_{DD} G(x,t;x',t_o) \iint_{DD} \left[P_o^{\dagger}(x',x") + M(x',x",t)\right]^{\dagger} \frac{\partial}{\partial t}\left[M(x",y",t)\right]$$

$$\cdot\left[P_o^{\dagger}(y",y') + M(y",y',t)\right]^{\dagger} G^T(y,t;y',t_o)\, dy"dx"\, dy'dx'$$

$$= -\iint_{DD} G(x,t;x',t_o) \iint_{DD} \left[P_o^{\dagger}(x',x") + M(x',x",t)\right]^{\dagger} \left[\sum_{i,j=1}^{m} G^T(n_i,t;x",t_o)\, H_i^T(t)\right.$$

$$\left.\cdot(R^{-1}(t))_{ij}\, H_j(t) G(n_j,t;y",t_o)\right] \left[P_o^{\dagger}(y",y') + M(y",y',t)\right]^{\dagger} G^T(y,t;y',t_o)$$

$$dy"dx"\, dy'dx'$$

$$= -\sum_{i,j=1}^{m} \left\{\int_D \int_D G^T(x,t;x',t_o)\left[P_o^{\dagger}(x',x") + M(x',x",t)\right]^{\dagger} G^T(n_i,t;x",t_o)\, dx"dx'\right\}$$

$$\cdot\left\{H_i^T(t)(R^{-1}(t))_{ij}\, H_j(t)\right\}\left\{\iint_{DD} G(n_j,t;y",t_o)\left[P_o^{\dagger}(y",y') + M(y",y',t)\right]^{\dagger}\right.$$

$$\left.\cdot G^T(y,t;y',t_o)\, dy"dy'\right\}$$

$$= -\sum_{i,j=1}^{m} \left\{\bar{P}(x,n_i,t)\right\}\left\{H_i^T(t)(R^{-1}(t))_{ij}\, H_j(t)\right\}\left\{\bar{P}(n_j,y,t)\right\}$$

Thus we get

$$\frac{\partial \bar{P}(x,y,t)}{\partial t} = A_x\, \bar{P}(x,y,t) + \bar{P}(x,y,t)\, A_y^T - \sum_{i,j=1}^{m} \bar{P}(x,n_i,t) H_i^T(t)(R^{-1}(t))_{ij}$$

$$\cdot H_j(t)\bar{P}(n_j,y,t)$$

(B.4)

The expression (2.58) for $\overline{P}(x,y,t)$ thus obeys the partial differential equation (2.55) with initial condition and boundary conditions given by (2.56) and (2.57).

APPENDIX C

In this appendix, we derive the discrete equations (3.37) - (3.38) for the tubular reactor. As expressed in (3.35) the first and second derivatives of concentration at the collocation points s_i, i = 1,2,..., N' where N' = N+2, are given by

$$\left.\frac{\partial c}{\partial s}\right|_{s_i} = \sum_{j=1}^{N'} A_{ij}\, c_j(t)$$

$$\left.\frac{\partial^2 c}{\partial s^2}\right|_{s_i} = \sum_{j=1}^{N'} B_{ij}\, c_j(t) \qquad (C.1)$$

The boundary conditions at s=0 and s=1 provide the equations

$$\sum_{j=1}^{N'} A_{1j}\, c_j = P_{e_m}\,(c_1 - 1) \qquad (C.2)$$

$$\sum_{j=1}^{N'} A_{N'j}\, c_j = 0 \qquad (C.3)$$

Equations (C.2) and (C.3) allow us to express the concentrations c_1 and $c_{N'}$ at the boundaries in terms of the concentrations at the interior collocation points.

$$c_1 = \eta_1 \left[\sum_{k=2}^{N+1} (A_{1N'}A_{N'k} - A_{N'N'}A_{1k})\, c_k - P_{e_m}\, A_{N'N'} \right] \qquad (C.4)$$

$$\text{and} \quad c_{N'} = \eta_1 \left[\sum_{k=2}^{N+1} (A_{N'1}\, A_{1k} - (A_{11} - P_{e_m})\, A_{N'k})\, c_k + P_{e_m} A_{N'1} \right] \qquad (C.5)$$

where

$$\eta_1 = 1 \Big/ \left[A_{N'N'}(A_{11} - P_{e_m}) - A_{1N'} A_{N'1} \right]$$

Using (C.1) and (3.8), we find that the concentrations c_j at the interior collocation points are governed by the equations

$$\frac{dc_j}{dt} = \sum_{k=1}^{N'} B_{jk} c_k - P_{e_m} \sum_{k=1}^{N'} A_{jk} c_k - \alpha r(c_j, T_j) \qquad (C.6)$$

$$(j = 1,2,\ldots, N')$$

The equations (C.4) and (C.5) can be used to eliminate c_1 and $c_{N'}$. Thus, we get

$$\frac{dc_j}{dt} = \sum_{k=2}^{N+1} D_{jk} c_k - \alpha r(c_j, T_j) + p_j \qquad (C.7)$$

$$(j = 2,3,\ldots, N+1)$$

where

$$\begin{aligned}
D_{jk} &= (B_{jk} - P_{e_m} A_{jk} + \eta_1 W_{jk}) \\
p_j &= \eta_1 P_{e_m} \left[A_{N'1}(B_{jN'} - P_{e_m} A_{jN'}) - A_{N'N'} (B_{j1} - P_{e_m} A_{j1}) \right] \\
W_{jk} &= (B_{j1} - P_{e_m} A_{j1})(A_{1N'} A_{N'k} - A_{N'N'} A_{1k}) \\
&\quad + (B_{jN'} - P_{e_m} A_{jN'}) \left[A_{N'1} A_{1k} - (A_{11} - P_{e_m}) A_{N'k} \right]
\end{aligned} \qquad (C.8)$$

The equations for temperature T_j at the interior collocation points can similarly be obtained. We get

$$Le \frac{dT_j}{dt} = \sum_{k=2}^{N+1} S_{jk} T_k + \alpha\beta r(c_j,T_j) + \gamma(T_a-T_j) + q_j \qquad (C.9)$$

$$(j = 2,3,\ldots, N+1)$$

where

$$S_{jk} = B_{jk} - P_{e_h} A_{jk} + \eta_2 W'_{jk}$$

$$q_j = \eta_2 P_{e_h} \left[A_{N'1}(B_{jN'} - P_{e_h} A_{jN'}) - A_{N'N'}(B_{j1} - P_{e_h} A_{j1}) \right] \qquad (C.10)$$

$$W'_{jk} = (B_{j1} - P_{e_h} A_{j1})(A_{1N'} A_{N'k} - A_{N'N'} A_{1k})$$

$$+ (B_{jN'} - P_{e_h} A_{jN'}) \left[A_{N'1} A_{1k} - (A_{11} - P_{e_h}) A_{N'k} \right]$$

and

$$\eta_2 = 1 \Big/ \left[A_{N'N'}(A_{11} - P_{e_h}) - A_{1N'} A_{N'1} \right]$$

for the case of Le = 1, we get

$$\frac{dT_j}{dt} = \sum_{k=2}^{N+1} S_{jk} T_k + \alpha\beta r(c_j,T_j) + \gamma(T_a-T_j) + q_j \qquad (C.11)$$

In fact for this case $S_{jk} = D_{jk}$ and $q_j = p_j$.