THE THEORY OF MULTIPLE MEASUREMENTS TECHNIQUES IN DISTRIBUTED PARAMETER SYSTEMS

BY

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ABSTRACT

A comprehensive theory of multiple measurements for the optimum on-line state estimation and parameter identification in a class of noisy, dynamic distributed systems, is developed in this study. Often in practical monitoring and control problems, accurate measurements of a critical variable are not available in a desired form or at a desired sampling rate. Rather, noisy independent measurements of related forms of the variable may be available at different sampling rates. Multiple measurements theory thus involves the optimum weighting and combination of different types of available measurements. One of the contributions of this work is the development of a unique measurement projection method by which off-line measurements may be optimally utilized for on-line estimation and control.

The analysis of distributed systems often requires the establishment of monitoring stations. Another contribution of this study is the development of a measurement strategy, based on statistical experimental design techniques, for the optimum spatial monitoring stations in a class of distributed systems.

By incorporating in the optimization criterion, terms representing the realistic costs of making observations, an algorithm is developed for an estimator indicator whose values dictate an observation strategy for the optimum number and temporal intervals of observations. This, along with the optimum measurement stations thus provides a comprehensive monitoring policy on which the estimation and control of a distributed system may be based.

By employing the measurement projection scheme and the monitoring policy, algorithms are further developed for Kalman-type distributed filters for the estimation of the state profiles based on all available on-line and off-line measurements.

In the interest of a realistic engineering application, the developments in this study are based on a specific class of distributed systems representable by the mass transport models in environmental pollution systems. However, the techniques developed are equally applicable to a broader class of systems, including process control, where measurements may be characterized by noisy on-line instrumentation and off-line empirical laboratory tests.

Although pertinent field data were not available for the research, the multiple measurements techniques developed were applied to several simulated numerical examples that do represent typical engineering problems. The results obtained demonstrate the consistent superiority of the techniques over existing estimation methods. Methods by which the results of this work may be integrated into real engineering problems are also discussed.

APPROVAL OF DISSERTATION

THE THEORY OF MULTIPLE MEASUREMENTS TECHNIQUES

IN DISTRIBUTED PARAMETER SYSTEMS

BY

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THIS WORK IS DEDICATED WITH
UTMOST LOVE AND AFFECTION, TO
MY MOTHER, MY GRANDMOTHER,
MY FATHER AND ALL MY BROTHERS
AND SISTERS

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CHAPTER I

INTRODUCTION AND OBJECTIVES

The classical problem of estimation is that of extracting a signal from noise corrupted measurements. However, in practical monitoring problems, the direct measurements of a critical variable may not be available at a desired sampling rate. Rather, noisy independent measurements of related forms of the variable may be available at different sampling rates. Further, a frequent limitation of conventional on-line control methods is that only a few parameters may be measurable on-line.

The optimum weighting and combination of all available types of measurements thus underlies the basic concepts of the theory of multiple measurements developed in this study. In distributed systems, the measurements are spatial and temporal in nature; hence the techniques of multiple measurements include the optimization of the measurement rates and stations.

The scope of this research is the development of a comprehensive multiple measurements theory for the on-line optimum state estimation and parameter identification in noisy distributed systems. The specific goals include

(i) the development of a method by which off-line measurements may be optimally utilized in an on-line estimation or control problem.

(ii) the development of a comprehensive measurement strategy that includes

a) the determination of the optimum spatial monitoring stations and

b) an observation strategy for the optimum number and temporal intervals of measurements.

(iii) the development of multiple Kalman-type distributed filters for optimum state estimation.

(iv) the optimum identification of parameters based on all available measurements.

(v) the application of the multiple measurements techniques developed to a class of real engineering problems.

The study presents an interesting interdisciplinary approach to the engineering problems of modeling, analysis and control of environmental pollution systems. The developments are based on a class of distributed systems representable by the mass transport models of polluted stream and estuary systems. However, the techniques developed are equally applicable to a broader class of systems for which there exists a representative mathematical model and a realistic understanding of the measurement characteristics.

Owing to the interdisciplinary nature of this work, it is found necessary to include the review of the pertinent background theory and prior work in each chapter. The text is organized in an order that may represent the sequence of the problems in monitoring a dynamic distributed system. The characteristics of the models, including the state-of-the-art methods of measurements are presented in the early chapters. The solution techniques applicable to the models are then presented as a prelude to the development of the optimum monitoring policy. Algorithms are later developed for the estimation of the state profiles and the critical parameters based on various combinations of off-line and on-line measurements.

Because pertinent field data were not available for the research, special efforts are made to employ numerical examples that do typify the realistic engineering problems. The results obtained in the specific class of problems treated demonstrate the superiority of the techniques developed over existing estimation and monitoring methods. It is hoped that in future studies, the results of this work would find useful applications in real engineering monitoring and control problems.

CHAPTER II

DEVELOPMENT OF WATER QUALITY MODELS FOR ESTUARIES AND RIVERS

In contrast with the several definitions that have been given to the term model in scientific literature [148], it is defined here as the mathematical formulation and solution techniques of processes that determine the distribution of variables of interest in a system. The systems to be modeled here consist of estuaries and rivers.

Among the various resources associated **with** these systems are waterway transportation, shipping and harbor, fresh water supply, habitat for countless aquatic cultures and recreation. These activities attract to the boundaries of the water systems municipal and industrial complexes causing pollutional load. It is this principal role of estuaries and rivers as receiving waters for municipal and industrial wastes that underlies the development of the models discussed in this chapter.

The specific variables chosen to define water-quality models vary with the intended uses of that reach of the water system. Specific models may feature such variables as [38]:

(i) toxic materials and heavy metal ions

(ii) Soluble organics that cause taste and odor in water supply

(iii) color and turbidity

(iv) pH: alkalinity and acidity

(v) refractory materials that cause foaming

(vi) nitrogen and phosphorous content that cause eutrophication of lakes

(vii) suspended solids

(viii) excessive temperature resulting in thermal pollution

(ix) salinity

The models considered here emphasize the depletion of dissolved oxygen content of the natural estuary or river as a result of the biodegradable organic content of the municipal and industrial waste loads and urban runoff. Dissolved oxygen (DO) and biochemical oxygen demand (BOD) are the critical water quality defining variables considered in the models.

A detailed modeling of an estuary from first principles involves two separate packages. One package would include the derivation of equations for such hydrodynamic processes as water elevation and tidal velocity from conservation of mass and momentum. The other package would include equations of the hydrodynamic and reaction processes that jointly result in the mass balance of dissolved pollutants. Along with the simultaneous solution of the equations in the two packages, a complete model requires knowledge of several other parameters such as

(i) physical dimensions of the estuary

(ii) distribution of atmospheric pressure and surface wind stresses

(iii) values of all initial and boundary conditions including the dynamics of all boundary transfer processes, sources and sinks.

Although such elaborate models are available for some estuaries [43], simplifications such as those necessary in analysis have been assumed in the models presented in the sequel. Water elevation dynamics are generally ignored. Treatment of tidal velocity is given in the next chapter. The rest of this chapter presents models which represent the mass balance of dissolved oxygen and biochemical oxygen demand in

(i) a three-dimensional estuary

(ii) a two-dimensional stratified estuary

(iii) a one-dimensional tidal river.

Water Quality Model In A Three-Dimensional Estuary

The mass balance of a dissolved constituent such as DO or BOD is determined by the principle of conservation of matter and may be stated qualitatively as [156].

$$\begin{bmatrix}\text{time rate of accumulation of constituent in a fluid element}\end{bmatrix} = \begin{bmatrix}\text{net rate of flow of constituent into fluid element}\end{bmatrix} + \begin{bmatrix}\text{time rate of net production of constituent in fluid element}\end{bmatrix} \quad (2.1)$$

The differential equation governing the distribution of each constituent in a three-dimensional model may be written as

$$\frac{\partial \tilde{c}}{\partial t}(x, y, z, t) = -\nabla(\tilde{\underline{u}}\,\tilde{c}) + D\left[\frac{\partial^2 \tilde{c}}{\partial x^2} + \frac{\partial^2 \tilde{c}}{\partial y^2} + \frac{\partial^2 \tilde{c}}{\partial z^2}\right] + r_s \quad (2.2)$$

where $\tilde{c}$ and $\tilde{\underline{u}}$ are instantaneous concentration and velocity vector respectively. r_s represents the net production rate due to internal and external sources and sinks to be discussed shortly. The effects of the transport processes fall into two categories. The gradient term represents the effects of local fluid velocity while the second term represents effects of molecular diffusion.

Owing to the turbulent nature of an estuary, both $\tilde{c}$ and $\tilde{\underline{u}}$ are stochastic processes each having deterministic and random parts represented as

$$\tilde{c} = c + c'$$

$$\tilde{\underline{u}} = \underline{u} + \underline{u}'$$

While each of the random variables c' and $\underline{u}'$ may be considered as having an ensemble mean of zero, the mean of the cross product $(\underline{u}'\ c')$ may not be zero. Taking the ensemble average of equation (2.2) results in a more useful form written as

$$\frac{\partial \tilde{c}}{\partial t} = -\nabla (\underline{u}\ c) - \nabla (\underline{u}'\ c') + D\left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right] + r_s \qquad (2.3)$$

Among the simplifying assumptions usually applied to the above process are

(i) by invoking Fick's diffusion-type approximation, each component of the turbulent term $\underline{u}'\ c'$ may be written as a linear proportion of the concentration gradient; for example, in the x-direction

$$(\underline{u}'_x\ c') = -E_x \frac{\partial c}{\partial x}$$

where E_x is the coefficient of eddy diffusion.

(ii) The contribution resulting from molecular diffusion is several order of magnitude less than that of eddy diffusion and may be neglected, that is $D \approx 0$.

(iii) The incompressibility of the fluid and the principle of conservation of mass result in an approximation

$$\nabla \underline{u} = 0$$

For estuaries where density shows a strong dependence of salinity and temperature, Boussinesq-type approximation results in a similar simplification [113]

Employing the approximations above reduce equation (2.3) to a form which may represent the distribution of DO or BOD in a three-dimensional estuarine water quality model

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[E_x \frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial y}\left[E_y \frac{\partial c}{\partial y}\right] + \frac{\partial}{\partial z}\left[E_z \frac{\partial c}{\partial z}\right]$$

$$- U_x \frac{\partial c}{\partial x} - U_y \frac{\partial c}{\partial y} - U_z \frac{\partial c}{\partial z} + r_s \qquad (2.4)$$

Among the sources of DO are natural reaeration and photosynthesis. Reaeration occurs as oxygen transfers from air into water across the estuary surface. It increases with surface turbulence [34] and natural mixing of the estuary. This process may be represented as

$$r_s = Ka\ (C_s - C)$$

where Ka is the coefficient of reaeration, C is the instantaneous DO concentration and C_s is the DO saturation level of the estuary. The term $(C_s - C)$ is often referred to as the DO deficit in the literature of water quality studies. In general, Ka is temporally and spatially distributed and may be related to the mean non-tidal advective velocity and depth as in the following empirical reaeration equation

$$Ka = \text{constant X } \frac{(\text{mean velocity})^n}{(\text{depth})^m}$$

Several authors [90, 73, 33, 10] have evaluated the numerical values of the constant and the exponents in the above formular for several cases of estuaries and streams.

Photosynthesis is a process by which oxygen is transfered between the water and the suspended algae. This oxygen source exhibits a diurnal variation with sunlight [99]. and also increases with temperature and the amount of nutrients available to the algae. It is represented as P in the sequel.

Among the sinks associated with DO are deoxygenation, nitrification, respiration demand and benthal deposit demand. Deoxygenation is a first-order reaction representing the oxidation of soluble organic waste. It may be represented as

$$r_s = - K_d \ L$$

where L is the concentration of BOD. Coefficient of deoxygenation K_d increases with longitudinal mixing and bottom growth [13] Nitrification represents the oxygen utilization for endogenous metabolism of the microorganism present in the estuary. This oxygen demand may be significant in an estuary segment subjected to well-oxidized effluent loading and may be represented by a first order decay reaction with a time-lag [42].

Respiration demand (R) results from consumption of oxygen by aquatic plants for respiration. This contribution varies with turbulence and available nutrients. Benthal deposit demand (B) occurs mostly as a result of the diffusion of the anaerobic decomposition from the bottom deposits.

The source and sink associated with the BOD process are due to runoff (La) and BOD-removing processes (K_r) which may include oxidation, sedimentation and flocculation.

All the above transport and reaction processes are included in the following dynamic water quality model of a three-dimensional estuary

$$\frac{\partial L(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x}\left[E_x \frac{\partial L}{\partial x}\right] + \frac{\partial}{\partial y}\left[E_y \frac{\partial L}{\partial y}\right] + \frac{\partial}{\partial z}\left[E_z \frac{\partial L}{\partial z}\right]$$

$$- U_x \frac{\partial L}{\partial x} - U_y \frac{\partial L}{\partial y} - U_z \frac{\partial L}{\partial z} - K_r L + La \qquad (2.5)$$

$$\frac{\partial C}{\partial t}(x, y, z, t) = \frac{\partial}{\partial x}\left[E_x \frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial y}\left[E_y \frac{\partial C}{\partial y}\right] + \frac{\partial}{\partial z}\left[E_z \frac{\partial C}{\partial z}\right]$$

$$- U_x \frac{\partial C}{\partial x} - U_y \frac{\partial C}{\partial y} - U_z \frac{\partial C}{\partial z} - K_d L - K_a C$$

$$+ K_a C_s + P - R - B \qquad (2.6)$$

Water Quality Model In A Stratified Estuary

In many application problems, two dimensional estuary models have been considered [102, 52, 83, 116]. In addition to easing analysis, this model may represent the water-quality characteristics of two common estuary types namely stratified and non-stratified estuaries. Stratification is the variation of density with depth resulting from salinity instrusion This density variation influences the tidal velocity distribution and determines the rate of vertical mixing of dissolved constituents.

Complete vertical mixing characterizes non-stratified estuaries. Such a system may be represented by a vertically averaged version of the three-dimensional equations (2.5) and (2.6). This simplication results in a system of equations

$$\frac{\partial L}{\partial t}(x, y, t) = \frac{\partial}{\partial x}\left[E_h \frac{\partial L}{\partial x}\right] + \frac{\partial}{\partial y}\left[E_h \frac{\partial L}{\partial y}\right]$$

$$- U_x \frac{\partial L}{\partial x} - U_y \frac{\partial L}{\partial y} - K_r L + La \qquad (2.7)$$

$$\frac{\partial C(x, y, t)}{\partial t} = \frac{\partial}{\partial x}\left[E_h \frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial y}\left[E_h \frac{\partial C}{\partial y}\right]$$

$$- U_x \frac{\partial C}{\partial x} - U_y \frac{\partial C}{\partial y} - K_d L - K_a C$$

$$+ K_a C_s + P - R - B \qquad (2.8)$$

The parameter E_h is known as the effective horizontal diffusivity coefficient and is generally less than the eddy diffusion coefficients in the three-dimensional model [113].

Stratified estuaries on the other hand are usually shallow and exhibit vertical mixing at a rate comparable with the tidal period [123, 101]. Vertical distribution of velocity and concentration of dissolved constituents must be represented while the lateral distribution may be averaged. The lateral averaged version of equations (2.5) and (2.6) representing the water quality model in a two dimensional stratified estuary may be written as

$$\frac{\partial L(x, z, t)}{\partial t} = \frac{\partial}{\partial x}\left[E_x \frac{\partial L}{\partial x}\right] + \frac{\partial}{\partial z}\left[E_z \frac{\partial L}{\partial z}\right]$$

$$- U_x \frac{\partial L}{\partial x} - U_z \frac{\partial L}{\partial z} - K_r L + La \qquad (2.9)$$

$$\frac{\partial C(x, z, t)}{\partial t} = \frac{\partial}{\partial x}\left[E_x \frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial z}\left[E_z \frac{\partial C}{\partial z}\right]$$

$$- U_x \frac{\partial C}{\partial x} - U_z \frac{\partial C}{\partial z} - K_d L - K_a C$$

$$+ K_a C_s + P - R - B \tag{2.10}$$

Water Quality Model In A Tidal River

A one-dimensional model most appropriately applies to the segment of the estuary that may be considered vertically and laterally homogeneous. This condition characterizes the tidal river where salinity intrusion is minimum. The mathematical model may be obtained by spatially averaging equations (2.5) and(2.6) over the cross section (A) of the estuary. This results in

$$\frac{1}{A(x)} \frac{\partial}{\partial t} [A(x)\ L(x,t)] = \frac{1}{A} \frac{\partial}{\partial x} [A\ E_L\ \frac{\partial L}{\partial x}] - \frac{1}{A} \frac{\partial}{\partial x} [AUL] - K_r L + L_a \tag{2.11}$$

$$\frac{1}{A} \frac{\partial}{\partial t} [A(x)\ C(x,t)] = \frac{1}{A} \frac{\partial}{\partial x} [A\ E_L\ \frac{\partial C}{\partial x}] - \frac{1}{A} \frac{\partial}{\partial x} [AUC] - K_d L - K_a C + K_a C_s + P - R - B \tag{2.12}$$

The longitudinal dispersion coefficient E_L results from the spatial variation in velocity and concentration over the cross section and is several order higher in magnitude than the eddy diffusion coefficients in equations (2.5) and(2.6), [135, 50].

Equations (2.11) and (2.12) represent a general form of the model that has been widely used in the one-dimensional analysis of estuaries [91,95] .

The effect of longitudinal dispersion is most pronounced in the tidal saline segment of an estuary. It is less important but still significant in the analysis of tidal non-saline segment of the estuary. However, upstream where tidal effect can be negligible, the dispersion term may also be neglected in the model. Publication [34] shows an analysis of the relative significance of the dispersion and advective terms in estuaries and streams. Also, quite often as in the case of the Passaic and Raritan Rivers in New Jersey upstream is decoupled from tidal effects by dams in the river.

This approximation reduces equations (2.11) and (2.12) to the forms which have been used in the analysis of one-dimensional water-quality stream models namely

$$\frac{\partial L}{\partial t}(x, t) = -\frac{1}{A}\frac{\partial}{\partial X}[AUL] - K_r L + L_a \qquad (2.13)$$

$$\frac{\partial C}{\partial t}(x,t) = -\frac{1}{A}\frac{\partial}{\partial x}[AUC] - K_d L - K_a C$$

$$+ K_a C_s + P - R - B \qquad (2.14)$$

In many studies, terms $\overline{P}$, $\overline{R}$ and $\overline{B}$ have been used in the above equation to represent the daily-averaged values of the photosynthetic, respiration and benthal deposits effects in the streams [134].

Steady-State Water Quality Models

The models presented in the preceeding sections represent the dynamics of polluted esturies and streams including the effects of the unsteady time and spatially varying tidal velocity. Because of the difficulties associated with the analysis of such models, several investigators have considered modified models based on different concepts of the tidal velocity.

The works of Ketchum [69, 68] and Phelps et al [112] were based on the concept of tidal prism exchange where a segment of the estuary may be considered completely mixed within each tidal period. Stommel [127] studied the distribution of concentrations averaged over a tidal period by considering a velocity term that represents only the effects of non-tidal fresh water flow. O'Connor [95, 93] developed a different non-tidal model to derive concentration distribution under slack-time conditions in esturies with varying cross-section. The equations of the models resulting from these non-tidal advective approximations have the same forms as equations (2.11) and(2.12) for one-dimensional cases. However, the interpretations and the values of the parameters and concentration distributions vary from one model to another.

An estuary model may be considered at steady state when the concentration distribution does not change from one point in the tidal period to the next. In this case the derivatives $\frac{\partial L}{\partial t}$ and $\frac{\partial C}{\partial t}$ may be set to zero. Under this condition, equations (2.11) and (2.12) reduce to

$$\frac{1}{A}\frac{\partial}{\partial x}\left[A E_L \frac{\partial L}{\partial x}\right] - \frac{1}{A}\frac{\partial}{\partial x}\left[AUL\right] - K_r L + La = 0 \qquad (2.15)$$

$$\frac{1}{A}\frac{\partial}{\partial x}\left[A E_L \frac{\partial C}{\partial x}\right] - \frac{1}{A}\frac{\partial}{\partial x}\left[AUC\right] - K_d L$$

$$- K_a C + K_a C_s + P - R - B = 0 \qquad (2.16)$$

A similar form of this model has been used in a case study of the East River in New York [96]

The development of some of the mathematical models employed in the studies of water quality systems have been presented in this chapter. Present methods of evaluating some of the variables and parameters in the models are discussed in the next chapter. In later chapters, techniques are developed and applied for optimum on-line estimation of critical variables and parameters in some specific examples of these models.

CHAPTER III

EVALUATION AND MEASUREMENTS OF VARIABLES AND PARAMETERS IN WATER QUALITY SYSTEMS

A brief review of the state-of-the-art methods of measuring and evaluating some of the critical water quality variables and parameters, is presented in this chapter. The principal objective is to explore the validity and limitations, in a practical engineering sense, of some of the assumptions that usually characterize theoretical and analytical approaches. An understanding of some of the aspects of engineering practice is particularly essential for a meaningful application of an interdisciplinary approach, such as this study, to the analysis of water quality systems.

Determining which variables are the most critical to the successful management of polluted water systems is a subject of extensive debate among researchers in this field [2]. This is because of the multipurpose use of the water resources and the variability of the pollutional contents in the municipal, industrial and agricultural wastes to which a water system may be subjected. The discussion in this chapter is limited to those variables and parameters that characterize the mathematical models presented in the previous chapter. They emphasize the interplay between the amount of dissolved oxygen (DO) available in a natural waterbody and the various oxygen depletion processes, which may include biochemical oxygen demand (BOD), respiration demand for aquatic plants (R) and benthal deposit demand (B).

A detailed discussion on apparatus, pretreatment of polluted water samples, procedures and instrumentation for measurements in water quality systems, is beyond the scope of this study. Such information may be obtained from a reference text on Standard Methods [128] and from manuals provided by various instrument manufacturers [8 , 48 , 63]. The interest here is to delineate some of the practical features of the multiple measurements estimation techniques developed in the later chapters of this study. These include

(i) independent measurements of the multiple forms of a variable

(ii) availability of on-line measurements of certain variables

(iii) measurement error characteristics.

The application of the multiple measurements techniques to water quality systems is contingent upon the independent measurements of various forms of the same variable, such as: BOD, total organic carbon (TOC), chemical oxygen demand (COD) and total oxygen demand (TOD). The relationships between the various oxygen demands are explored in the sequel. Furthermore, a part of the objectives of this study is to develop an on-line optimum estimation method that may be integrated into an on-line control of a polluted water system. Hence, interest also is focused here on the on-line and off-line methods of measuring dissolved oxygen and the various oxygen demands. In addition, some of the practical problems associated with measurements are discussed. An attempt is made, wherever possible, to determine typical values of the standard deviations that may be associated with measurement errors. This is the basis on which measurement variance terms, used later in numerical examples, are established.

In general, only a few of the parameters that describe the hydrodynamic and biochemical processes in a water system can be measured directly. Therefore, empirical methods based on field data of such variables as DO, BOD, temperature and salinity are used. For other parameters such as tidal velocity and reaeration coefficient, empirical formulae based on the physical properties of the water systems have been developed. The presentation that follows includes methods used in practice as well as those that have been applied in recent theoretical and analytical works.

Measurements Of Variables

Biochemical Oxygen Demand.

BOD is a measure of the biodegradable organic content of a polluted river or estuary. It is determined by recording the amount of oxygen utilized by organisms for aerobic decomposition and stabilization of the organic content in a water sample. The standard laboratory procedure involves seeding the polluted water sample with a microbial population in a BOD bottle. It is then incubated in a water bath or a special air incubator, in the dark at a temperature of 20° C.

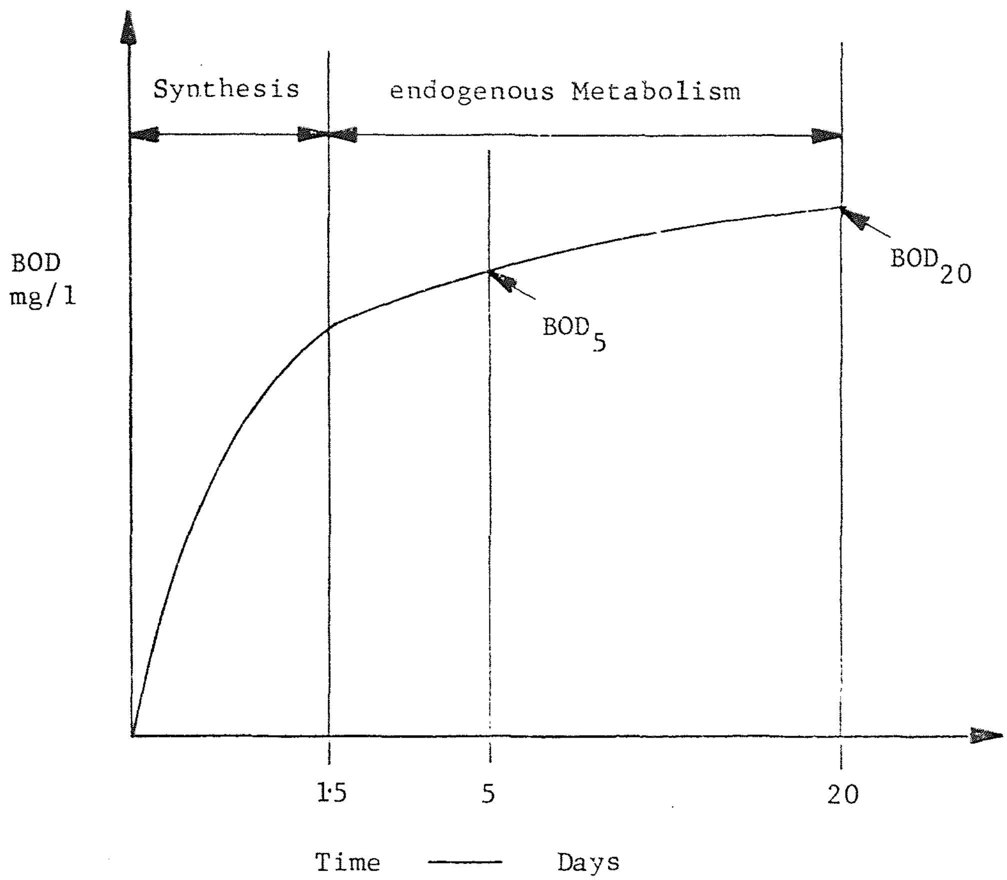


FIGURE III-1. Aerobic Reaction in a BOD Test

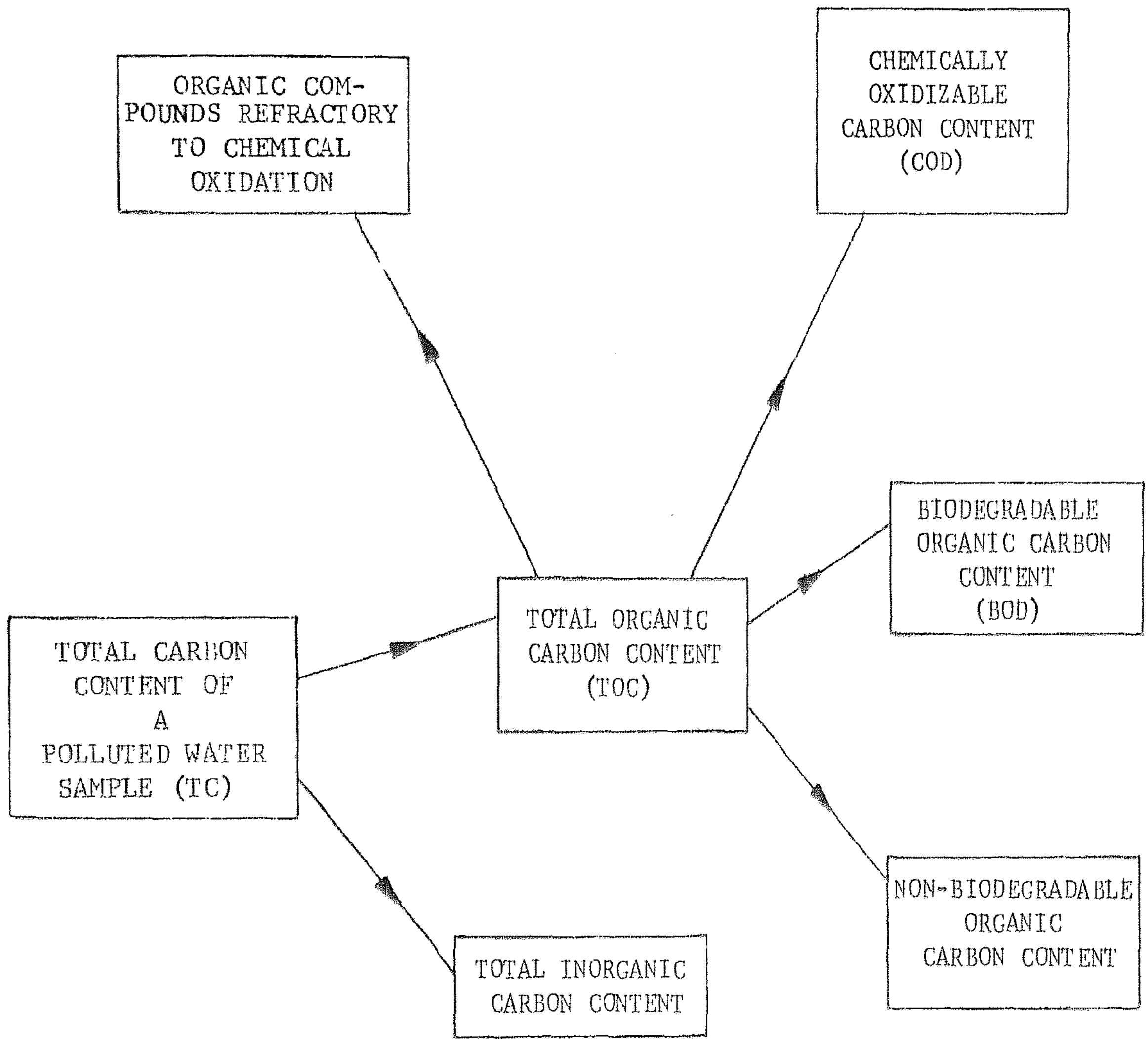


FIGURE III-2. Relationship Between Oxygen Demands in a Polluted Water Sample

Figure III-1 gives a qualitative illustration of the carbonoceous reaction in a BOD test. During the synthesis stage, the microorganisms utilize oxygen and the organic content in the water sample for energy and growth. The rate of growth decreases with the amount of nutrient available and may terminate after about 36 hours of incubation. During endogenous metabolism, more oxygen is consumed, however at a slower rate, for the utilization of stored metabodies and the cell component of dead organisms. Complete oxidation of the biodegradable organic content in the BOD bottle may last up to twenty days. The standard BOD measurement is the amount of oxygen utilized after five days of incubation (BOD_5); oxygen consumed for the complete carbonaceous oxidation is often referred to as the ultimate BOD (BOD_{20}).

<u>Possible causes of errors in BOD measurements</u>.

Among the several factors that may affect BOD measurements are

(i) disparity between the natural and laboratory environments

(ii) seeding

(iii) nitrification

(iv) toxicity

and (v) human qualitative judgements.

The apparatus and procedure for a BOD test are not conducive to measurements in the natural environment of the polluted water system. However, laboratory BOD measurements may not adequately report the effects of such natural environmental conditions as turbulence, temperature, dissolved oxygen concentration and sunlight. Algae for example, if present in a water sample, may die for lack of sunlight during incubation and the resulting organic matter may increase the apparent BOD reading. Among the recent studies of the effects of temperature changes on BOD reaction is [122].

Organisms from settled domestic sewage are by standard, used for seeding waste water samples. However, in the case of a polluted stream dominated by industrial wastes, organisms taken close to the waste outfall are used. In some other cases, it may be necessary to cultivate a special microbial population capable of oxidizing a particular waste characteristic. If the organisms are not acclimated to the waste, a lag results in the BOD reaction and an error may be introduced into the BOD reading. Graphical illustrations of the effects of seed concentration and acclimation are provided in figures (2.6) and (2.7) of [38]

Oxygen demand due to nitrification results from the utilization of the nitrogen content of organic waste by nitrifying bacteria. This process usually follows the carbonaceous oxidation process. However, in the case of a stream subjected to well oxidized effluents, both processes may occur simultaneously. The use of polluted river water for seed, therefore, may increase the apparent BOD measurement.

The presence of heavy metal ions in an industrial waste or the toxic contamination of dilution water may inhibit the activities of the oxidizing microorganisms and result in an apparent decrease in BOD readings. The effect of toxicity on BOD readings has been studied by [87]

BOD measurement is an empirical test where the result accuracy often depends on the experience and judgement of the analyst to properly identify and pretreat the undesirable components of a water sample. Although various reagents are available to minimize the effects of some of the above processes, BOD is basically a noisy measurement. The variability of the sources of errors seems to justify the characterization in later chapters, of the measurement errors as random and zero mean. Table 219(1) of [128] in reporting the effect of seed on BOD readings shows typical standard deviation values of about 5% of the mean BOD reading. The overall precision of BOD measurement also is given as about 17%. The standard deviation values used in the simulation of BOD measurements in this study range from 5% to 20% of the expected measurements.

The five day delay in obtaining a BOD reading is an undesirable factor in the automatic control of a treatment plant or a polluted water system. Other forms of oxygen demand and their relationship to BOD are discussed next.

Chemical Oxygen Demand.

Again a qualitative figure III-2 is given to illustrate the relationships between various oxygen demands. COD measures the total organic carbon content of a polluted water system, except for some chemical compounds such as benzene which are refractory to chemical oxidation. The standard test employs potassium dichromate with temperature reflux to chemically oxidize the organic content in a water sample. COD measurement takes about two hours by standard method; however, other faster methods based on incomplete oxidation of some of the constituent organics are available [64]. In addition, a linear relationship has been observed between BOD and COD readings for some specific organic compounds [44, 114].

Possible causes of error in COD measurements.

One of the major causes of error in a COD measurement is the additional oxidation of inorganic compounds such as ferrous iron, sulfites and nitrogen. A useful reading, therefore, requires the proper identification of the constituent pollutants in a water sample.

Total Organic Carbon.

As shown in Figure III-2, TOC is a measure of the total organic content of a polluted stream. The test procedure involves the combustion of the organic content to water vapor and carbondioxide and the analysis of the latter to obtain the TOC value. By the wet chemistry method, the water sample is oxidized in acid prior to combustion and the CO_2 output is analyzed using an absorption train [38].

The more recent methods involve a high temperature (900 - 100^{o} C) catalytic oxidation of the organic content and the use of an infra-red spectrophotometer to analyze the resulting CO_2 to obtain a total carbon (TC) measure. The inorganic carbon such as carbonates, present in the water sample may be removed with acid prior to injection into the combustion tube. Methods of removing volatile organics are also available [120]. However, the most recent TOC analyzers contain an additional low temperature (150^{o} C) combustion tube where only the inorganic carbon content is removed in presence of acid and again in form of CO_2. The total organic carbon is then determined by taking the difference between the total carbon reading and the total inorganic carbon reading.

According to Helfgott et al in [3] TOC measurement takes between five to fifteen minutes. In addition, several investigators also have established a linear relationship between BOD and TOC for some industrial [44] and domestic wastes. The ratio of BOD to TOC values varies with the specific wastes being tested with typical values ranging between 1.35 and 2.62 for industrial and municipal wastes [38]. The linear function used later in this study to relate BOD and TOC measurements are based on the preceding reports.

Possible causes of errors in TOC measurements.

An incomplete removal of the inorganic carbon content of the water sample by pretreatment may introduce errors in the TOC readings. Also, the presence of anions such as NO_3^- may interfere with the absorption pattern of the spectrophotometer [38] In addition, the dry phase high temperature oxidation technique in modern TOC analyzers may not adaquately represent the wet environment of the natural water system. Furthermore, in formalizing the linear function between BOD and TOC, the error of linear approximation should be considered, as done later in this study.

Dissolved Oxygen.

Dissolved oxygen is a measure of the amount of oxygen available in a stream to sustain the survival and the activities of microorganisms and other aquatic life. The quality criteria for various water usage are based in part, on the concentration of dissolved oxygen.

The methods available for DO measurements fall into two categories; namely, the Winkler Test and the Membrane Electrode methods [128]. In the Winkler Test, the dissolved oxygen in a water sample is used to oxidize a precipitate of manganous hydroxide. Upon acidification of the mixture in presence of iodide ions, iodine equivalent to the concentration of DO in the water sample is produced. The amount of iodine produced may be determined by titration or the use of an absorption spectrophotometer.

The Winkler Test is an off-line measurement process; however, instrumation capable of on-line DO measurements are now commercially available. The recent DO meters are based on the chemical reduction of oxygen in a solution and its diffusion across special semipermeable membranes. Two types of DO meters are available namely, Galvanic type [81] and the Polarographic type. In the former, the reduction process causes a current flow which may be calibrated for the DO concentration. The polarographic meter employs an external emf (usually .8 v) for the polarization of the indicator electrode.

Possible causes of errors in DO measurements.

Errors may be introduced into the empirical Winkler Test by the presence in the water sample, of organic compounds that may interfere with the oxidation of the iodide ions or the production of the hydroxide precipitate. In addition, great care is often required in sampling to prevent agitation and contact of the water sample with air, as these may drastically influence the DO concentration level.

The response of a DO meter is based on the activities of the oxygen molecules. Therefore, DO readings are very sensitive to temperature changes and the presence of salinity in the water samples. Sensitivity of DO meters also has been found to decrease with age in a comparative study of DO measurement methods [84]. An accuracy of about 0.1 mg/liter has been specified by several manufacturers manuals.

Hydrodynamic Variables

Tidal Velocity.

The successful management of a polluted water system requires an adequate knowledge of the hydrodynamic characteristics of the system, including tidal velocity distribution and the dispersion coefficients. Extensive research has been conducted in recent years on the tidal velocity distribution in several estuary cases. In general, three different approaches have been applied namely, [55]

(i) continuity and momentum equation approach

(ii) cubature method

(iii) direct measurement

Tidal velocity may be evaluated from first principles by the simultaneous solution of a pair of non-linear hyperbolic first-order partial differential equations which represent mass and momentum conservation in the estuary. For a one-dimensional case, these equations may be written as

$$b \frac{\partial h}{\partial t} + \frac{\partial Q}{\partial x} = 0 \tag{3.1}$$

$$\frac{\partial Q}{\partial t} + U \frac{\partial Q}{\partial x} + g \frac{\partial h}{\partial x} A + \frac{g\, Q\, Q}{A\, C_h^2\, R} = 0 \tag{3.2}$$

where U is the tidal velocity; Q is the flow rate; h is the instantaneous tidal height; b and A are the width and cross sectional area; g is the gravitational acceleration and (C_h^2 R) represents the roughness property of the estuary. Various forms of equations have been derived by several investigators [37 , 54] and the solutions usually obtained by finite-difference methods, have been applied to several estuaries [126 , 150 , 151]. Field measurements of the tidal elevations at the ocean boundary and the freshwater flow at the head of the tide region are usually applied as the boundary conditions in solving equations (3.1) and (3.2).

If data on the distributions of tidal amplitude and phase are available, the tidal velocity distribution may be obtained by integrating the continuity equation (3.1). This is known as the cubature method. Analysis based on this method and the assumption of a harmonic tidal flow has been applied to obtain tidal velocity distributions in a one-dimensional model of the Delaware Estuary [51] and a two-dimensional model of the Galveston Bay [116].

Although the results in [51] demonstrated that the tidal velocity in a constant density region of an estuary may not be a harmonic function of the tidal period, harmonic approximation of the form

$$U(x,t) = U_F(x) + U_T(x) \,\mathrm{Sin}\left(wt - F(x)\right) \qquad (3.3)$$

has been used in many studies. This may provide a useful representation in analysis, especially when direct field measurements are available for the freshwater flow $U_F(x)$, maximum tidal velocity $U_T(x)$ and the tidal phase $F(x)$.

Tidal velocity distribution resulting from vertical transport in the salinity intrusion region of a two-dimensional estuary has been studied in recent years. Experimental data collected from the salinity intrusion flume at Waterway Experiment Station [52 , 53] show a time-averaged tidal velocity distribution with a logarithmic vertical profile. Similar results were obtained in a study of velocity profiles [123]. The results from these reports are presented later in Chapter VI and used in a numerical example of a saline two-dimensional estuary.

Dispersion Coefficient.

Because dispersion of pollutants is a result of the spatial variations in the tidal velocity over a cross-section, more research has been performed on the latter phenomenon. Early studies on evaluating longitudinal dispersion are represented by the work of Taylor [135] and Elder [39]. Various forms of Taylor's equation [55]

$$E_L = 77\, \eta\, U\, R_h^{5/6} \tag{3.4}$$

have been employed to determine the dispersion term E_L for a undirectional flow in a pipe. A modified form of this equation for an oscillatory flow was developed in [54] and has been used successfully to predict distribution in a dye experiment on the Pomomac River [56].

However, in general empirical methods are used to evaluate the dispersion in the natural water systems. Usually, the dispersion distribution is obtained by curve-fitting field measurements of the salinity distribution. The later also may be represented by equation (2.11) except that the decay rate $K = 0$ for a conservative constituent such as salinity. By this approach, the spatial variation in longitudinal dispersion coefficient also may be obtained.

Biochemical Parameters

BOD Removing Coefficient (K_r).

The biological stabilization of the organic content of a polluted water body may be considered a first-order reaction of the form

$$\frac{dL}{dt} = -K_r L \qquad (3.5)$$

where L is the BOD concentration of the unstabilized organics. The reaction rate K_r represents all the BOD removing processes which may include carbonaceous oxidation, sedimentation, flocculation and volatilization. The numerical value of K_r may decrease along the stretch of a stream as the suspended solids, volatile organics and flocculants are removed.

Deoxygenation Coefficient (K_d).

Deoxygenation is the process by which dissolved oxygen in a stream is depleted as a result of carbonaceous oxidation. This process may be written as

$$\frac{dc}{dt} = -K_d L$$

where c is the DO concentration. In the absence of sedimentation and other non-oxidation processes $K_d = K_r$.

In practice, empirical methods are employed to evaluate both K_r and K_d, and data of the DO and BOD distributions under steady state low-flow conditions are used. The numerical values for K_r and K_d are computed form best-fit logarithmic plots of the DO and BOD distributions. To properly represent the steady state conditions, ultimate BOD values (BOD_{20}) are usually used in the analysis, and empirical temperature coefficients to adjust for temperature changes are applied [38]. A recent study relating K_d to the reaction rate in a BOD bottle test is contained in [13].

Reaeration Coefficient (K_a).

Reaeration coefficient may be computed from the empirical reaeration equation presented in Chapter II. On the other hand, it may be computed directly from BOD and DO data by the curve-fitting method. Among the recent studies using the latter method is [30].

Sources and Sinks.

Photosynthesis has been shown to be representable by a summation of diurnal harmonic function [99]. The coefficients of each harmonic may then be evaluated by applying the curve-fitting method to field data of DO taken on a diurnal basis.

It may also be evaluated from chlorophyll measurements in cases of isolated algae region. Respiration and benthal deposit rates may also be computed by the curve-fitting method tied in with bottom deposit respiration methods

Application of the curve-fitting method in most of the cases above require a proper identification of the regions along the river in which each process dominates. In addition, the evaluation is an off-line process and numerical values often represent steady state stream conditions. The reliability of such determination is not considered very good, and, thus Environmental Protection Agency, Region II Headquarters refused to release such information to Dr. Perlis . In Chapter VIII, on-line estimation for some of these parameters is developed both for steady and non-steady state conditions. A review of measurements and parameter evaluations in water quality systems has been given in this chapter. Some of the practical features in measurements that have been discussed in the preceding, are incorporated in the developments in later chapters.

CHAPTER IV

SOLUTION TECHNIQUES OF WATER QUALITY MODELS

In later chapters, algorithms are derived to optimally estimate the state profiles and parameters in some water quality models. This development requires the solution of equations similar to the parabolic partial differential equations presented in Chapter II. In addition to presenting the solution techniques used in this study, this chapter includes a brief review of techniques that have been applied by other investigators.

The solution techniques for water quality models fall into two broad categories namely

(i) analytical close-form approach

(ii) numerical approach

Analytical approach was used extensively in early pollution studies of stream models such as the classical Streeter-Phelps equation [131]. In more recent studies O'Connor [96,98] and Thomann [141 , 140 , 138 , 139] have applied different analytical solution methods to steady-state water quality systems segmented into reaches in which the physical hydraulic and reaction rate parameters are constants or well defined.

Time-varying analytical solutions have been derived mostly for simple one-dimensional systems subject to slug or constant load at the boundary. Such a solution is used in the measurements projection scheme presented in Chapter V.

As the time and spatial variations in parameters and inputs are included in a model, analytical solutions become complex, impractical and in most cases unavailable. In these cases, various finite-difference approximation techniques have been applied using high-speed digital computers [41, 156, 36]. Analog [94] and hybrid computers [147 , 133] also have been applied in some case studies.

For the stream and estuary cases considered in this study, the explicit-finite difference method was used. The problems of stability and boundary conditions associated with finite-difference methods are also discussed in this chapter.

Analytical Solutions

Continuous solution approach to steady state problems.

The solution to the steady state DO and BOD equations in a one-dimensional, constant parameter tidal river presented in equations (2.15) and (2.16) may be written as

$$L(x) = Lo\, e^{j_1 x} \tag{4.1}$$

$$C(x) = -\frac{k_d\, Lo}{ka - kr}\left[e^{j_1 x} - e^{j_2 x} \right] + C_o\, e^{j_2 x}$$

$$+ \left(C_s + \frac{P}{Ka}\right)\left(1 - e^{j_2 x}\right) \tag{4.2}$$

where

$$j_1 = \frac{u}{2E}\left[1 \pm \sqrt{1 + \frac{4\, k_r E}{u^2}}\right] \tag{4.3}$$

$$j_2 = \frac{u}{2E}\left[1 \pm \sqrt{1 + \frac{4\, k_a E}{u^2}}\right] \tag{4.4}$$

The minus signs in the j terms apply to regions $x > o$.

In general, each equation may be written in a form

$$C(x) = A\, e^{jx} + B\, e^{gx} \tag{4.5}$$

where g is the corresponding j term for $x < o$. This last equation applies to segmented reaches of a river or estuary at steady state, and the complete concentration profiles is obtained by matching appropriate boundary conditions This method developed by O'Connor [92] has been applied successfully in the analysis of the Delaware Estuary [98] and the East River in New York [96].

Finite section approach to steady state problems.

This approach developed by Thomann [138] may be considered a subset of the finite-difference method discussed in the sequel. Rather than applying an analytical closed form solution, this method approximates the differential equations between the segments. The basic equation relating the parameters and concentration distribution of a pollutant L in three adjacent well-mixed river segments i - 1, i and i + 1 may be written as

$$
\begin{aligned}
V_i \frac{dLi}{dt} = {} & Q_{i-1,i} [\alpha_{i-1,i} L_{i-1} + (1 - \alpha_{i-1,i}) L_i] \\
& - Q_{i,\,i+1} [\alpha_{i,\,i+1} L_i + (1 - \alpha_{i,\,i+1}) L_{i+1}] \\
& - E^1_{i-1,i} [L_{i-1} - L_i] + E^1_{i,\,i+1} [L_{i+1} - L_i] \\
& - k_r V_i L_i
\end{aligned}
\qquad (4.6)
$$

where V_i is the volume of segment i, $Q_{i-1,i}$ is the net flow and $\alpha_{i-1,i}$ is a dimensionless mixing coefficient between segments i - 1 and i. Coefficients $E^1_{i-1,i}$ is defined as the bulk dispersion and differs in value from the longitudinal dispersion term discussed Chapter II.

Applying this method to a steady state problem reduces the system differential equations to n simultaneous algebraic equations where n is the number of segments. This method has the advantage of coping with systems with spatially varying parameters. This approach has also been extended to solving time-varying problems [104].

However, the emphasis in this study is an on-line estimation which requires transient solutions as well. Therefore, the preceding steady state methods were used only in the preliminary stages of this study.

Real time solutions.

In general, complete closed-form solutions including the transient response are not available for many practical problems in water quality analysis. However, when available for simple cases, they provide a valuable tool for verifying the accuracies of solutions obtained by other approximations for more complex problems. The presentation here is limited to the two types of real time solutions employed in the measurements projection schemes developed in Chapter V.

For the constant parameter, one-dimensional stream with negligible dispersion considered in Chapter VII, the state equations of the BOD and DO profiles may be written as in (2.13) and (2.14)

$$\frac{\partial L(x,t)}{\partial t} = -u\frac{\partial L(x,t)}{\partial x} - k_r L(x,t)$$

$$\frac{\partial C(x,t)}{\partial t} = -\frac{\partial C(x,t)}{\partial x} - K_r L(x,t) - k_a C(x,t)$$

$$+ k_a C_s + P(x,t).$$

Using solution method of characteristics [33 , 71], the response of the homogeneous system to an initial condition at (x_o, t_o) may be written as

$$\underline{V}(x,t) = \underline{\Phi}(t, t_o) \; \underline{V}(x_o, t_o) \tag{4.7}$$

where

$$\underline{\Phi}(t, t_o) = \begin{bmatrix} e^{-k_r (t-t_o)} & 0 \\ -\frac{k_d}{k_a - k_r}\left[e^{-k_r (t-t_o)} - e^{-k_a (t-t_o)}\right] & e^{-k_a (t-t_o)} \end{bmatrix}$$

$$x(t) = x_o + U(t-t_o) \tag{4.8}$$

and

$$\underline{V}(x,t) = \begin{bmatrix} L(x,t) \\ C(x,t) \end{bmatrix} \tag{4.9}$$

The solution is along the characteristics x_o, t_o and only three of the variables x, t, x_o and t_o may be specified independently. The foregoing solution is used later in Chapter V to project an off-line noisy measurement taken at point $(x_o, t - T)$ to an on-line estimation point (x_m, t).

The responses of BOD distribution to a slug input in the specific estuary cases to be treated later are now presented. The differential equation describing the BOD distribution in a well-mixed one-dimensional estuary with constant dispersion and decay terms is written as

$$\frac{\partial L(x,t)}{\partial t} = E \frac{\partial^2 L}{\partial x^2} - U(x,t) \frac{\partial L}{\partial x} - k_r L$$

Under steady flow condition, U may be assumed constant and the transient response of the system to an instantaneous load W (lb/ area) released at point (x_o, t_o) may be written as

$$L(x,t) = \frac{W}{\sqrt{4\pi E (t-t_o)}} \exp \left[\frac{-a^2}{4 E (t-t_o)} - c \right]$$

where

$$a = (x - x_o) - U_f (t-t_o)$$

$$b = \frac{U_t}{w} (\cos wt - \cos wt_o)$$

$$c = k_r (t-t_o) \qquad (4.10)$$

In the tidal region of the estuary, the velocity $U_{(x,t)}$ may be approximated by a harmonic function

$$U_{(x,t)} = U_f + U_t \text{ S in } wt \qquad (4.11)$$

Under this condition, the transient BOD response becomes [55]

$$L(x,t) = \frac{W}{\sqrt{4\pi E(t-to)}} \exp\left\{ -\frac{[(x-x_o) - U_f\ (t-to) + U_t(\cos wt - \cos wto)]^2}{4\ E\ (t-to)} - k_r\ (t-to) \right\} \quad (4.12)$$

Similarly, BOD distribution in a two dimensional estuary may be represented as

$$\frac{\partial L}{\partial t}(x,z,t) = Ex\frac{\partial^2 L}{\partial x^2} + Ez\frac{\partial^2 L}{\partial z^2} - U_{(x,z,t)}\frac{\partial L}{\partial x} - V_{(x,z,t)}\frac{\partial L}{\partial z} - k_r L \quad (4.13)$$

In the specific example treated later, a one-dimensional flow is assumed

$$v_{(x,z,t)} = 0$$

Although spatially varying tidal velocity $U_{(x,z,t)}$ also is considered, it suffices for the purpose of this presentation to assume a spatially averaged velocity of the form in equation (4.11). The transient response of the two dimensional estuary under the foregoing conditions to a slug load W (lb/ depth) may then be written as [55, 156].

$$L\ (x,z,t) = \frac{W}{4\pi(t-to)\sqrt{E_x\ E_z}} \exp\left\{ -\frac{[a+b]^2}{4E_x(t-to)} - \frac{[z-zo]^2}{4E_z\ (t-to)} - c \right\} \quad (4.14)$$

where a,b, and c are defined in (4.10)

The transient responses in equations (4.10), (4.12) and (4.14) are programmed to project off-line BOD measurements taken at a general point (x_o, z_o, t_o) to an on-line estimation point (x_m, z_m, t).

Finite-Difference Techniques

Availability of high speed and large memory size computers has increased the application of finite-difference solution techniques to water quality problems. Basically, finite difference representation of a partial derivative is a truncated Taylor series approximation.

In this study, temporal partial derivatives are represented using a forward difference formulation

$$\frac{\partial L}{\partial t}(x,t) = \frac{1}{\Delta t}\left[L_{x,\ t+\Delta t} - L_{x,t}\right] \quad (4.15)$$

and spatial derivates are represented using a central difference formulation

$$\frac{\partial L}{\partial x}(x,t) = \frac{1}{2\Delta x}\left[L_{x+\Delta x,t} - L_{x-\Delta x,t}\right] \quad (4.16)$$

$$\frac{\partial^2 L}{\partial x^2}(x,t) = \frac{1}{(\Delta x)^2}\left[L_{x+\Delta x,t} - 2L_{x,\ t} + L_{x-\Delta x,t}\right] \quad (4.17)$$

Δx and Δt are the spatial and temporal grid increments.

When the finite-difference representation of a differential equation is such that the value of a variable $L_{x,\ t+\Delta t}$ is expressed only in terms of its values at a previous time step L (x,t), an explicit finite difference formulation results. However, when the values of $L_{(x,\ t+\Delta t)}$ at various spatial points are related in an equation, an implicit formulation results.

The explicit finite difference formulation was found appropriate for the on-line state estimation schemes developed in this study. However, the implicit finite difference methods have been applied in other water quality studies such as [156] .

In the following, the explicit finite difference equations of some specific estuary conditions are presented. For an example of a one-dimensional well mixed, non-saline estuary system with constant dispersion and decay terms, application of (4.15), (4.16), (4.17) to (2.11) and (2.12) yields.

$$L_{x,t+1} = \frac{E \Delta t}{(\Delta x)^2} [L_{x+1,t} - 2L_{x,t} + L_{x-1,t}]$$

$$- \frac{U_{x,t} \Delta t}{2 \Delta x} [L_{x+1,t} - L_{x-1,t}]$$

$$- \Delta t K_r L_{x,t} + L_{x,t} \qquad (4.18)$$

$$C_{x,t+1} = \frac{E \Delta t}{(\Delta x)^2} [C_{x+1,t} - 2C_{x,t} + C_{x-1,t}]$$

$$- \frac{U_{x,t} \Delta t}{2 \Delta x} [C_{x+1,t} - C_{x-1,t}]$$

$$- K_r \Delta t L_{x,t} + K_a \Delta t (C_s - C_{x,t})$$

$$+ \Delta t P_{x,t} + C_{x,t} \qquad (4.19)$$

For the two-dimensional stratified estuary system treated in Chapter IX, the explicit finite difference representation of equations (2.9) and (2.10) become

$$L_{x,z,t+1} = \frac{E_x \Delta t}{(\Delta x)^2} \left[L_{x+1,z,t} - 2L_{x,z,t} + L_{x-1,z,t}\right] + \frac{E_z \Delta t}{(\Delta z)^2} \left[L_{x,z+1,t} - 2L_{x,z,t} + L_{x,z-1,t}\right] - U_{x,z,t} \frac{\Delta t}{2\Delta x} \left[L_{x+1,z,t} - L_{x-1,z,t}\right] - \Delta t\, K_r L_{x,z,t} + L_{x,z,t} \tag{4.20}$$

and

$$C_{x,z,t+1} = \frac{E_x \Delta t}{(\Delta x)^2} \left[C_{x+1,z,t} - 2C_{x,z,t} + C_{x-1,z,t}\right] + \frac{E_z \Delta t}{(\Delta z)^2} \left[C_{x,z+1,t} - 2C_{x,z,t} + C_{x,z-1,t}\right] - U_{x,z,t} \frac{\Delta t}{2\Delta x} \left[C_{x+1,z,t} - C_{x-1,z,t}\right] - \Delta t\, K_r L_{x,z,t} + K_a \Delta t\, (C_s - C_{x,z,t}) + C_{x,z,t} \tag{4.21}$$

where a one-dimensional tidal flow in the x-direction is assumed and the photosynthetic and other zero-order sources are neglected.

Boundary Conditions and Stability Requirements

Stability criteria.

A major problem that may plague a finite difference computational scheme, if care is not exercised, is the instability of solutions resulting from uncontrollable amplification of numerical errors. These errors are usually introduced by the finite-difference approximations of the system differential equations and inappropriate initial and boundary conditions.

Avoidance of this problem was crucial to successful development of the computer programs used in this study because

(i.) The distinct effect of simulated measurement noise was being investigated.

(ii.) On-line parameter estimates based on noisy measurements might violate the stability conditions especially during the initial time steps of an iteration scheme.

Care had to be taken, especially in the study of the two-dimensional estuary with non-linear distributed tidal velocity (Chapter IX) to ensure that the maximum expected parameter estimate errors satisfy the stability criteria.

Leendertae [78] and Lily [80] have presented detailed analysis of stability problems in finite difference solutions of some mass transport equations. Dresnack and Dobbin [36] have also developed a two-step explicit method by which the convective process is operated in one-step and the the dispersive and other processes are operated in the computation of distribution profiles in a tidal river.

The preceeding methods guarantee that the coefficients of the individual concentration in (4.18) and (4.19) are positive. The positiveness of the coefficients has been chosen as the basis for establishing stability criteria in this and many other studies [156].

Applying this conditions to (4.18) and (4.10), yields

$$\frac{E \Delta t}{(\Delta x)^2} - \frac{U \Delta t}{2 \Delta x} > 0$$

and

$$- \frac{2 E \Delta t}{(\Delta x)^2} - \Delta t K + 1 > 0$$

from which the stability criteria for the one-dimensional tidal estuary are derived as

$$\Delta x < \frac{2 E}{U_{max}} \tag{4.22}$$

$$\Delta t < \frac{(\Delta x)^2}{2E + (\Delta x)^2 [K_r, K_a]_{max}}$$

U_{max} is the maximum tidal velocity and $[K_r, K_a]_{max}$ is the larger of the two decay rates which usually is K_a.

For the two-dimensional estuary with zero vertical velocity, the stability criteria become

$$\Delta x < \frac{2 E_x}{U_{max}} \tag{4.24}$$

and

$$\Delta t < \frac{(\Delta x)^2 \; (\Delta z)^2}{2 E_x (\Delta z)^2 + 2 E_z (\Delta x)^2 + [K_a \; K_r]_{max} (\Delta x)^2 \; (\Delta z)^2}$$

Boundary conditions.

The central difference formulation employed in this study allows computation of concentrations only at the internal points of the spatial-temporal grid. Conditions that satisfy the appropriate transfer processes at the boundaries are required for complete solutions. Several methods of extrapolation of solutions at the boundaries of finite difference grids have been investigated by [156].

In this study, upstream boundary conditions are assumed to be determined from measurements and are implemented in the sequel by the addition of simulated random noise to a specific boundary value. The grid downstream boundary conditions are readily established for the case of a stream with negligible dispersion.

It is known from the behavior of the physical system that steady state conditions are reached shortly after the time required to flush the stream reach has elapsed, that is at

$$t > \frac{ss}{U}$$

where ss is the length of the reach and U is the velocity of flow. It is sufficient, therefore, to choose a grid with a downstream boundary located a few grid points beyond the physical boundary of the reach. By this technique, an arbitrary downstream boundary condition may be assumed without introducing errors into the computation. This approach has been successfully applied in [36].

The time it takes a solution to reach essential steady state in a dispersive-advective system depends on the relative values of the coefficients. If the coefficients are known, it is possible to determine the size of the grid required such that arbitrary boundary conditions may be applied as mentioned above. A system with comparable effects of the dispersive and advective terms may require a very large grid to satisfy this condition.

An alternative approach is to approximate the value of the solution at the boundary of the grid by linear extrapolation of the values at adjacent internal grid points. In this study an approximation of the type

$$L_{xf,\, t+1} = 2\, L_{xf-1,t+1} - L_{xf-2,t+1} \qquad (4.26)$$

is used, where x_f is the downstream boundary of the grid.

For the two-dimensional estuary considered, it is assumed that no transfer of pollutants occurs across the surface or the bottom of the system. This is a common assumption in the analysis of water-quality systems, although the gradient of dissolved oxygen concentration at the bottom has been equated with benthal demand in some cases [1]. The extrapolation approximation (4.26) is applied in this case where benthal deposit is negligible, to determine the solution values at the surface and boundary grid points based on the generated values at the internal points.

This chapter has presented a review of solution techniques applicable to many water-quality systems. In addition, the finite-difference and real time solutions of some specific models to be treated in later chapters have been developed.

CHAPTER V

MULTIPLE MEASUREMENTS AND ESTIMATION THEORY IN WATER QUALITY MODELS

Multi-disciplinary approaches have been applied in recent years to the problems of modeling, analysis and control of polluted rivers and estuaries. In addition, improvements in instrumentation design have advanced efforts towards the automation of waste water treatment plants and on-line control of polluted water systems.

As part of the contributions of this study, estimation theory developed and normally used in communication and control systems is extended in this and subsequent chapters to water quality systems. Multiple measurements techniques are developed and applied to obtain Kalman type filters for optimum state estimation in a class of distributed systems.

The overall objective is to derive optimum on-line estimates of biochemical oxygen demand (BOD) and dissolved oxygen (DO) concentration profiles in polluted streams and estuaries. The special techniques developed emphasize those features such as model structure, measurement procedure and cost functions which may be unique to water quality systems.

There are several motivations for applying filtering theory to problems in water quality systems. Because of the turbulence in a natural water body, mass transport and distribution of dissolved pollutants are inherently stochastic processes. Although deterministic models are often used in water pollution analysis, stochastic models have been developed and applied in some cases [121 , 29 , 131 , 144]. As the stochastic modeling of these systems expands, so will the importance of stochastic estimation and control theory in water quality application problems.

Random instrument noise is another factor suggesting the application of filtering theory in water quality analysis. For model verification, important parameters such as the dispersion and reaction rates coefficients cannot be measured directly. Instead they are derived analytically from measured distribution of such variables as BOD, DO and salinity (Chapter III). An instrument subject to strong winds, currents and other adverse environmental conditions or an analytical laboratory measurement procedure subject to human qualitative judgments may produce random results. Without a proper estimation approach, this may produce serious errors in subsequent computations and analysis based on the noisy measurements.

There are two types of water quality standards namely stream standards and effluent standards [38]. Stream standards establish the allowable threshold values of such variables as dissolved oxygen based on the intended uses of that segment of the water system. It is desirable to apply a filtering technique in monitoring these variables to ascertain that established standards are not violated. This is particularly important because of the stochastic nature and the sensitivity of the pollutant distribution to density and temperature changes.

In urban areas, several municipal and industrial complexes use the same river or estuary as receiving water for their wastes. The establishment of an equitable policy for the allocation of loads and degree of effluent treatment among users requires the knowledge of the on-line response of the river to the various loads.

In addition, considerable research has been conducted by Perlis and associates [108 , 109], Tarassov et al [134] and Thomann et al [141] on optimum control of polluted water systems. An on-line adaptive control scheme obviously requires on-line optimum estimates of the state profiles as inputs.

Although the foregoings are sound arguments for applying filtering theory to water quality analysis, these systems present some unique problems. The dynamics of DO and BOD are coupled in one of the state equations, however, the variables are not measurable at the same rate. Instrumentation is available for measuring DO concentration in a matter of minutes, hence DO monitoring may be considered an on-line process. On the other hand, the measurement of BOD requires a laboratory process of seeding and incubation of water samples which may take between five to twenty days. This delay in BOD monitoring obviously creates a handicap to conventional on-line estimation or control techniques. In addition, water samples for BOD measurements are usually taken at several hours intervals in practice.

Other forms of oxygen demand such as chemical oxygen demand (COD) and total organic carbon (TOC) have been established to be functions of BOD concentrations for specific streams and under certain conditions. Whenever available measurements of such variables provide addition information on BOD distribution with a particular advantage that they can be measured relatively fast. TOC which for a particular water body under fairly steady load is known to be approximately a linear function of BOD can be measured in a matter of minutes [40 , 114] and may also be considered as an on-line process [49].

One aspect of the multiple measurements theory developed in this study concerns the optimization of the various weights (filters) to be associated with both the noisy on-line DO and TOC measurements and the off-line BOD measurements to obtain an on-line estimation of BOD and DO state profiles. This subject is covered in Chapters VIII and IX for stream and estuary models.

Water quality variables are generally distributed both temporally and spatially. However, instrumentation capable of making distributed measurements are not available. This leads to the question of spatial location of measuring instruments. Another contribution of the study is the development of a comprehensive theory for determining the optimum monitoring stations in a class of distributed parameter systems. This theory based on statistical experimental design techniques is applied to examples of estuary systems in Chapter VI.

A special method is required for the combination of various types of measurements available at different sampling rates. In the third section of this chapter, a unique method is presented by which off-line BOD measurements may be projected to the time of on-line estimation for specific stream and estuary systems.

The cost function to be optimized in the estimation developments is presented in the fourth section. The function is formulated to represent realistic engineering cost considerations in water quality analysis. It includes the variance of the estimate errors which represents the costs of uncertainties in estimates and an additional term representing the costs of making observations (instrument cost, labor and so on). However, before these considerations, a brief review of pertinent prior work on estimation theory in lumped and distributed systems and earlier applications of the multiple measurements concept are presented in the next two sections.

Estimation Theory In Lumped Parameter Systems

Steady state lumped systems.

Wiener [153] pioneered the procedure of designing an optimum, physically realizable filter to extract and predict a signal from a continuous stationary noise-contaminated measurement. The predicting process is summarized in figure V.1 where s(t) is the true signal which is contaminated by a random noise n(t) in the measurement y(t). The desired output signal $s^*(t)$ is a known function of s(t) where H(p) and h(t) are the frequency and impulsive responses of the ideal predictor.

Owing to the random noise and in some cases physical unrealizability of the ideal predictor the actual output signal estimate $\hat{s}(t)$ contains an estimate error $\epsilon(t)$. K(p) and k(t) are the frequency and impulsive responses of the actual filter.

Wiener's development based on the minimization of the ensemble variance of the estimate error $\epsilon(t)$ yielded a linear filter of infinite memory. Later investigations by Zadeh and Ragazzini [157] produced a more practical finite-memory optimum filter. Franklin [45] and Lees [79] similarly developed infinite memory and finite-memory filters for noisy discrete measurement processes. Among the other early applications of Wiener's theory were the processing of an analog signal from noisy digital measurements [89] and the use of spectial factorization to develop Wiener-type linear filters for multivarible systems [67].

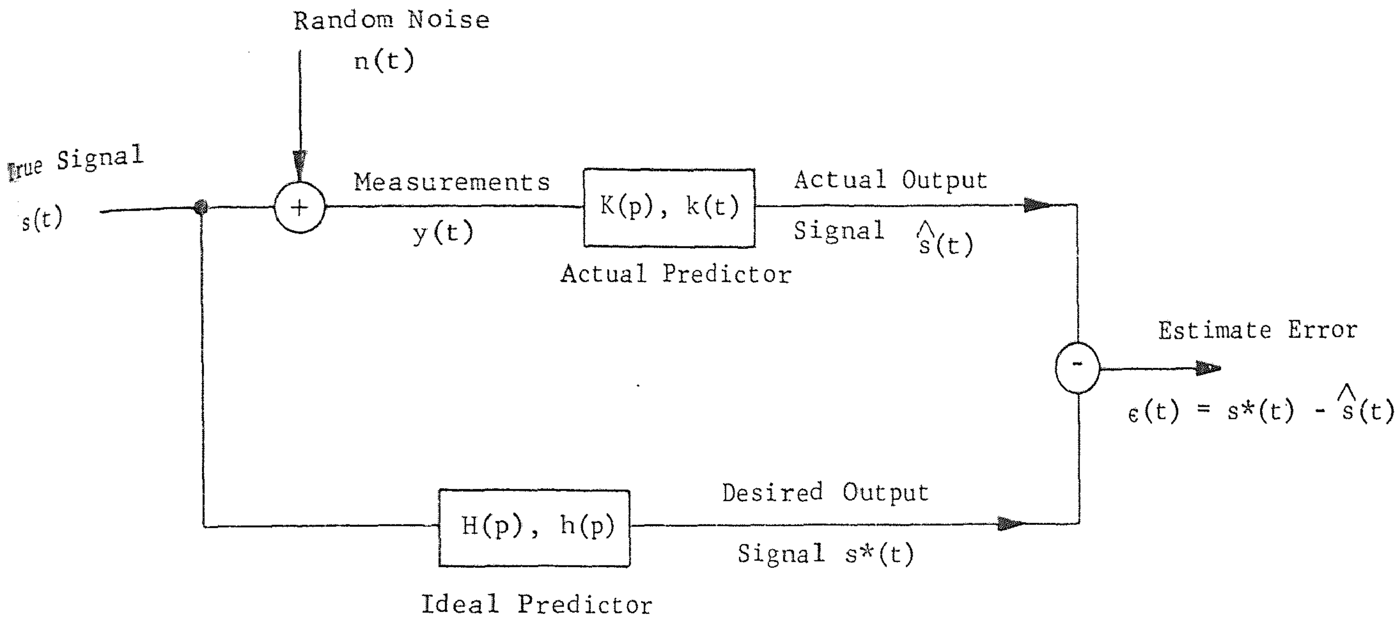


FIGURE V-1. Prediction Process in Wiener's Theory

The definition of multiple measurements technique in this study is the use of noisy independent measurements of related forms of a signal for the optimum estimation of the signal. From this point of view one of the earliest estimation problems involving multiple measurements was by Bendat [8] wherein the author extended Wiener's procedure to obtain linear time-invariant filters for the optimum filtering of two related signals. Bendat's problem is summarized in Figure V.2 where $y_1(t)$, $y_2(t)$ are independent noisy measurements of signals $s_1(t)$, $s_2(t)$ which are related through the response function F(p). The figure shows the process for the optimum filtering of signal $s_2(t)$ using the Wiener-type optimum filtered estimate $\hat{s}_1(t)$. Chang [19] solved a similar problem using the method of spectral factorization. The above multiple measurement techniques have found application in missile guidance systems [130] where simultaneous measurements of position and acceleration were used to minimize the position deviation of a load of primary inertia.

Hung [61 , 60] derived equivalent filters for discrete noisy measurements having different sampling rates and from a combination of continuous and discrete noisy monitorings of the same signal. His results are useful in trajectory tracking where it may be necessary to reduce the load capacity of a processing digital computer by taking analog and digital measurements in parallel.

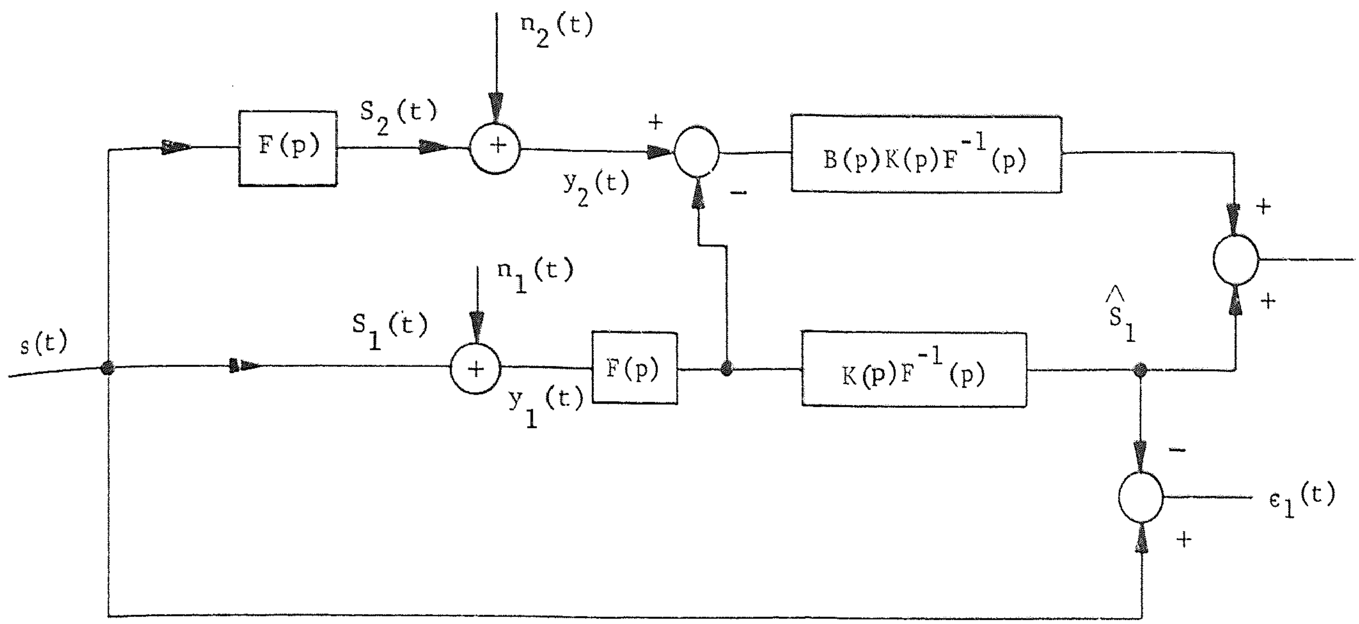


FIGURE V-2. Summary of Bendat's Multiple Filtering Process

Dynamic Lumped Systems.

Often, the form of a signal is known only through a model of the differential equation describing its dynamics. State estimation in lumped dynamic systems was initiated by Kalman [65] in deriving finite-time optimal filter for linear systems with noise stationary noises. Kalman and Bucy [66] extended a similar procedure to discrete-time linear systems with Gaussian white noises. These two pioneering works utilized a Bayesian approach of estimation and have set a framework for numerous later investigations.

Extensive literature is available on recent developments in estimation theory; one comprehensive reference textbook is by Sage and Melsa [118]. A detailed review of estimation theory is not the interest of this study, suffice to say that various classes of problems have been studied including

(i) linear systems [65, 66, 26]

(ii) non-linear systems [32, 132]

(iii) time delay systems [15]

and (iv) stochastic systems [58, 155]

with various types of system and measurement noises among which are

(i) Non-Gaussian noises [46]

and (ii) State-correlated noises [17].

For non-linear systems an optimal filter is generally infinite-dimensional. Some investigators have achieved more practical finite-dimensional filters by utilizing some of the following approximations

(i) Taylor series expansion [5]

(ii) Stochastic linearization [57] [119]

and(iii) quasi-linearization [132] [21].

The existing approaches to estimation problems in dynamic systems include

(i) minimization of the mean square error [124]

(ii) minimization of integral weighted square error [32]

(iii) minimum variance method [20] [4]

(iv) Bayesian approacy [65, 66, 58]

(v) optimal control theory [4, 77]

(vi) characteristic function approach [143]

(vii) orthogonal-projection lemma [142]

and (vii) Fokker-Plank equation approach [144]

The procedures of solving the derived filtered equation may include

(i) analytical solution [8]

(ii) numerical analysis method [86]

and (iii) dynamic programming [26]

Most of the preceding publications have developed estimation schemes based on noisy measurements of only one form of the state vector. From the point of view of this study, multivariate measurement vectors and discretized measurements of the same form of the state vector are considered special cases of single measurements techniques.

Very few researchers have actually applied the techniques of multiple measurements or provided precedures adaptable to multiple measurements concepts. With a shaping filter a system having state-correlated noises (colored noise) may be reduced to an augumented system in which all measurements either contain additive white noise or are noise-free. Bryson and Johansen [17] using a matrix partitioning method have estimated state vector from such a mixture of measurements.

Chang [20] developed an algorithm for state vector estimation based on noisy discretized measurements. At zero limit of the time interval, the algorithm reduces to a filter for continuous measurements. A combination of both results yielded a state filtering algorithm based on multiple discrete and continuous measurements of the state vector. This particular paper represents a good application of the multiple measurements techniques and sets a basis for the theory developed in this study for distributed parameter systems.

The theory of multiple measurements has been applied in some cases of real engineering problems. For a class of linear augmented system representable by a steerable antenna control system Perlis [106] used the spectral factorization method to develop sub-optimal filters based on continuous and discrete noisy measurements of the same signals. Also, Mehra [86] has applied a similar multiple measurements approach to parameter identification in an aircraft using noisy measurements of the state vector and its derivatives.

Estimation Theory In Distributed Parameter Systems

Tzafestas and Nightingale have contributed significantly to the literature on estimation in distributed systems. In [142], optimum state estimate in a class of distributed system was derived from noisy distributed (spatially and temporally) measurements. The estimate, formulated as a linear transformation of the measurements, was obtained by utilizing an orthogonal-projection lemma technique. A characteristic function approach was applied in [143] to a similar problem to obtain results for state-correlated noises. Another publication [144] by the same authors considered a Bayesian maximum likelihood approach to the filtering problem in non-linear distributed systems. Differential dynamic programming was applied to solve the filtered equations.

An important limitation of the preceding studies is the assumption of distributed form of measurements. In practice, as in the case of water quality systems, distributed measurements are not available. Meditch [85] coped with this difficulty partially by considering a scanner-type measurement which is only distributed in time. Thau [136] has considered a more practical scheme where measurements are taken at a point in the spatial domain. The results of the work have been further developed in this study to include cases of multivariate systems with several monitoring stations. In addition, the problem of the optimum number and the optimum spatial locations of monitoring stations considered by Pell [103], Seinfield [125] and Perlis [107] is studied with a comprehensive approach and presented in detail in Chapter VI.

The preceding sections have presented a review of the status of estimation theory and multiple measurements application in prior works. In the next two sections, the measurements projection schemes and the cost functions to be employed in the development of the multiple measurements techniques in this study are presented.

Off-line Measurements Projection In Water Quality Systems

Application to a stream model.

A special scheme is required to properly utilize off-line measurements in an optimum on-line estimation or control problem. In the following, measurements projection techniques developed to project an off-line BOD measurement to the point of on-line estimation in a specific stream model, is presented.

Figure V-3 shows the definition of the time variables employed in the development. For a specific stream or estuary system, the approximate linear function relating TOC and BOD concentrations is represented by

$$TOC\ (x,t) = TG * BOD\ (x,t) + TIN \qquad (5.1)$$

where TG is the slope and TIN is the intercept. Numerical values for TG and TIN depend on the characteristics of the pollutional load to which the stream or estuary is subjected and, therefore, may vary for different streams or over different reaches of the same stream. These constants may be evaluated from the readings of the values of TOC and BOD in a particular segment and under steady state and steady load conditions. Typical values for TG range between 1.55 and 2.55 [44 , 40 , 114].

The set of TOC and DO readings taken on-line at point $(x_{m},\ i\ T)$ is then represented in terms of the state vector as

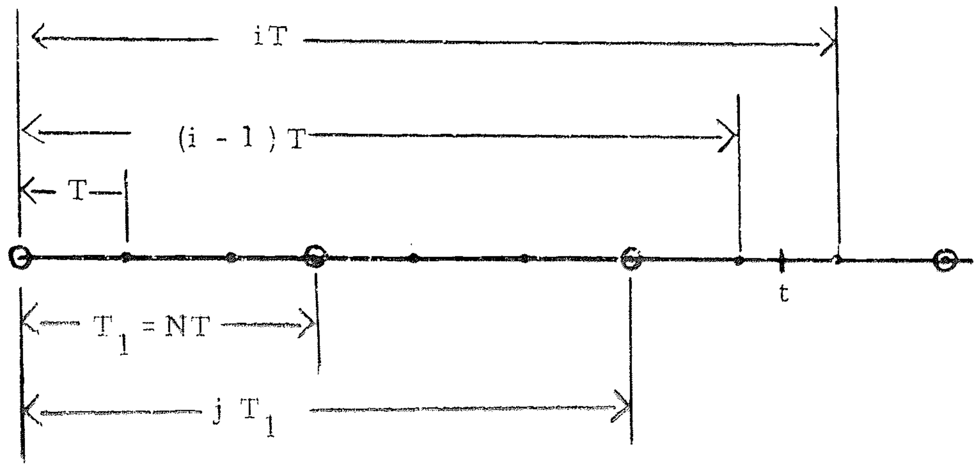


FIGURE V-3. Definition of Time Variables for Delayed Measurement Projection

$$\underline{Y}(x_m, iT) = \underline{H}(iT)\ \underline{V}(x_m, iT) + \underline{\xi}(iT) \qquad (5.2)$$

$$\text{for } i = 0, 1, 2, ---$$

where T is the on-line sampling period which usually has a range from a few minutes to a few hours. The first component of $\underline{Y}$ is the result of substracting TIN from the TOC readings. The measurements noise vector $\underline{\xi}$ (i T) is represented as a zero mean white noise with a variance term

$$E\left\{\underline{\xi}(iT)\,\underline{\xi}^T(iT)\right\} = \underline{R}_i(iT)$$

ξ_1 (i T), the noise associated with the TOC measurements represents the lumped effects of both the linear approximation and the instrument errors.

In practice, water samples for BOD measurements are taken at several hours interval. This rate is shown as T_1 in Figure V.3 where for convenience T_1 is considered to be an integral multiple of T. In addition, there is a fixed time delay, T_D before the values of BOD readings are obtained. For an on-line estimation or control analysis it is desired to write the delayed measurements taken at $(x_D, j T_1 - T_D)$ in terms of the state vector values at the on-line estimation point $(x_m, j T_1)$.

The delayed measurements in terms of the state aector value at $(x_D, j T_1 - T_D)$ is represented by

$$\underline{T}\ (x_D,\ j\ T_1 - T_D) = \underline{O}\ (x_D,\ j\ T_1 - T_D)\ \underline{V}\ (x_D,\ j\ T_1 - T_D) + \underline{\eta}\ (j\ T_1 - T_D) \tag{5.3}$$

for $\quad j\ T_1 > T_D$ and $j = 1,2,3,$ ---

where vector $\underline{T}$ includes off-line BOD and DO (added for symmetry of vector representation) readings. Again, the noise element is considered zero-mean white type with variance

$$E\left\{\underline{\eta}\ (j\ T_1)\ \ \eta^T\ (j\ T_1)\right\} = \underline{N}\ \ (j\ T_1)$$

The expected value of the state vector from (5.3) becomes

$$\overline{\underline{V}}\ \ (x_D,\ j\ T_1 - T_D) = \underline{O}^{-1}\ (x_D,\ j\ T_1 - T_D)\ \underline{T}\ (x_D,\ j\ T_1 - T_D) \tag{5.4}$$

By substituting in Chapter IV

$$to = t - \frac{(x - x_D)}{U}$$

from (4.8)into (4.7), it follows that for a stream with negligible dispersion, the current state profile $\underline{V}$ (x,t) may be written in terms of its previous values at x_D as

$$\underline{V}\ (x,t) = \underline{\Phi}\ [t,\ t - \frac{(x - x_D)}{U}\ ]\ \underline{V}\ [x_D,\ t - \frac{(x - x_D)}{U} \tag{5.4}$$

for $x_D \leq x \leq Ut$

At $(x_m,\ j\ T_1)$ equation (5.4) yields

$$\underline{V}(x_m, j\,T_1) = \underline{\Phi}\left[j\,T_1, j\,T_1 - \frac{(x - x_D)}{U}\right] \underline{V}\left[x_D, j\,T_1 - \frac{(x_m - x_D)}{U}\right] \quad (5.5)$$

If x_D is chosen such that

$x_m = x_D + U\,T_D$, then (5.5) becomes

$$\underline{V}(x_m, j\,T_1) = \underline{\Phi}[j\,T_1, j\,T_1 - T_D]\,\underline{V}[x_D, j\,T_1 - T_D] \quad (5.6)$$

Similarly, the expected state vector $\bar{\underline{V}}(x_D, j\,T_1 - T_D)$ from the delayed measurements in (5.3) may be projected to $(x_m, j\,T_1)$ using (5.6) as follows

$$\bar{\underline{V}}(x_m, j\,T_1) = \underline{\Phi}[j\,T_1, j\,T_1 - T_D]\,\underline{O}^{-1}[x_D, j\,T_1 - T_D]\,\underline{T}[x_D, j\,T_1 - T_D] \quad (5.7)$$

Substituting (5.3) and then (5.6) into (5.7)

$$\bar{\underline{V}}(x_m, j\,T_1) = \underline{V}(x_m, j\,T_1) + \underline{\Phi}[j\,T_1, j\,T_1 - T_D]\,\underline{O}^{-1}(x_D, j\,T_1 - T_D)$$

$$\underline{\eta}(j\,T_1 - T_D)$$

The above is rewritten as

$$\underline{Z}(x_m, j\,T_1) = \underline{M}(j\,T_1)\,\underline{V}(x_m, j\,T_1) + \underline{\rho}(j\,T_1) \quad (5.8)$$

$$\text{for } j\,T_1 > T_D \quad j = 1, 2, ---$$

Where for the above assumptions $\underline{M}(j\,T_1) = \underline{I}$ (unitary matrix)

The noise is still zero-mean

$$\underline{\rho}\ (j\ T_1) = \underline{A}\ \ \underline{N}\ (j\ T_1 - T_D) \qquad (5.9)$$

with a variance

$$E\left\{\underline{\rho}\ (j\ T_1)\ \underline{\rho}^T\ (j\ T_1)\right\} = \underline{A}\ \underline{N}\ (j\ T_1 - T_D)\ \underline{A}^T \qquad (5.10)$$

where

$$\underline{A} = \underline{\Phi}\ (j\ T_1,\ j\ T_1 - T_D)\ \underline{Q}^{-1}\ [x_D,\ j\ T_1 - T_D] \qquad (5.11)$$

Thus, the delayed measurements represented by (5.3) may now be represented on-line as formulated in (5.8). At $i\ T \neq j\ T_1$, only one set of measurements is available to the on-line estimation scheme as represented by (5.2). However, at $i\ T = j\ T_1$ both sets of measurements (5.2) and (5.8) are available and may both be used as on-line measurements.

Application to estuary models.

It may be observed by comparing (5.3) and (5.8) in the preceding development that the projection scheme results in the modification of the noise component through an operation of the impulsive response $\Phi\ (j\ T_1,\ j\ T_1 - T_D)$. The contributions at $(x_m,\ j\ T_1)$ of the errors in the delayed measurements have the same effects as instantaneous initial conditions imposed on the system at $(x_D,\ j\ T_1 - T_D)$. This result is very useful in that it may then be extended to the estuary models in which the impulsive responses are known.

In the following, only the projection of off-line BOD measurements are considered because of the complexity of the DO impulsive response. BOD distribution responses to slug inputs have been derived for various cases of estuary conditions in (4.10), (4.12) and (4.14). Equation (4.10) may be rewritten as [55]

$$L(x, t) = L_o\, u\, \phi(x, t; x_o, t_o) \tag{5.11}$$

where L_o is a reference initial concentration

$$L_o = \frac{w}{Au}$$

A is the cross-sectional area of the estuary and ϕ is a transition function

$$\phi(x,t; x_o, t_o) = \frac{1}{\sqrt{4\pi E(t - t_o}} \exp\left\{- \frac{[(x-x_o) - u(t - t_o)]^2}{4E(t - t_o)} - K_r (t - t_o)\right\} \tag{5.12}$$

If the delayed BOD measurement, taking at a point $(x_D, j T_1 - T_D)$, is represented as

$$T(x_D, j T_1 - T_D) = L(x_D, j T_1 - T_D) + \eta(x_D, j T_1 - T_D) \tag{5.13}$$

it follows from equation (5.8) and (5.13) that the corresponding on-line representation at $(x_m, j T_1)$ becomes

$$Z_1(x_m, j T_1) = L(x_m, j T_1) + \rho_1(j T_1) \tag{5.14}$$

where the modified noise component is

$$\rho_1 \, (j\, T_1) = u\, \phi\, (x,\, t;\, x_D,\, j\, T_1 - T_D)\, \eta\, (x_D,\, j\, T_1 - T_D) \tag{5.15}$$

with a variance

$$E\, [\rho_1^2\, (j\, T_1)\,] = u^2\, \phi^2\, (x, t;\, x_D,\, j\, T_1 - T_D)\, N_1\, (x_D,\, j\, T_1 - T_D) \tag{5.16}$$

The expressions for the on-line representation of off-line BOD measurements in other cases of estuary conditions are similar to equations (5.14), (5.15) and (5.16) with the following modifications

(i) for the tidal river with oscillatory flow (equations (4.10), (4.11)), the term u in (5.15) is replaced by u_F, the velocity of fresh-water flow.

Also, the transition function ϕ becomes the coefficient of W in equation (4.12) evaluated at $x = x_m$, $x_o = x_D$, $t = j\, T_1$, and $t_o = j\, T_1 - T_D$.

(ii) for the two-dimensional estuary example in equations (4.13) and (4.14) the term u in (5.15) is replaced by u_F and the transition function ϕ is the coefficient of W in equation (4.14) evaluated as above.

This concludes the development of the off-line measurements projection to the time of on-line estimation. Although only delayed BOD measurements are considered in the estuary cases, other laboratory methods of measuring DO may include a fixed time delay. In that case, a similar projection scheme may be developed based on the DO transient response, when available for an estuary model. Without loss of generality, another set of on-line DO measurements are assumed in later chapters to enable the use of measurement vectors such as in equation (5.8).

Optimization Criterion

The general formulation of the optimization criterion to be employed for the on-line estimation problems treated in later chapters is now presented. The formulation aims at a realistic representation of the cost considerations in water pollution problems.

The cost function used in this study is written as

$$P\,(x_m,\ i\,T^+) = \int_{x_o}^{x_f} E\left\{\left[\lambda(x)\ \underline{\tilde{V}}\ (x,\ i\ T^{\,+})\right]\right\}\ dx$$

$$+\ e\ (x_m,\ i\ T)\ \left[\delta(i\ T - j\ N\ T_1)\ \underline{\beta}\ \underline{C}_D\ (x_D)\right.$$

$$\left. +\ \underline{\alpha}\ \ \underline{C}\ (x_m)\right] \qquad (5.17)$$

The variance term represents the costs of possible damage to such benefits as recreational facilities, aquatic life and so on, due to uncertainties in estimates. This may be regarded as the economics of irreplaceable assets [59 , 70]. The remaining terms represent costs of observation which may include instrument and operational costs.

More detailed definitions and the methods by which the various cost factors ($\underline{\lambda}, \underline{\delta}$ and $\underline{\alpha}$), may be evaluated are discussed in Chapter X. The development of the estimator indicator $e(x_m, i\,T)$ whose optimum values dictate measurements strategy (such as the optimum number and temporal intervals between measurements) is also presented in that chapter. The estimation problems presented prior to Chapter X employ only the variance part of the cost function.

This chapter has presented the background literature on which the estimation techniques developed in this study are based. In addition, the role of this study in the general state-of-the-art of water pollution analysis has been discussed. Also, a projection technique for the optimum utilization of off-line measurements for on-line estimation and control in water quality systems has been presented as part of the contributions of this investigation. Subsequent chapters include other important aspects of the multiple measurement techniques developed in this study namely

(i) optimum measurement strategy (Chapter VI and X)

(ii) optimum parameter estimation (Chapter VI and VII)

(iii) optimum Kalman-type filtering in distributed systems (Chapter VIII and IX).

Numerical results obtained from the application of the multiple measurements techniques developed here, to state and parameter estimation in some specific stream and estuary examples are also presented.

CHAPTER VI

OPTIMUM SPATIAL MONITORING STATIONS IN DISTRIBUTED PARAMETER SYSTEMS

An important engineering problem in modeling and control is that of estimating the state and parameters of a dynamic system from field data which as often corrupted with noise. Consequently, the numerical accuracy of any estimated variable depends both on the quality of the data used and the strategy by which the data are acquired.

For estimation in a lumped parameter system with continuous monitoring, the problem of measurement strategy is that of determining the optimum length of time over which measurements may be taken. In the case of discrete monitoring, the problem becomes determining the optimum number and sampling intervals of measurements on which an estimation scheme is based. One approach to this problem is presented in Chapter VI of [118] for a non-dynamic system with colored noise.

The question of measurement strategy is even more critical in dynamic distributed systems because instruments capable of temporally and spatially continuous monitoring are rare in practice. The scanner-type of measurements suggested in [85] is applicable only to special cases of distributed systems with large time constants such as heat transfer systems or to a steady-stream having a known mean velocity. It may be inadequate for a two-dimensional dynamic estuary.

While extensive literature is available on state and parameter estimation in systems of various types, very few contain a systematic approach to determining where and when measurements may be taken. Field engineers tend to rely on experience with emphasis on the constraints imposed on measurements by the physical nature of the system being considered. Theoretical papers often assume either continuously distributed measurements or an arbitrary number of samples taken at equal intervals.

Among the merits of these approaches is the ease of analysis. However, when an important factor such as cost of making measurements is considered, neither of these approaches is optimum. This point is well illustrated in the publications by Berthouex and Hunter [10], [11] where an analytical approach is presented for planning BOD experiments in a steady-state scalar BOD equation. Nahi [88], Cooper [24], Cooper and Nahi [25], Aoki and Li [6] have obtained the optimum number of observations for estimation and control of various examples of lumped-parameter stochastic systems. Senfield and Chen [125] and Thau [ ] are among authors who have considered the problem of optimum spatial monitoring location in specific examples of distributed systems.

In this chapter, statistical experimental design techniques [11] are applied to develop a general method to determine the optimum spatial monitoring locations for sequential filtering and parameter estimation in a non-linear, dynamic multivariate distributed system. The filtering and parameter estimation schemes are presented in later chapters. The results of the development in this chapter are formalized by two theorems given for the optimum number and the locations of spatial stations for simultaneous monitoring of each component of the state vector.

Recognizing that close-form solutions may not exist for the partial differential equations representing many water quality and other distributed systems of interest, the development in the sequel is based on an explicit finite difference representation (Chapter IV). Deterministic models with constant or time-varying but spatially uniform parameters are treated. A model of this type may represent a segment of a stream or estuary with constant dispersion and decay rates coefficients. Such segments may be combined by matching appropriate boundary conditions for a treatment of a more general system [96] wherein parameters vary spatially.

Both types of instantaneous and delayed measurements in Chapter V are considered. In each case, additive guassian white measurement noise is assumed. The basic concepts of the measurement strategy theory is first developed using an example of the scalar equation representing the dynamics of biochemical oxygen demand in a simple one-dimensional estuary. The theory is then extended to a multivariate system distributed in one spatial dimension. It is further extended to a multivariate system distributed in a multi-dimensional space. For the last two cases, the development is illustrated through specific systems used in numerical examples in later chapters.

Scalar One-Dimensional Distributed System

Consider a deterministic system

$$\frac{\partial L(x,t)}{\partial t} = E \frac{\partial^2 L(x,t)}{\partial x^2} - U \frac{\partial L(x,t)}{\partial x} - K_r L(x,t) \qquad (6.1)$$

which represents the dynamics of biochemical oxygen demand concentration L (x,t) in a simple estuary or a tidal river with constant coefficients. An explicit finite-difference representation of the state profile at any time t based on the profile at a prior time t - 1 is

$$L_{x,t} = \frac{E\Delta t}{(\Delta x)^2}(L_{x+1,t-1} - 2L_{x,t-1} + L_{x-1,t-1})$$

$$- \frac{U\Delta t}{2\Delta x}(L_{x+1,t-1} - L_{x-1,t-1})$$

$$- \Delta t K_r (L_{x,t-1}) + L_{x,t-1} \qquad (6.2)$$

This may be written in compact form as

$$L_{x,t} = \underline{g}^T_{x,t} \underline{P} + f_{x,t} \qquad (6.3)$$

where $$\underline{P} = \begin{bmatrix} E \\ U \\ K_r \end{bmatrix}, \quad f_{x,t} = L_{x,\, t-1}$$

$$\underline{g}_{x,t} = \begin{bmatrix} \dfrac{\Delta t}{(\Delta x)^2} \left(L_{x+1,\, t-1} - 2L_{x,\, t-1} + L_{x-1,\, t-1} \right) \\ -\dfrac{\Delta t}{2(\Delta x)} \left(L_{x+1,\, t-1} - L_{x+1,\, t-1} \right) \\ -\Delta t \left(L_{x,\, t-1} \right) \end{bmatrix}$$

and Δx and Δt are the spatial and temporal incrementation $x - (x-1)$, $t - (t-1)$, respectively.

It is desired to obtain the optimum number and interval of spatial locations at which BOD ($L_{x,t}$) may be monitored for an on-line filtering or parameter estimation at any time, t. As discussed in Chapter V, a linearly related variable, TOC can be monitored on-line, and this will be used here.

Initially, an arbitrary number M of guassian white noise corrupted instantaneous measurements taken simultaneously at spatial locations $x_1, x_2, \text{---}, x_M$ are assumed. The measurements may be expressed as

$$y_{x_m,\, t} = h_{x_m,\, t}\, L_{x_m,\, t} + \eta_{x_m,\, t} \tag{6.4}$$

$$m = 1, 2, \text{---}, M$$

where the variance of the measurement noise

$$E\left\{\eta_{x_{m},t}\ \eta_{x_{j},t}\right\} = \sigma^2_{m,t}\ \delta\ (x_m - x_j)$$

is assumed to be given, and $h_{x_{m},t}$ is a constant of measurement.

Since a deterministic model is assumed, a Bayesian estimation cannot be obtained as discussed Chapter VI of [118] Instead, a maximum likelihood estimate of $L_{x,t}$ is considered. For this, the conditional density function $p_{y_{x_{m},t}/Lx,t}$ is needed.

From equation (6.4) expressions for the following mean and variance terms may be derived.

$$E\left\{y_{x_{m},t}/Lx,t\right\} = h_{x_{m},t}\ L_{x_{m},t} \tag{6.5}$$

$$\mathrm{Var}\left\{y_{x_{m},t}/Lx,t\right\} = \sigma^2_{m,t} \tag{6.6}$$

Because guassian white noise is being considered, the conditional density function may be written as

$$p_{y_{x_{m},t}/Lx,t} = \frac{1}{\sqrt{2\pi\ \sigma^2_{m,t}}} \exp\left\{-\tfrac{1}{2}\ \frac{\left[y_{x_{m},t} - h_{x_{m},t}\ L_{x_{m},t}\right]^2}{\sigma^2_{m,t}}\right\} \tag{6.7}$$

In addition, because the measurement are considered statistically independent, the joint density function for all M measurements taken at time t becomes

$$p_{y_{x_{m},t},\ m=1,2\ --\ M/Lx,t} = \frac{1}{\sqrt{2\pi}\ \prod_{m=1}^{m} \sigma_{m,t}} \exp\left\{-\frac{1}{2} \sum_{m=1}^{M} \frac{[y_{x_{m},t} - h_{x_{m},t} L_{x_{m},t}]^2}{\sigma_{m,t}^2}\right\} \tag{6.8}$$

Maximum likelihood estimate is defined as the estimate of $L_{x,t}$ that maximized the density function $p_{y_{x_{m},t},\ m=1,2\ --\ M/Lx,t}$

Only the expression in the exponent needs to be optimized, since only this expression depends on $L_{x,t}$ in the density function. If it can be assumed that the profile $L_{x,t-1}$ is known exactly, then it follows from equation (5.2) that only the estimates of the parameters E, U and K_r are required for optimization. Usually, only estimates $\hat{L}_{x,\ t-1}$ of $L_{x,\ t-1}$ are known with an associated variance of estimate error. This is the subject of later chapters. Without loss of generality it is assumed here that $L_{x,\ t-1}$ is known exactly.

For the density function to be maximum with respect to the parameters, it is sufficient that each element in the summation sign be zero. That is

$$y_{x_{m},t} - h_{x_{m},t} \hat{L}_{x_{m},t} = 0 \text{ for } m = 1,2\ --\ M$$

This condition may be expanded using equation (6.3) as

$$\underline{G}^T \hat{\underline{P}} = [\, \underline{H}^{-1} \underline{Y} - \underline{F} \,] \qquad (6.9)$$

where $\underline{G}^T$ is an M x N matrix

$$\underline{G}^T = \begin{bmatrix} g^T_{x_1,t} \\ g^T_{x_2,t} \\ \vdots \\ g^T_{x_M,t} \end{bmatrix}$$

$\underline{H}$ is a M x M matrix

$$\underline{H} = \begin{bmatrix} h_{x_1,t} & 0 & 0 & - & - \\ 0 & - & h_{x_2,t} & 0 & - \\ 0 & 0 & - & - & - & h_{x_M,t} \end{bmatrix}$$

$\underline{Y}$ and $\underline{F}$ are M x 1 vectors

$$\underline{Y} = \begin{bmatrix} y_{x_1,t} \\ y_{x_2,t} \\ \vdots \\ y_{x_M,t} \end{bmatrix} \qquad \underline{F} = \begin{bmatrix} f_{x_1,t} \\ f_{x_2,t} \\ \vdots \\ f_{x_M,t} \end{bmatrix}$$

and N is the dimension of the parameter vector.

It follows from matrix theory [100] that the M x N matrix $\underline{G}^T$ must have a minimum rank of N for a complete solution of the N x 1 parameter vector $\hat{\underline{P}}$. It follows then that the minimum number of spatial independent measurements is N. This is equivalent to a single replicate of Box-Lucas design [14]. In practice, it is desirable to have as much data as possible subject only to the cost of acquiring and processing additional data, so as to increase the confidence of estimates. Where additional measurements are possible, they may be taken at spatial points that satisfy the criterion of replication of Box-Lucas optimum design [149], [45] [79].

The estimate of the parameter vector P is unbaised because

$$E \left\{ \hat{\underline{P}} \right\} = \underline{P}$$

and it has a variance

$$\mathrm{Var}\ (\underline{P} - \hat{\underline{P}}) = [\underline{G}\ \underline{H}^T\ \underline{R}^{-1}\ \underline{HG}^T]^{-1} \tag{6.10}$$

where

$$\underline{R} = \begin{bmatrix} \sigma_1^2 & 0 & 0 & - - & - & - \\ & \sigma_2^2 & 0 & - & - & - \\ & & & & & \\ 0 & 0 & - & - & - & \sigma_m^2 \end{bmatrix}$$

Having established the minimum number of spatial measurement stations as N, the optimum values of $x_1, x_2 --- x_N$ are desired. These are determined to minimize a measure of the variance matrix. It is chosen, for computational convenience to maximize the trace of the inverse of the variance matrix. Other measures such as the determinant of the matrix may be used [11]. The trace term may be written as

$$J = \text{Trace}\,[\underline{G}\,\underline{H}^T\,\underline{R}^{-1}\,\underline{HG}^T] \tag{6.11}$$

Expanding J yields

$$J = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{h^2_{x_{i},t}\, g^2_{jx_{i},t}}{\sigma^2_{j,t}} \tag{6.12}$$

where $g_{jx\,i,t}$ is the j^{th} component of the $\underline{g}_{x_{i},t}$ vector. The trace term is maximum at the spatial points x_j, j = 1 --- N where the absolute value of the j^{th} element of the sensitivity vector $\underline{g}$ is maximum in the spatial domain.

For the specific numerical example used in the section, the optimum number spatial monitoring point at time t is 3 and the measurements points are

$$XM(1) = \max_x \left[\frac{\Delta t}{(\Delta x)^2}\,(\hat{L}_{x+1,\,t-1} - 2\hat{L}_{x,\,t-1} + \hat{L}_{x-1,\,t-1})\right]^2 \tag{6.13}$$

$$XM(2) = \max_x \left[-\frac{\Delta t}{2\Delta x}\,(\hat{L}_{x+1,\,t-1} - \hat{L}_{x-1,\,t-1})\right]^2 \tag{6.14}$$

$$XM(3) = \max_{x} \left[-\Delta t \left(\hat{L}_{x,\ t-1} \right) \right]^2 \tag{6.15}$$

where $h_{x,t}$ and $\sigma^2_{x,t}$ are considered constants.

In case of multiple measurements, additional data taken at time (t - T) may be available at time t (Chapter V). This data may be represented as

$$Z_{x_{m},\ t-T} = O_{x_{m},\ t-T}\ L_{x_{m},\ t-T} + \beta_{x_{m},\ t-T}$$

$$m = 1, \cdots N$$

A similar analysis shows that the optimum monitoring locations at $t - T$ maximize the terms $[g_{j,x,\ t-T}]^2$. In addition, the optimum monitoring stations at time t remain the same. However, the optimum parameter vector estimate using both sets of measurements y_{x_m}, z_{x_m} and following the analysis in the next section becomes

$$\underline{P} = [(\underline{R}^{-1}\ \underline{H}\ \underline{G}^T)_t + (\underline{B}^{-1}\ \underline{O}\ \underline{G}^T)_{t-T}]^{-1}\ [\{\underline{R}^{-1}\ (\underline{Y} - \underline{H}\ \underline{F})\}_t$$

$$+ \{\underline{B}^{-1}\ (\underline{Z} - \underline{O}\ \underline{F})\}_{t-T}]$$

where $\underline{O}$ and $\underline{B}^{-1}$ contain the measurement constants and variances and $\underline{Z}$ represents the measurement vector at time $t - T$.

Multivariate One-Dimensional Distributed System

The measurement theory developed in the previous section is now extended to a two-dimensional state system distributed in one spatial dimension. An example of such system is the coupled dynamics of dissolved oxygen (DO) and biochemical oxygen demand (BOD) in a one-dimensional estuary. The partial differential equations are (Chapter II).

$$\frac{\partial L}{\partial t}(x,t) = E \frac{\partial^2 L(x,t)}{\partial x^2} - U_{(x,t)} \frac{\partial L(x,t)}{\partial x} - K_r L(x,t) \tag{6.16}$$

$$\frac{\partial C}{\partial t}(x,t) = E \frac{\partial^2 L(x,t)}{\partial x^2} - U_{(x,t)} \frac{\partial C(x,t)}{\partial x} - K_d L(x,t) - K_a C(x,t) + K_a C_s + P(x,t) \tag{6.17}$$

Various considerations necessary for the representation of tidal velocity $U_{(x,t)}$ and photosynthesis $P(x,t)$ have been discussed in Chapter III. For the purpose of this section, it suffices to represent them as

$$U_{(x,t)} = U_F + U_T \operatorname{Sin} \omega_T t \tag{6.18}$$

$$P(x,t) = P_H \operatorname{Sin} \omega_D t \tag{6.19}$$

where U_F is the velocity of freshwater flow, U_T is the maximum tidal velocity and P_H is the maximum rate of dissolved oxygen contribution due to photosynthesis. ω_T and ω_D are tidal angular frequency and diurnal angular frequency respectively. It is also assumed that $K_d = K_r$.

The explicit finite-difference representation of $L_{x,t}$ is given by equation (6.2) and $C_{x,t}$ may be written as

$$
\begin{aligned}
C_{x,t} = {} & \frac{E\,\Delta t}{(\Delta x)^2}\left(C_{x+1,\,t-1} - C_{x+1,\,t-1} + C_{x-1,\,t-1}\right) \\
& - \frac{U_{x,\,t-1}\,\Delta t}{2\,\Delta x}\left(C_{x+1,\,t-1} - C_{x-1,\,t-1}\right) \\
& - K_r\,\Delta t\,(L_{x,t-1}) + K_a\,\Delta t\,(C_s - C_{x,\,t-1}) \\
& + \Delta t\,P_{x,t-1} + C_{x,\,t-1}
\end{aligned}
\qquad (6.20)
$$

Equations (6.2) and (6.20) may be written in compact forms as

$$
V_{x,t}^{(i)} = \underline{g}_{x,t}^{(i)T}\,\underline{P} + f_{x,t}^{(i)} \qquad i = 1,2 \qquad (6.21)
$$

where

$$
\underline{P} = \begin{bmatrix} E \\ U_F \\ U_T \\ K_r \\ K_a \\ P_H \end{bmatrix} = \begin{bmatrix} P^{(12)} \\ ---- \\ P^{(22)} \end{bmatrix}
\qquad \left.\begin{matrix} E \\ U_F \\ U_T \\ K_r \end{matrix}\right\} P^{(1)}
\qquad \left.\begin{matrix} E \\ \vdots \\ P_H \end{matrix}\right\} P^{(2)}
$$

$$g^{(1)}_{x,t} = \begin{bmatrix} \frac{\Delta t}{(\Delta x)^2} (L_{x+1,\ t-1} - 2L_{x,\ t-1} + L_{x-1,\ t-1}) \\ - \frac{\Delta t}{2\Delta x} (L_{x+1,\ t-1} - L_{x-1,\ t-1}) \\ - \frac{\Delta t}{2\Delta x} \text{Sin}\ \omega_T\ (t-1)\ (L_{x+1,\ t-1} - L_{x-1,\ t-1}) \\ - \Delta t\ (L_{x,\ t-1}) \\ 0 \\ 0 \end{bmatrix}$$

$$g^{(2)}_{x,t} = \begin{bmatrix} \frac{\Delta t}{(\Delta x)^2} (C_{x+1,\ t-1} - 2C_{x,\ t-1} + C_{x-1,\ t-1}) \\ - \frac{\Delta t}{2\Delta x} (C_{x+1,\ t-1} - C_{x-1,\ t-1}) \\ - \frac{\Delta t}{2\Delta x} \text{Sin}\ \omega_T\ (t-1)\ (C_{x+1,\ t-1} - C_{x-1,t-1}) \\ - \Delta t\ (L_{x,\ t-1}) \\ \Delta t\ (C_s - C_{x,\ t-1}) \\ \Delta t\ \text{Sin}\ \omega_D\ (t-1) \end{bmatrix}$$

$$f^{(1)}_{x,t} = L_{x,\ t-1}$$

$$f^{(2)}_{x,t} = C_{x,\ t-1}$$

The dimensions of the preceding vectors vary with the parameters that need to be updated in the estimation scheme. In general, the parameter vector may be written as

$$\underline{P} = \begin{bmatrix} P^{(11)} \\ P^{(12)} \\ P^{(22)} \end{bmatrix} \quad \begin{matrix} \left.\begin{matrix} \\ \end{matrix}\right\} P^{(1)} \\ \left.\begin{matrix} \\ \end{matrix}\right\} P^{(2)} \end{matrix}$$

where $P^{(1)}$, $P^{(2)}$ are $r^{(1)} \times 1$ and $r^{(2)} \times 1$ vectors that include the parameters in each of equations (6.16) and (6.17). $P^{(11)}$, $P^{(22)}$ are $r^{(11)} \times 1$ and $r^{(22)} \times 1$ vectors containing the parameters unique to each equation and $P^{(12)}$ is a $r^{(12)} \times 1$ vector containing those parameters contained in both equations. The motivation for this matrix partitioning scheme will become obvious in the sequel.

By an analogy to the scalar system of the previous section, an arbitrary number M of on-line measurements of each state variable $v^{(1)}$, $v^{(2)}$ are available at time t as

$$y^{(i)}_{x_m, t} = h^{(i)}_m \, v^{(i)}_{x_m, t} + \eta^{(i)}_{m,t} \tag{6.22}$$

$m = 1, 2, ---, M$

$i = 1,2$

with measurement error variance $\sigma^{(i)^2}_m$, $i = 1,2$.

The equivalent optimization criterion for a maximum likelihood estimation may be written as

$$S = \sum_{i=1}^{2} \sum_{m=1}^{M} \frac{[y^{(i)}_{x_{m},t} - h^{(i)}_{m} \; V^{(i)}_{x_{m},t}]^2}{\sigma^{(i)\,2}_{m}}$$

Beyond the assumption in the previous section, the above formulation further assumes that the measurement errors of each variable are statistically independent. In practice, this assumption may be hard to justify. Box et al [15] and Hunter [62] have considered some problems associated with measurements correlation in multivariate systems. The latter discusses conditions under which the optimization criterion may be formulated as done above and also proposes a more realistic criterion that depends on measured expected errors.

The sufficient condition that maximizes the joint density function in this case yields

$$\underline{L}^{(i)\,T} \; \underline{P}^{(i)} = \underline{H}^{(i)-1} \; \underline{Y}^{(i)} - \underline{F}^{(i)}$$

The matrixes $\underline{R}^{(i)}$, $\underline{H}^{(i)}$, and vectors $\underline{Y}^{(i)}$, $\underline{F}^{(i)}$ are similar to those in the previous section for each state equation. In addition, the M x $r^{(1)}$ and M x $r^{(2)}$ matrixes $\underline{L}^{(1)T}$, $\underline{L}^{(2)T}$ contain all non-zero elements of matrixes $\underline{G}^{(1)T}$ and $\underline{G}^{(2)T}$. For example

$$\underline{L}^{(1)T} = \begin{bmatrix} g^{(1)}_{1, x_1, t} & \cdots\cdots & g^{(1)}_{r^{(1)}, x_1, t} \\ \vdots & & \\ g^{(1)}_{1, x_M, t} & \cdots\cdots & g^{(1)}_{r^{(1)}, x_M, t} \end{bmatrix}$$

A complete solution of $\underline{\hat{P}}^{(i)}$ requires that the $M \times r^{(i)}$ matrix $\underline{L}^{(i)T}$ have a minimum rank of $r^{(i)}$. It follows that the minimum number of spatially independent measurement of variable $v^{(i)}_{x,t}$ for optimum filtering and parameter estimation at time t be $r^{(i)}$, the number of unknown independent parameters in the i^{th} state equation. Thus this can be formalized by the following theorem.

Theorem I: For on-line filtering and parameter estimation in a multivariate distributed system, the optimum number of spatially independent measurement of a variable at time t is the same as the number of independent parameters unknown in the state equation of that variable at time t.

Equation (6.23) may be rewritten for each variable as

$$\underline{L}^{(1)T} \underline{\hat{P}}^{(11)} + \underline{L}^{(1)T} \underline{\hat{P}}^{(12)} = \underline{H}^{(1)-1} \underline{Y}^{(1)} - \underline{F}^{(1)}$$

$$\underline{L}^{(2)T} \underline{\hat{P}}^{(22)} + \underline{L}^{(2)T} \underline{\hat{P}}^{(12)} = \underline{H}^{(2)-1} \underline{Y}^{(2)} - \underline{F}^{(2)}$$

With no coupling parameters, $\underline{P}^{12} = \underline{O}$, the above equations reduce to

$$\underline{\hat{P}}^{(ii)} = \underline{L}^{(ii)T^{-1}} [\underline{H}^{(ii)^{-1}} \underline{Y}^{(i)} - \underline{F}^{(ii)}] \tag{6.24}$$

The resulting variance terms are

$$\mathrm{Var}\,(P^{(ii)} - \hat{P}^{(ii)}) = [\,\underline{L}^{(ii)}\ \underline{H}^{(ii)T}\ \underline{R}^{(ii)^{-1}}\ \underline{L}^{(ii)T}\,]^{-1} \tag{6.25}$$

These results reduce to those obtained in the last section for $i = 1$. Similarly, the trace of the variance term

$$J^{(ii)} = \mathrm{Trace}\,[\,\underline{L}^{(ii)}\ \underline{H}^{(ii)T}\ \underline{R}^{(ii)^{-1}}\ \underline{H}^{(ii)}\ \underline{L}^{(ii)T}\,]^{-1} \tag{6.26}$$

is maximum at spatial points $x_j^{(i)}$ where the sensitivity coefficient $[g_{j,x}^{(i)}]^2$ is maximum for $j = 1, --- r^{(ii)}$.

For the coupling parameter $\underline{P}^{(12)}$, equation (6.23) yields

$$[\underline{R}^{(12)^{-1}}\ \underline{H}^{(12)}\ \underline{L}^{(12)T} + \underline{R}^{(21)^{-1}}\ \underline{L}^{(21)^{T}}]\ \underline{P}^{(12)}$$

$$= \underline{R}^{(12)^{-1}}\ [\,\underline{Y}^{(12)} - \underline{H}^{(12)}\ \underline{F}^{(12)}] + \underline{R}^{(21)^{-1}}\ [\,\underline{Y}^{(21)} - \underline{H}^{(21)}\ \underline{F}^{(21)}] \tag{6.27}$$

The trace of inverse of the variance of the coupling parameter vector $P^{(12)}$ after some matrix manipulation becomes

$$J^{(12)} = \mathrm{Trace}\,[\underline{A}\ (\underline{R}^{(12)} + \underline{R}^{(21)-1})\ \underline{A}^{T}] \tag{6.28}$$

where

$$\underline{A} = [\underline{L}^{(12)}\ \underline{H}^{(12)T}\ \underline{R}^{(12)-1} + L^{(21)}\ H^{(21)T}\ R^{(21)-1}]$$

Similarly, this trace term is maximum at the spatial points where the sensitivity coefficients $\left[\frac{\partial V_{x,t}^{(i)}}{\partial P_j^{(12)}}\right]^2$ is maximum in the spatial domain. The preceding results also may be formalized by the following theorem.

<u>Theorem II</u>: For optimum filtering and parameter estimation in a multivariate system in which the i^{th} state variable is written as $V^{(i)}(x,\underline{P}^{(i)})$, the optimum monitoring locations of each variable $V^{(i)}$ are such that the sensitivity coefficients $\left[\frac{\partial V^{(i)}}{\partial P_j^{(i)}}\right]^2$ are maximum for each i and j, where $P_j^{(i)}$ is the j^{th} element of the parameter vector $\underline{P}^{(i)}$.

Although this was generated in a very general way, the results of the theorem resemble the results obtained in the crude work of McCormack and Perlis [ ].

For the example used in this section, the monitoring locations for the variable $V^{(1)}$ at time t are

$$XM^{(1)}(1) = \underset{x}{\text{Max}}\left[\frac{\Delta t}{(\Delta X)^2}\left(L_{x+1,\ t-1} - 2\,L_{x,t-1} + L_{x+1,t-1}\right)\right]^2$$

$$XM^{(1)}(2) = \underset{x}{\text{Max}} \left[\frac{-\Delta t}{2\Delta x} (L_{x+1,t-1} - L_{x-1,t-1})\right]^2$$

$$XM^{(1)}(3) = \underset{x}{\text{Max}} \left[\frac{-\Delta t}{2\Delta x} \text{Sin}\ \omega_T\ (t-1)\ (L_{x+1,t-1} - L_{x-1,t-1})\right]^2$$

$$XM^{(1)}(4) = \underset{x}{\text{Max}} \left[-\Delta t\ (L_{x,t-1})\right]^2 \qquad (6.29)$$

and for variable $V^{(2)}$

$$XM^{(2)}(1) = \underset{x}{\text{Max}} \left[\frac{\Delta t}{(\Delta x)^2} (C_{x+1,t-1} - C_{x,t-1} + C_{x-1,t-1})\right]^2$$

$$XM^{(2)}(2) = \underset{x}{\text{Max}} \left[\frac{-\Delta t}{2\Delta x} (C_{x+1,t-1} - C_{x-1,t-1})\right]^2$$

$$XM^{(2)}(3) = \underset{x}{\text{Max}} \left[\frac{-\Delta t}{2\Delta x} \text{Sin}\ \omega_T\ (t-1)\ (C_{x+1,t-1} - C_{x-1,t-1})\right]^2$$

$$XM^{(2)}(4) = \underset{x}{\text{Max}} \left[-\Delta t\ (L_{x,t-1})\right]^2$$

$$XM^{(2)}(5) = \underset{x}{\text{Max}} \left[\Delta t\ (C_s - C_{x,t-1})\right]$$

$$XM^{(2)}(6) = \underset{x}{\text{Max}} \left[\Delta t\ \text{Sin}\ \omega_D\ (t-1)\right]^2 \qquad (6.30)$$

<u>Multivariate System Distributed In A Multi-dimensional Space</u>.

The optimum monitoring theory developed in previous sections is now extended to the distribution of pollutants in a salinity intrusion region of a two-dimensional estuary with a one-dimensional flow represented by

$$\frac{\partial L(x,z,t)}{\partial t} = Ex \frac{\partial^2 L}{\partial x^2} + Ez \frac{\partial^2 L}{\partial z^2} - Ux,z,t \frac{\partial L}{\partial x} - KrL \qquad (6.31)$$

$$\frac{\partial C(x,z,t)}{\partial t} = Ex \frac{\partial^2 C}{\partial x^2} + Ez \frac{\partial^2 C}{\partial z^2} - Ux,z,t \frac{\partial C}{\partial x}$$

$$- K_r L - K_a C + K_a C_s \qquad (6.32)$$

In a study of velocity profiles and dispersion in estuarine flow, Segall and Gidlund [123] concluded that for an estuary wherein the period of vertical mixing may be much greater than the tidal period, the vertical variation in velocity may be represented as

$$U\ (z,t) = \frac{K}{\sigma} [e^{-\lambda z} \text{Sin } (\sigma,t - \lambda z) - \text{Sin } \sigma\ t]$$

λ is a function of eddy diffinity and tidal frequency σ. In addition, Ippen and Harleman [52] have shown that time-averaged tidal velocity has a logarithmic vertical profile in saline estuary. These two effects are combined in the following approximate representation of tidal velocity to be used in equation (6.31) and (6.32).

$$U_{(x,z,t)} = U_F [1 + 2\ (2 \frac{z}{zo} - 1) \frac{x}{xo}] + \frac{x}{xo} U_T \text{ Sin } \omega_T t \qquad (6.34)$$

where zo is the estuary depth and xo is the length.

As illustrated in the last section, the system equation (6.31) and (6.32) may be written in explicit finite difference forms as

$$V_{s,t}^{(i)} = g_{s,t}^{(i)T} \underline{P} + f_{s,t}^{(i)} \qquad (6.35)$$

$$i = 1,2$$

where subscript s represents the coordinates of a general spatial point (x,y,z), which in this case is (x,z), and $\underline{P}$ is a vector containing unknown parameters of the system.

With this formulation, the development of the optimum measurement stations is identical to the one given in the last section and the given theorems apply. For a parameter vector,

$$\underline{P} = \begin{bmatrix} E_x \\ E_z \\ U_F \\ U_T \\ K_r \\ K_a \end{bmatrix}$$

and similar types of measurements given in the last section. The optimum measurements stations at time t for this system becomes, for $V_{s,t}^{(1)}$

$$SM^{(1)}(1) = \underset{x,z}{\text{Max}} \left[\frac{\Delta t}{(\Delta x)^2} (L_{x+1,t-1} - 2L_{x,z,t-1} + L_{x-1,z,t-1}) \right]^2$$

$$SM^{(1)}(2) = \underset{x,z}{\text{Max}} \left[\frac{\Delta t}{(\Delta z)^2} (L_{x,z+1,t-1} - 2L_{x,z,t-1} + L_{x,z,-1,t-1}) \right]^2$$

$$SM^{(1)}(3) = \underset{x,z}{\text{Max}} \left[-\frac{\Delta t}{2\Delta x} \; a \; (L_{x+1,z,t-1} - L_{x-1,z,t-1})\right]^2$$

$$SM^{(1)}(4) = \underset{x,z}{\text{Max}} \left[-\frac{\Delta t}{2\Delta x} \; \frac{X}{Xo} \; \text{Sin} \; \omega_T \; (t-1) \; (L_{x+1,z,t-1} - L_{x-1,z,t-1})\right]^2$$

$$SM^{(1)}(5) = \underset{x,z}{\text{Max}} \left[-\Delta t \; (L_{x,z,t-1})\right]^2 \tag{6.36}$$

and for $V^{(2)}_{s,t}$

$$SM^{(2)}(1) = \underset{x,z}{\text{Max}} \left[\frac{\Delta t}{(\Delta x)^2} \; (C_{x+1,z,t-1} - 2C_{x,z,t-1} + C_{x-1,z,t-1})\right]^2$$

$$SM^{(2)}(2) = \underset{x,z}{\text{Max}} \left[\frac{\Delta t}{(\Delta z)^2} \; (C_{x,z+1,t-1} - 2C_{x,z,t-1} + C_{x,z-1,t-1})\right]^2$$

$$SM^{(2)}(3) = \underset{x,z}{\text{Max}} \left[-\frac{\Delta t}{2\Delta x} \; a \; (C_{x+1,z,t-1} - C_{x-1,z,t-1})\right]^2$$

$$SM^{(2)}(4) = \underset{x,z}{\text{Max}} \left[-\frac{\Delta t}{2\Delta x} \; \frac{X}{Xo} \; \text{Sin} \; \omega_T \; (t-1) \; (C_{x+1,z,t-1} - C_{x-1,z,t-1})\right]^2$$

$$SM^{(2)}(5) = \underset{x,z}{\text{Max}} \left[-\Delta t \; (L_{x,z,t-1})\right]^2$$

$$SM^{(2)}(6) = \underset{x,z}{\text{Max}} \left[-\Delta t \; (C_s - C_{x,z,t-1})\right]^2 \tag{6.37}$$

where $a = \left[1 + 2 \left(2 \frac{z}{zo} - 1\right) \frac{x}{xo}\right]$ in (6.36 and (6.37

This chapter has presented a general method for determining the optimum spatial monitoring stations in a class of distributed parameter systems. The method is based on statistical experimental design techniques. In the development, the explicit finite difference representations of the systems are used; the extension of the results to systems with known analytical closed-form solutions is straight-forward. The results are formalized by theorems given for the optimum number and locations of monitoring stations. The implementation of the results for specific estuary models has also been presented.

CHAPTER VII

STREAM PARAMETER ESTIMATION EMPLOYING STOCHASTIC APPROXIMATION AND MULTIPLE MEASUREMENT TECHNIQUES

It is often of interest in water quality modeling, after the pertinent hydrodynamic and biochemical processes are formalized by mathematical equations, to determine the numerical values of the various parameters in the equations. This is an important part of modeling because management and control policies are often based on predictions from such models.

As discussed earlier, only a few variables in a water quality model can be measured directly and even fewer are measurable on-line. The present methods of evaluating such parameters as the BOD removing coefficient, reaeration and photosynthetic rates are off-line techniques based on empirical curve-fitting of BOD, DO and temperature readings [82, 30]. In addition, that type of analysis usually provides parameter values which represent steady state and steady load conditions. However, very few water systems remain under steady conditions for an appreciable length of time.

In this chapter, stochastic adjustment techniques are used to derive numerical values for the optimum estimates of the state and parameter profiles of a polluted stream reach. Estimation is based on a special class of multiple measurements treated in

Chapter V. These measurements include noisy on-line TOC and DO and the off-line analytical five-day noisy BOD measurements. For the purpose of this study, the relating function between TOC and BOD is assumed to be linear and the deviation from such approximation is considered a noise at the instant of measurement. The TOC measurement error thus consists of the calibration error and the instrument noise, and consequently, it is considered much higher than the noise in the corresponding BOD measurement.

The cost function to be optimized consists of the square of the instantaneous difference between measured concentrations and the concentrations predicted from the mathematical model. The optimum parameter minimizes the average of the cost function in the mean square scense.

Over restricted intervals of distance and time, the stream rate coefficients can be treated as constants.For this special case, the Robbins-Munro stochastic approximation technique [117] is employed. A similar problem was studied in [71] in which only the on-line DO data was used because of the five-day delay associated with BOD measurements. The multiple measurements techniques developed in this study copes well with this problem, and the results in this chapter show an improvement over the estimates and the rates of convergence that may be obtained from a single set of measurements.

In a real stream, the coefficients are not constant and sources and sinks for photosynthesis (P) and respiration (R) vary from their daily-averaged values. This chapter also considers the more realistic diurnal variations in temperature which, in turn, cause the rate coefficients and the P - R terms to vary with time. In this more general case, a stochastic tracking technique [19] is used. The sequential algorithms derived in both cases yield optimum parameter estimates that converge to their true values asymptotically and with probability one.

Two methods are used in this and subsequent chapters to include the additive measurement noise. One method considers a fixed error variance for each variable while the other considers a variance term that is a fixed proportion of the expected measured value of the variable. The latter represents more realistically the characteristic of measuring instruments as discussed in Chapter III.

The rate of convergence of the algorithms decreases with the level of the system disturbance and measurement noises. It also varies with the measurement locations. The results presented in this chapter include the studies of the choice of fixed measurement stations for both the daily-averaged case and the diurnal variations case with respect to various measurement noise levels.

A numerical example is given for each of the two cases discussed. In both examples improved estimates and faster rates of convergence are shown to result from using a multiple measurements technique.

Problem Formulation

Stream Dynamics.

A stream model of the type presented in equations (2.13) and (2.14) in which the dispersion coefficient (E) and the urban runoff term (La) are negligible is considered.

$$\frac{\partial L(x,t)}{\partial t} = -U\frac{\partial L}{\partial x} - K_r L \tag{7.1}$$

$$\frac{\partial C(x,t)}{\partial t} = -U\frac{\partial C}{\partial x} - K_d L - K_a C + K_a C_s + \overline{P} - \overline{R} - \overline{B} \tag{7.2}$$

where

$L(x,t)$ = BOD concentration mg/l

$C(x,t)$ = DO cencentration mg/l

U = stream velocity miles/d

K_r = BOD-removing coefficient 1/day

K_d = deoxygenation coefficient 1/day

K_a = reaeration coefficient 1/day

C_s = DO saturation level mg/l-day

$\overline{P},\overline{R},\overline{B}$ = daily-averaged photosynthetic, respiration and benthal deposit demand mg/l-day.

The stream is assumed to be subjected to a steady daily-averaged BOD loading (L_o) at the upstream boundary, and also has a constant DO boundary condition.

For the daily-averaged stream condition mentioned above, the parameters in (7.1) and (7.2) are considered as constants. For the case of the more realistic stream condition where the parameters vary with temperature changes, the following empirical expressions used by [134] are employed

$$K_r\ (\theta) = 2.35 \times 10^{-7} \times \exp\ (0.064\theta) \qquad (7.3)$$

$$K_a\ (\theta) = 0.43 \times \exp\ [0.025\ (\theta-273)] \qquad (7.4)$$

$$C_s\ (\theta) = 4 \times 10^3 \times \exp\ (-0.021\theta) \qquad (7.5)$$

$$\overline{P-R} = \frac{(\alpha - \pi)}{\pi(\alpha-1)} [25.0 - 0.028\ (\theta-303.0)^2] \qquad (7.5a)$$

where in this treatment

$\alpha = 3.5$

$K_d = K_r$

and the diurnal variation of temperature θ with time is represented as

$$\theta\ (t) = 290 + a_T \text{ Sin } \omega t \qquad (7.6)$$

θ is in degrees Kelvin and a_T is the amplitude of the sinusodial component.

Measurement Scheme.

Two fixed measurement stations are considered in this development; one station is located at the upstream boundary and the other at an internal point in the stream to be determined in an optimum fashion shortly. Off-line analytical noisy measurements of BOD and DO with a sampling period T_1 and a fixed-time dalay T_D are assumed to be taken at the upstream boundary,

$$y_{Lo}\ (mT_1) = Lo + \rho_L\ (mT_1) \tag{7.7}$$

$$y_{Co}\ (mT_1) = Co + \rho_C\ (mT_1) \tag{7.8}$$

$$m = 1, 2, ---$$

The measurement errors are treated as zero mean gaussian white type with variances

$$E\ [\rho_L^2\ ] = \sigma_L^2$$

$$E\ [\rho_C^2\ ] = \sigma_C^2$$

The measured values (7.7) and (7.8) are used as initial conditions along with current estimates of the parameters in (7.1) and (7.2) to predict the concentrations L_P (xM,nT), C_P (xM,nT) at any measurement point xM in the stream.

In addition, a multiple set of on-line TOC and DO noisy measurements and off-line BOD and DO measurements are assumed to be taken at xM. These latter readings are then compared with the predicted concentrations, and a measure of the instantaneous differences is optimized to update the parameter estimates. The off-line BOD and DO noisy measurements at xM are written as

$$y_L\ (xM,\ mT_1) = L\ (xM,\ mT_1) + \rho_L\ (mT_1) \qquad (7.9)$$

$$y_C\ (xM,\ mT_1) = C\ (xM,\ mT_1) + \rho_C\ (mT_1) \qquad (7.10)$$

$$m = 1,\ 2,\ ---$$

Similarly, the on-line TOC and DO noisy measurements with a different sampling period T, taken at xM are represented as

$$y_T\ (xM,\ nT) = h\ L\ (xM,\ nT) + \xi_T\ (nT) \qquad (7.11)$$

$$y_C\ (xM,\ nT) = C\ (xm,\ nT) + \xi_C\ (nT) \qquad (7.12)$$

By comparing (7.11) and (5.1), it is evident that y_T represents an adjusted TOC reading after the intercept constant TIN has been subtracted and h represents the slope of the linear function between BOD and TOC values. Again the measurement errors are considered zero-mean gaussian white type with variances

$$E\ [\ \xi_T^2\ ] = \sigma_T^2$$

$$E\ [\ \xi_C^2\ ] = \sigma_C^2$$

The measurement error ξ_T contains both the error of linear approximation and the instrument noise, thus it is considered to have a higher variance than ρ_L.

The objective here is to obtain estimates of the parameters L_o, K_r, K_a and $\overline{P - R}$ that optimize a specified cost function to be formulated in the next section, based on both sets of off-line measurements (7.7), (7.8), (7.9), (7.10) and the on-line measurements (7.11) and (7.12). For the sake of brevity, the $\overline{P - R}$ term is represented as K_p in the sequel.

Cost Function.

Optimization implies the existence of a criterion. In this chapter, the cost function considered is the weighted sum of the square of the instantaneous difference between the noisy measured concentrations and the predicted concentrations at the estimation station xM. The function is formulated for each variable as

$$J_1 (n) = W_1 [y_T (xM, nT) - h L_p (xM, \underline{K}^n, nT)]^2 + W_2 \delta_{nT - (mT_1 + T_D)} [y_L (xM, mT_1) - L_p (xM, \underline{K}^n, mT_1)]^2 \tag{7.13}$$

$$J_2 (n) = W_3 [y_C (xM, nT) - C_p (xM, \underline{K}^n, nT)]^2 + W_4 \delta_{nT - (mT_1 + T_D)} [y_C (xM, mT_1) - C_p (xM, \underline{K}^n, mT_1)]^2 \tag{7.14}$$

where W_1, W_2, W_3, W_4 are specified weight factors, the kroneker delta

$$\delta_{nT} - (mT_1 + T_D) = \begin{cases} 1 & \text{for } nT = mT_1 + T_D \\ 0 & \text{for } nT \neq mT_1 + T_D \end{cases}$$

and T_1/T is considered an integer R. It is evident in (7.13) and (7.14) that in addition to the on-line measurements, the cost formulations incorporate the off-line delayed measurements taken at mT_1 and available at $nT = mT_1 + T_D$. The vector $\underline{K}^n$ contains the parameters K_o, K_r, K_a and K_p and represents their estimated values at time nT. It is also noted that the predicted concentrations are functions of the parameter estimates.

Sequential algorithms are desired for the parameter estimates that minimize the sum of the cost functions.

$$J(n) = J_1\ (n) + J_2\ (n) \tag{7.15}$$

asymptotically and in the mean square sense.

Stochastic Approximation and Stochastic Tracking Algorithms

The derivation of the sequential algorithms is illustrated by considering the terms in the J_1 component of the cost function. In general, the solution of the system equations (7.1) and (7.2) at point xM and after a time $nT > \frac{xM}{u}$ depends only on the values of the boundary conditions and may be written as

$$L\ (xM,\ nT) = L_o \exp\left[-K_r\ (nT)\ \frac{xM}{u}\right] \tag{7.16}$$

$$C(xM, nT) = \frac{-K_r(nT)}{K_a(nT) - K_r(nT)} \left\{ \exp\left[-K_r(nT)\frac{xM}{u}\right] - \exp\left[-K_a(nT)\frac{xM}{u}\right] \right\}$$

$$+ C_o \exp\left[-K_a(nT)\frac{xM}{u}\right]$$

$$+ \frac{K_p(nT)}{K_a(nT)} \left\{ 1 - \exp\left[-K_a(nT)\frac{xM}{u}\right] \right\} \qquad (7.17)$$

$$\text{for } nT > \frac{xM}{u}$$

where L (xM, nT), C (xM, nT) represent the BOD and DO steady state solutions at specific points in the diurnal cycle. For the case of the daily-averaged conditions where the parameters are treated as constants, equation (7.17) reduces to

$$L(xM, nT) = L_o \exp\left[-K_r \frac{xM}{u}\right] \qquad (7.18)$$

Similarly, the predicted BOD value based on the measurements (7.7) at the upstream boundary and the current estimates of the parameters, may be written as

$$L_p(xM, nT) = \left[L_o + \rho_L (nT - T_D)\right] \exp\left[-K_r^n \frac{xM}{u}\right] \qquad (7.19)$$

By substituting (7.11), (7.18) and (7.19) into (7.13), the J_1 component of the cost function becomes

$$J_1(n) = W_1 \Big\{ h\, L_o \left[\exp\left(\frac{-K_r xM}{u}\right) - \exp\left(-K_r^n \frac{xM}{u}\right) \right]$$

$$+ \xi_T(nT) - h\, \rho_L(nT-T_D) \exp\left(-K_r^n \frac{xM}{u}\right) \Big\}$$

$$+ W_2 \cdot \delta \Big\{ L_o \left[\exp\left(-K_r \frac{xM}{u}\right) - \exp\left(-K_r^n \frac{xM}{u}\right) \right]$$

$$+ \rho_L(nT-T_D) - \rho(nT-T_D) \exp\left(-K_r^n \frac{xM}{u}\right) \Big] \Big\} \tag{7.20}$$

For a deterministic problem where ρ_L and ξ_T are zero at all times, it can be readily shown by setting

$$G(K_r^n) = \frac{\partial J_1(n)}{\partial K_r^n}$$

to zero that the estimate K_r^n converges to its true value K_r at the minimum of the cost function. In the case of the noisy system treated here, it is necessary, if the sequential algorithms are to yield unbiased parameter estimates, that the statistical average of the instantaneous gradient $G(K_r^n)$ be zero as K_r^n converges to K_r [18]. That is

$$m^1(K_r) = \underset{K_r^n \to K_r}{E} \left\{ G(K_r^n) \right\} = 0 \tag{7.21}$$

However, by taking the derivative of J_1 with respect to K_r^n and then taking the ensemble average at $K_r^n = K_r$, it is evident that

$$m^1 (K_r) = - h^2 \sigma_L^2 \exp [-2 K_r \frac{xM}{u}] \tag{7.22}$$

which is not necessarily zero. This inherent bias results from using the noisy measurements at the upstream boundary (7.7) for the concentration prediction; the bias may be removed by considering a modified instantaneous gradient

$$G (K_r^n) = \frac{\partial J_1 (K_r^n)}{\partial K_r^n} - E \left\{ \frac{\partial J_1 (K_r^n)}{\partial K_r^n} \right\} \tag{7.23}$$

which satisfies the condition in (7.21).

The Robbins-Munro approximation algorithm [117]

$$K_r^{n+1} = K_r^n - A_n G(K_r^n) \tag{7.24}$$

may then be employed to obtain the zero-crossing of the term $E \left\{ G (K_r^n) \right\}$. For the convergence of the parameter estimate K_r^n, A_n must satisfy the following conditions [117, 19]:

(i) $A_n > 0$

(ii) $A_n \to 0$ as $n \to \infty$

(iii) $\sum_{n=1}^{\infty} A_n^2 = \text{constant} < \infty$

In addition, for the parameter to converge to its true value

(iv) $\sum_{n=1}^{\infty} A_n \to \infty$

Detailed proof of these conditions are contained in [117] and the algorithm formulated as above has been shown [12] to converge in the mean square sense

$$\lim_{n \to \infty} \left\{ E\,[K_r^n - K_r]^2 \right\} = 0$$

and with probability one

$$\text{Prob} \lim_{n \to \infty} K_r^n = K_r$$

A sequence that satisfies these conditions, $A_n = \frac{1}{n}$ is used in this study.

The preceding development involves the estimation of a single parameter K_r in a constant parameter daily-averaged stream model. For the simultaneous estimation of all the parameters, the generalized algorithm follows from a similar procedure and may be written as

$$K_j^{n+1} = K_j^n - A_n\, G\,(K_j^n) \tag{7.25}$$

where

$$G\,(K_j^n) = \frac{\partial J\,(\underline{K}^n)}{\partial K_j^n} - E\left[\frac{\partial J(K^n)}{\partial K_j^n}\right] \tag{7.26}$$

and K_j^n represents the current estimate of each of the parameters L_o, K_r, K_a and K_p.

For the case of the diurnally varying system, the development differs to the extent that the instantaneous cost function J (n) is actually a function of a function. Its value depends not only on the instantaneous values of the parameters at nT but also on their values at previous times. That is

$$J\ (n) = J\ (\underline{K}\ (iT),\ i = 1,\ 2\ \text{---}\ n) \tag{7.27}$$

A change in J (n) could result both from the measurement error at nT and the change in the parameters due to temperature variation.

If it may be assumed that the tracking process to be developed would yield parameter estimates $\underline{K}^n$ which are close to their true trajectory $\underline{K}$ (nT), then $\underline{K}$ (nT) - $\underline{K}^n$ is small and the first order Taylor approximation of (7.27) becomes

$$J\ (n) = J\ (\underline{K}^n) + \sum_{i=1}^{n} \left[\frac{\partial J\ (\underline{K}^i)}{\partial \underline{K}^i} \right]^T [\underline{K}\ (iT) - \underline{K}^i] \tag{7.28}$$

where $\frac{\partial J\ (\underline{K}^i)}{\partial \underline{K}^i}$ represents the gradient vector of the cost function with respect to the parameter estimates at any time $iT \leq nT$.

By analogy to (7.23) and (7.26), the bias resulting from using measured concentration values instead of the unknown true values to predict the concentration level at the estimation point (xM, nT) must be subtracted from the gradient terms in (7.28)

$$G(K_j^i) = \frac{\partial J(\underline{K}^i)}{\partial K_j^i} - E\left[\frac{\partial J(\underline{K}^i)}{\partial K_j^i}\right] \quad (7.29)$$

for the j^{th} element of the parameter vector. The resulting stochastic tracking algorithm may then be written in form of (7.25) as

$$K_j^{n+1} = K_j^n - A_n \sum_{i=1}^{n} C_{i,j}\, G(K_j^i) \quad (7.30)$$

where $C_{i,j}$, i= 1, 2 --- n are the weighting factors associated with the all present and past measurements. The analysis for the optimum values of C_i for various examples of stochastic adaptive control problems is contained in [19].

This concludes the derivation of the stochastic approximation algorithms and the stochastic tracking algorithms for the constant parameter and diurnally varying stream systems treated here. Implementations of these algorithms are given in the following numerical examples.

Numerical Examples.

Judicious choice of A_n, $C_{i,j}$ determine the rate of convergence. The experience in the preparation of this work shows that

$$A_n C_{i,j} = \frac{1}{\sum_{j=1}^{N} G^2(K_j^i)}$$

provides optimum estimation in term of the accuracy of the final estimate, in equation (7.30), where N is the number of parameters being estimated. In addition,

$$A_n = \frac{1}{n}$$

provides optimum estimation in terms of rate of convergence in both (7.25) and (7.30). The weight factors W_1, W_2, W_3, W_4 chosen as the inverse of the corresponding measurement error variances in (7.13) and (7.14) are found to produce the least value of the mean square function [118]. For both numerical examples, the following stream parameters are assumed constant

stream reach = 5 miles

stream velocity = 0.75 miles/day

true upstream BOD load L_o = 30 mg/liter

true upstream DO boundary condition C_o = 6 mg/liter.

The on-line DO and TOC measurements are taken hourly and the off-line BOD and DO are taken every 12 hrs. with a 5-day delay. For the case of the constant parameter daily-averaged stream, the following true stream parameter were used in the simulation:

the daily-averaged temperature $\theta = 290^o$ K and the variation $a_T = 0$. This results in true stream coefficients

$K_r = 0.164$

$K_a = 0.658$

$C_s = 9.062$

$K_p = .921$

In one set of computer runs, the measurement errors simulated are assumed to have constant variances for each variable

$$\sigma_T^2 = (5)^2$$

$$\sigma_B^2 = (0.5)^2$$

$$\sigma_C^2 = (1.0)^2$$

Algorithms (7.25) are employed to simultaneously estimate the parameters L_o, K_r, K_a and K_P. Figure VII-1, illustrates the profiles of the K_r parameter estimates based on various combinations of measurements. It may be observed that both the convergence rate and the final accuracy (after 7 days of iteration) of the estimate based on the multiple measurements show considerable improvement over those of the estimates based on either set of single measurements.

In another example of the same system, measurement errors with standard deviations which are fixed proportions of the expected measured values are considered

σ_T = 20% expected TOC measurement

σ_L = 1% expected BOD measurement

σ_C = 10% expected DO measurement.

Figure VII-2 again shows the improvement both in the rates of convergence and in the final accuracy for the estimate of parameter L_o based on multiple measurements.

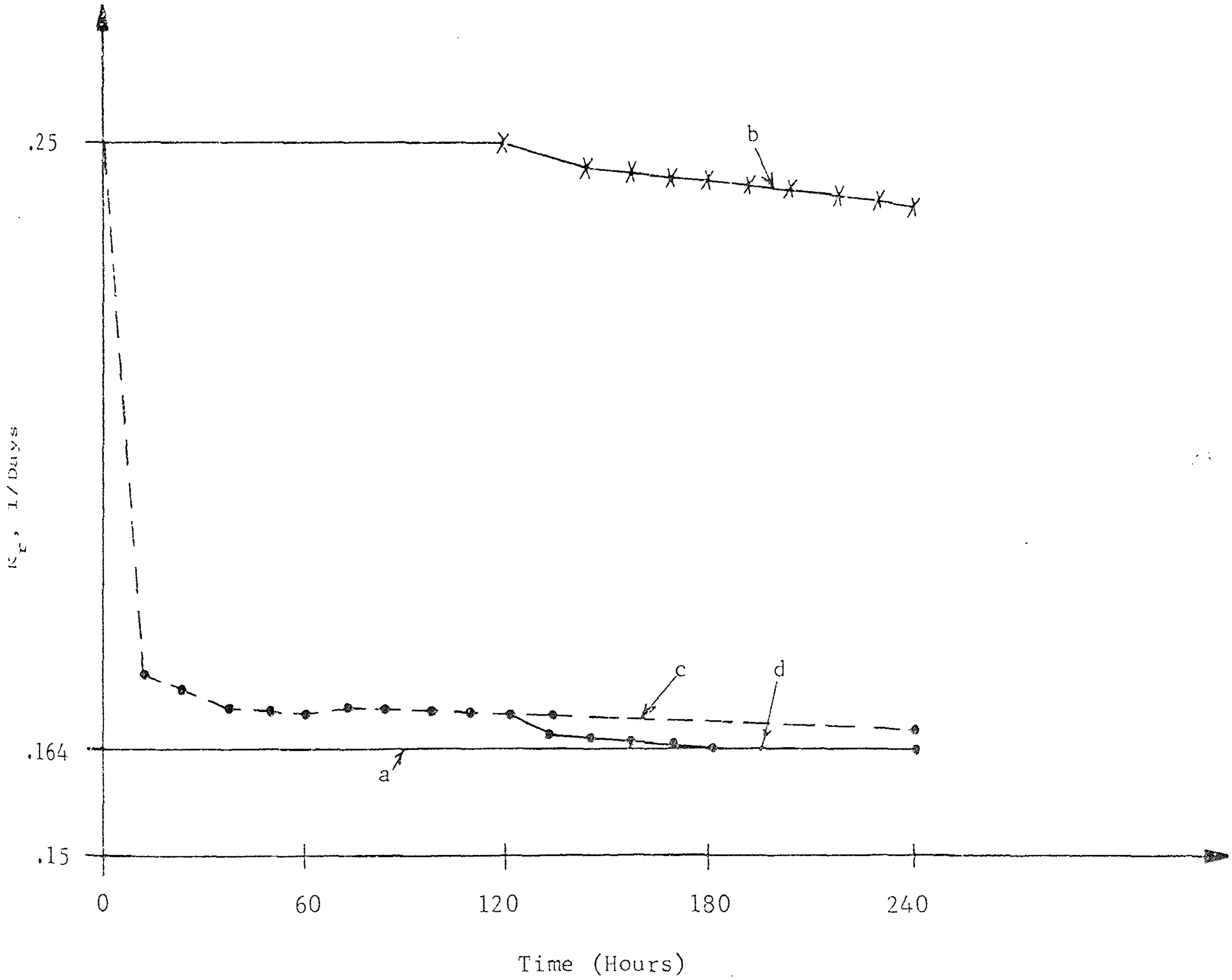


FIGURE VII-1. Parameter Estimation Using Stochastic Approximation with Constant Observation Error Variances.

a) True value of K_r.

b) Estimate of K_r from single (BOD-DO) measurements.

c) Estimate of K_r from single (TOC-DO) measurements.

d) Estimate of K_r from multiple (TOC-DO, BOD-DO) measurements.

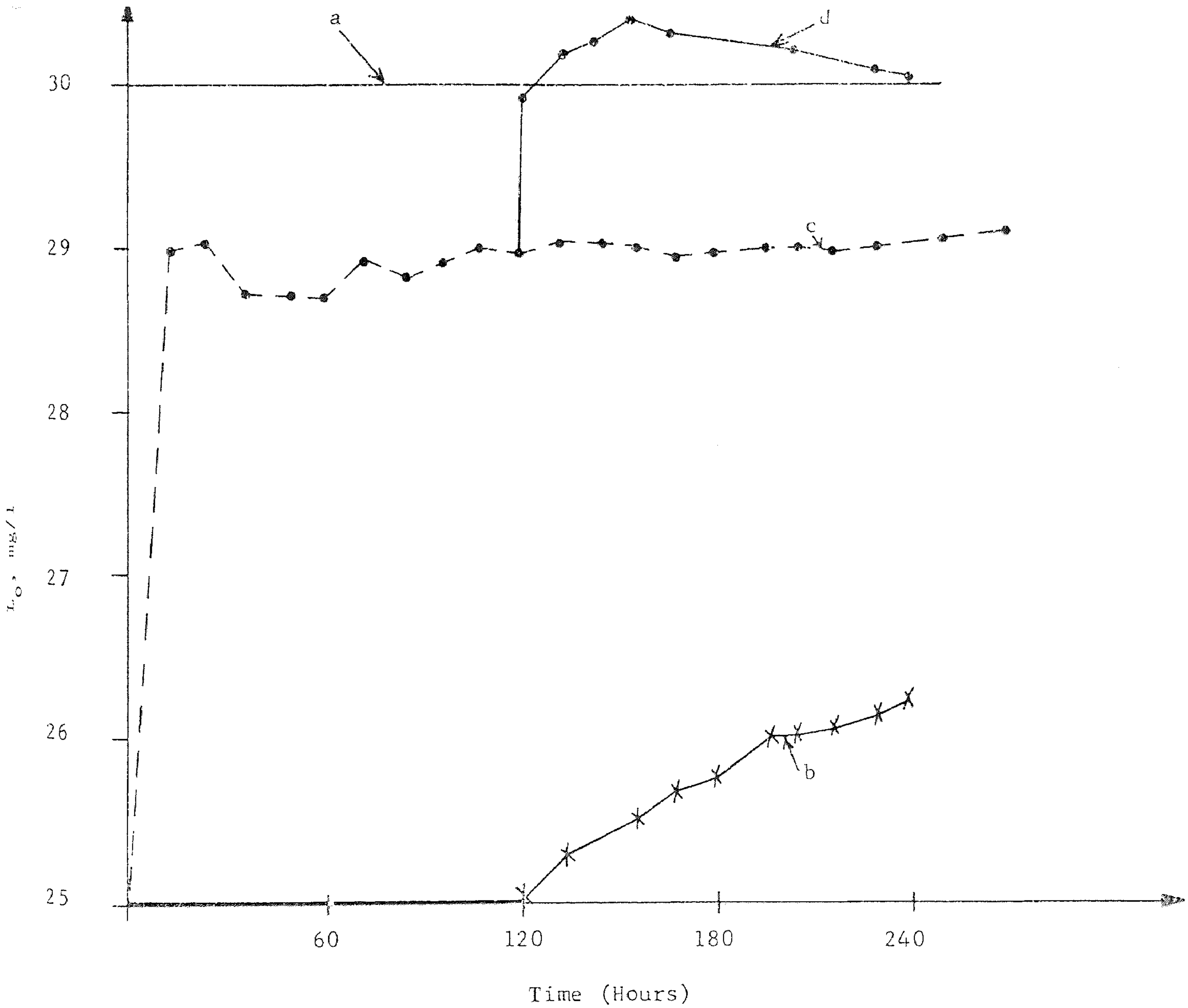


FIGURE VII-2. Parameter Estimation Using Stochastic Approximation with Constant Observation Error Variance-to-Signal Ratio.

a) True value of L_o.

b) Estimate of L_o from single (BOD-DO) measurements.

c) Estimate of L_o from single (TOC-DO) measurements.

d) Estimate of L_o from multiple (TOC-DO, BCD-DO) measurements.

For the more realistic diurnally varying stream example, temperature variation in (7.6) is employed to simulated the true parameter trajectories in (7.3), (7.4), (7.5) and (7.5a) A peak value of the sinusodial component $a_T = 10^{o}$ K and the period

$$T = \frac{2\pi}{\omega} = 24 \text{ hrs.}$$

Figure VII-3 shows the resultant K_r estimate profile for the same constant variance values of the measurement errors used above. Figure VII-4 shows the K_a profile for the diurnal varying system and measurement error with fixed standard deviation-to-expected measurement ratio. Again, in both examples improved estimates are obtained by using the multiple sets of measurements.

Optimum Measurement Station

In a previous chapter, an analysis of the optimum measurement stations was presented. However, in these examples an arbitrary number (2) of measurement stations is assumed. This may represent the situation in practice where a fixed number of stations already exists on a river system. The optimum location of the interior station xM for these examples is obtained by comparing the results for various values of xM in the stream spatial domain. Figure VII-5 shows a trade-off among the accuracies obtained for each parameter. The significance of each parameter based on the judgment of the engineer and the intended use of the stream determine the location to be used for minitoring.

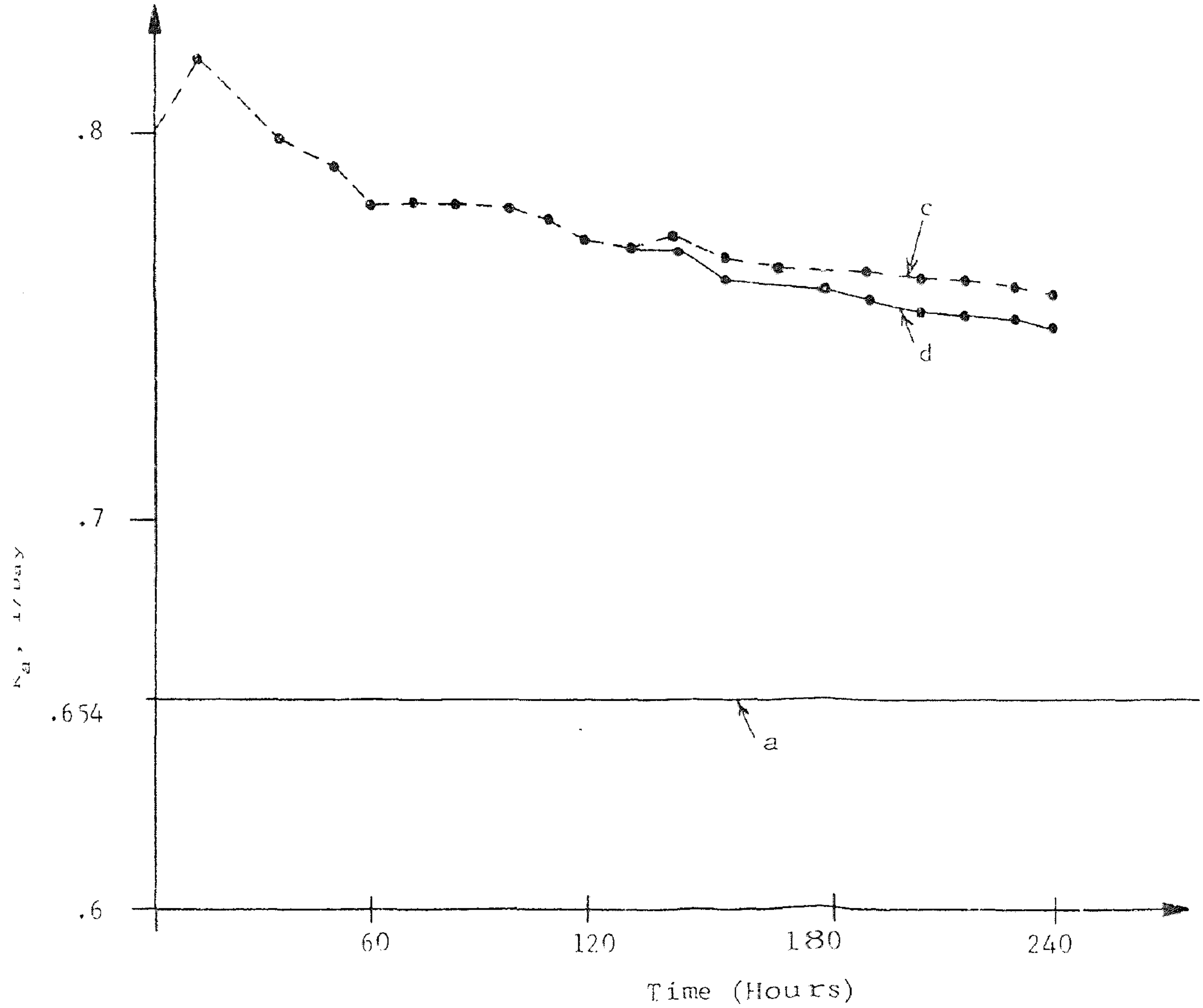


FIGURE VII-3. Parameter Estimation Using Stochastic Tracking Method with Constant Observation Error Variances

a) True value of the daily-averaged K_a.

b) Estimate of the daily-averaged K_a using single (BOD-DO) measurments - (off scale).

c) Estimate of the daily-averaged K_a using single (TOC-DO) measurements.

d) Estimate of the daily-averaged K_a using multiple (TOC-DO, BOD-DO) measurements.

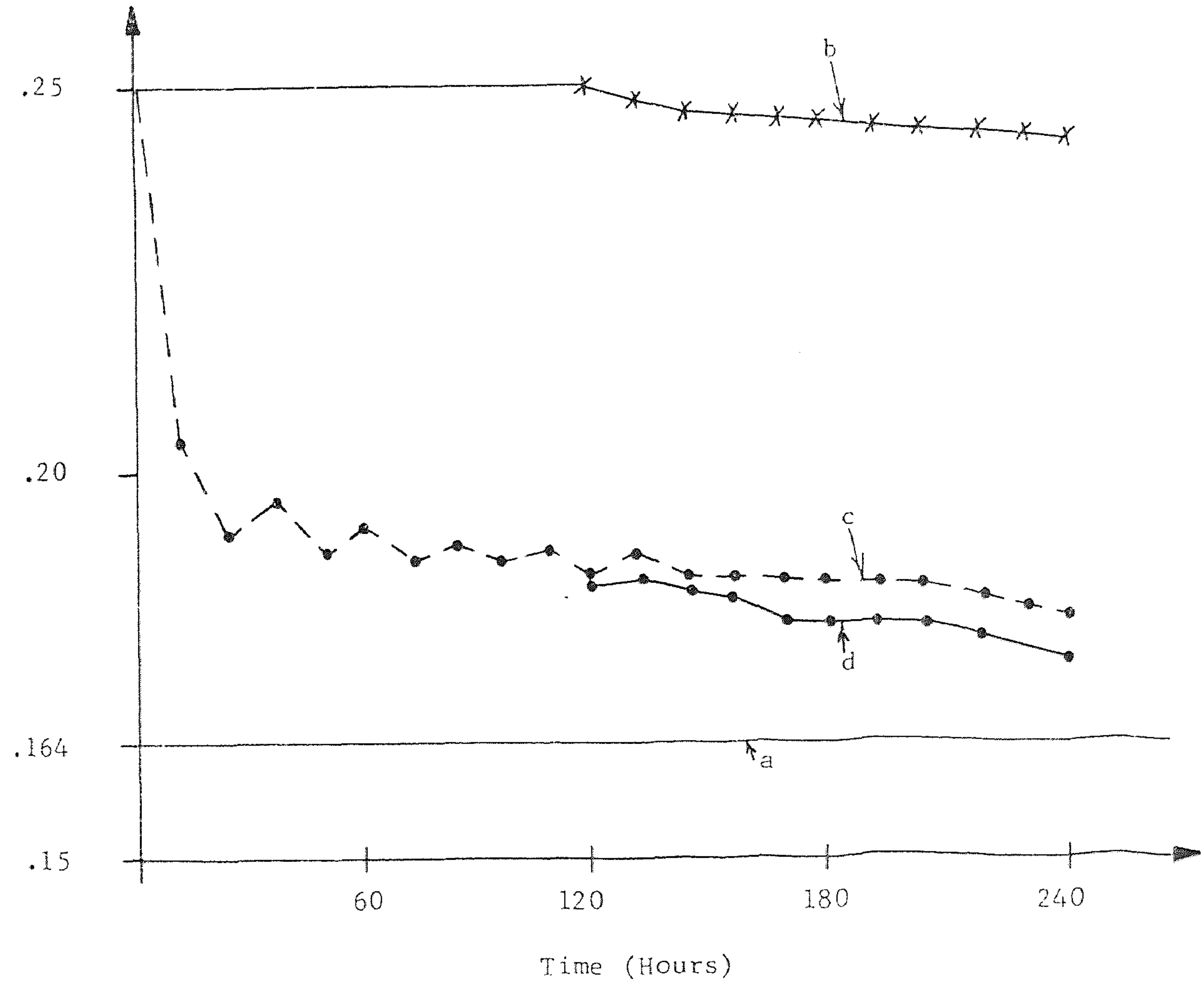


FIGURE VII-4. Parameter Estimation Using Stochastic Tracking Method with Constant Observation Error Variance-to-Signal Ratio

a) True value of the daily-averaged K_r.

b) Estimate of daily-averaged K_r using single (BOD-DO) measurements.

c) Estimate of daily-averaged K_r using single (TOC-DO) measurements.

d) Estimate of daily-averaged K_r using multiple (TOC-DO, BOD-DO) measurements.

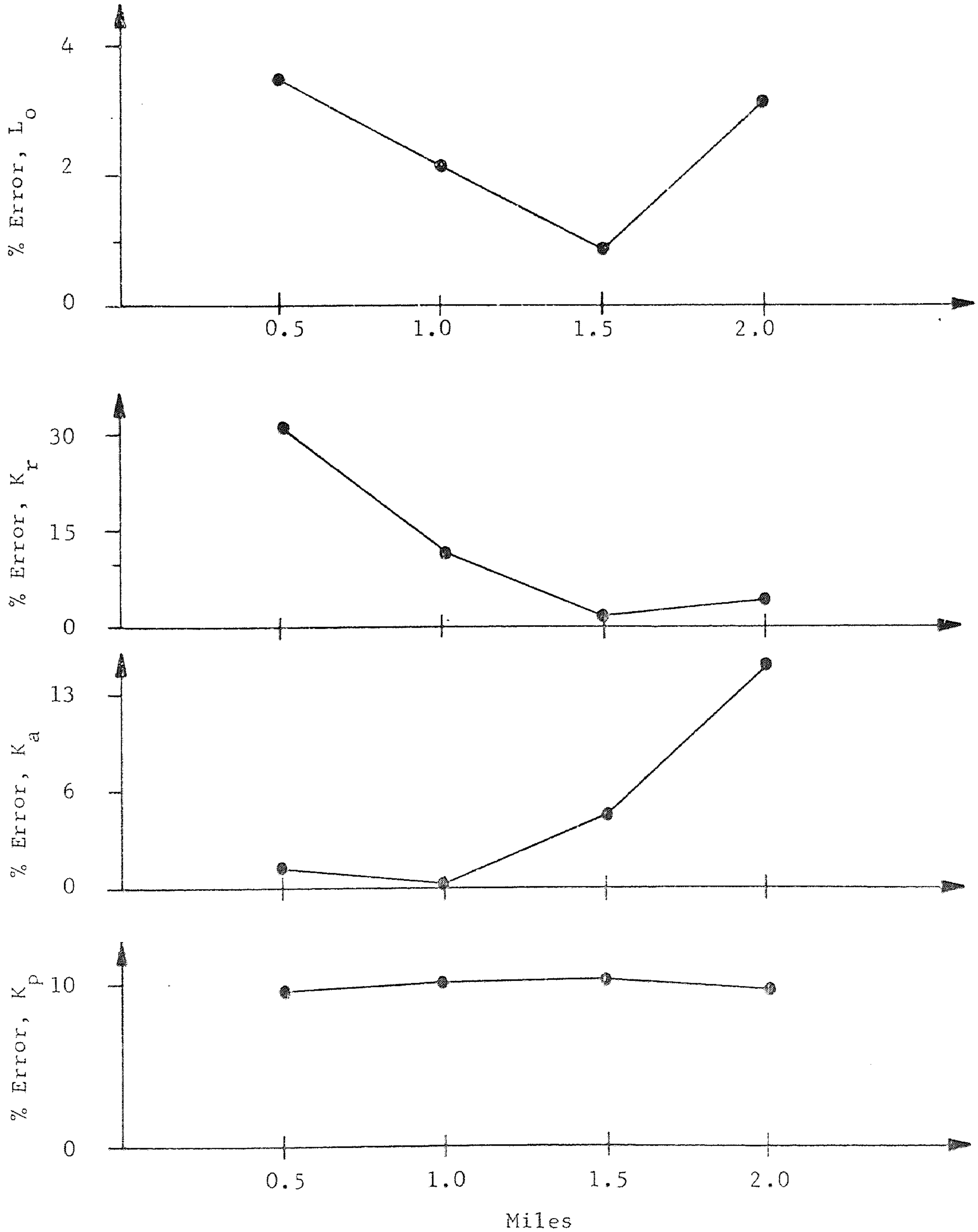


FIGURE VII-5. Optimum Measurement Stations for Parameter Estimation Using Stochastic Approximation and Constant Observation Error Variances

In this chapter stochastic adjustment methods have been successfully used to estimate stream parameters. By employing a multiple measurements technique developed in this study, the results show considerable improvement in estimated values and rates of convergence over single sets of measurements. The methods developed and the results obtained may be valuable in an on-line control of a polluted river in which it may be necessary to track the time variations of the critical parameters. The algorithms yield optimum estimates in a sequential fashion. This may not be desirable in practice in view of cost of making measurements. A more realistic cost function that includes instruments and operation costs is studied in a later chapter.

CHAPTER VIII

MULTIPLE KALMAN FILTERING IN A ONE-DIMENSIONAL STREAM SYSTEM

In this chapter, Kalman-type filters are derived for the optimum estimation of BOD and DO profiles in a one-dimensional polluted stream with negligible longitudinal dispersion. Modified forms of equations (2.11) and (2.12) which represent a stream model developed by O'Connor [97] are considered.

In a natural stream, parameters such as the velocity of flow, the decay rates and other sources and sinks are distributed temporally and spatially and may not be known a priori. Such cases are treated in other chapters of this study. For the purpose of this chapter, these parameters are treated as known constants and the effects of errors in modeling are lumped into driving functions which are represented as zero-mean Gaussian white noises.

Estimation is based on two sets of noisy independent measurement vectors. One set represents on-line readings of TOC and DO concentrations taken at short intervals of time. The other measurement vector represents off-line readings of BOD and DO concentrations taken at a different sampling rate and available after a fixed-time delay, T_D. The scheme for combining both sets of measurements employs the projection of the off-line measurements to the time of on-line estimation as presented in Chapter V.

The optimum estimates of the BOD and DO profiles are derived in two stages, namely propagation and measurements and correction [20 , 136]. The change in the estimate at sampling instant is formulated as a linear function of all expected errors of measurements.

The cost function considered is a subset of the general formulation presented in Chapter V. Here, algorithms are derived for multiple distributed Kalman-type filters which minimize weighted variances of the estimate errors. The problem of the optimum number of observations and their temporal spacing is treated later in Chapter X.

Optimization of measurement stations are obtained to satisfy a form of observability under steady-state conditions and the minimization of the cost function. The improvements in estimation obtained from using multiple measurements techniques are illustrated both in the development and in the results of some numerical examples studied. The effects of the levels of both system and measurement noises are also studied.

Problem Formulation

Stream Dynamics.

The stream model is described by the following system of partial differential equations

$$\frac{\partial V_1(x,t)}{\partial t} + \frac{U\partial V_1(x,t)}{\partial x} = -K_r V_1(x,t) + f_1(x,t)\,\omega_1(t) \tag{8.1}$$

$$\frac{\partial V_2(x,t)}{\partial t} + \frac{U\partial V_2(x,t)}{\partial x} = -K_d V_1(x,t) - K_a V_2(x,t) + K_a C_s$$

$$+ \bar{P} - \bar{R} - \bar{B} + f_2(x,t)\,\omega_2(t) \tag{8.2}$$

where

$V_1(x,t)$ = biochemical oxygen demand concentration mg/l

$V_2(x,t)$ = dissolved oxygen concentration mg/l

U = stream mean velocity miles/day

K_r = BOD removing rate coefficient 1/day

K_d = deoxygenation rate coefficient 1/day

K_a = reaeration rate coefficient 1/day

$\bar{P},\bar{R},\bar{R}$ = daily averaged photosynthetic, respiration and benthal deposits demand rates respectively (mg/l - day)

$f_1(x,t)$, $f_2(x,t)$ = functions representing the distribution of the lumped effects of errors in modeling

$\omega_1(t)$, $\omega_2(t)$ = zero-mean Gaussian white noises.

Equations (8.1) and (8.2) are written in a vector formulation as

$$\frac{\partial \underline{V}(x,t)}{\partial t} + \frac{U\partial \underline{V}(x,t)}{\partial x} = -\underline{k}\,\underline{V}(x,t) + \underline{S}(x,t) + \underline{D}(x,t) \tag{8.3}$$

where

$$\underline{V} = \begin{bmatrix} V_1 (x,t) \\ V_2 (x,t) \end{bmatrix}$$

$$k = \begin{bmatrix} K_r & 0 \\ K_d & K_a \end{bmatrix}.$$

$$S = \begin{bmatrix} 0 \\ K_a C_s + \bar{P} - \bar{R} - \bar{B} \end{bmatrix}$$

$$D = \underline{F} (x,t) \underline{\omega} (t)$$

$$\underline{\omega} (t) = \begin{bmatrix} \omega_1 (t) \\ \omega_2 (t) \end{bmatrix}$$

$\underline{\omega}$ (t) is a zero mean Gaussian white noise vector with a covariance matrix

$$E \left\{ \underline{\omega}(t) \, \underline{\omega}^T (\tau) \right\} = \underline{W} (t) \, \delta (t-\tau) \qquad (8.4)$$

The initial state profile is specified as

$$\underline{V} (x,t_o) = \underline{V}_o(x) \qquad (8.5)$$

and the upstream boundary condition as

$$\underline{V} (o,t) = \underline{V}_{oo}(t) \qquad (8.6)$$

In practice, only estimates of the initial and boundary conditions, usually established through measurements or prior analysis, are known. The estimates of the state profile at any time t is represented here by $\hat{\underline{V}}(x,t)$ and the effects of initial estimate errors are included in the analysis.

Following the development in [71], the solution of the system's differential equation (8.3) using the method of characteristics [33] becomes

$$\underline{V}\ (x,t) = \underline{\Phi}\ (t,to)\ \underline{V}\ (xo,\ to) + \int_{to}^{t} \underline{\Phi}\ (t,\ \tau)\ \underline{S}\ [x\ (\tau)\ \tau]\ d\ \tau$$

$$+ \int_{to}^{t} \underline{\Phi}\ (t,\ \tau)\ \underline{D}\ [x\ (\tau),\ \tau]\ d\ \tau \qquad (8.7)$$

where

$$x\ (t) = x\ (t_o)\ + U\ (t - t_o) \qquad (8.8)$$

For the example of the constant parameter stream model considered here, the $\underline{K}$ matrix is time-invariant, and hence, the transition matrix $\underline{\Phi}$ (t, to) becomes

$$\underline{\Phi}\ (t\text{-}to) = \begin{bmatrix} e^{-k_r(t-to)} & 0 \\ \frac{-k_d}{k_a-k_r} [e^{-k_r(t-to)}\ e^{-k_a}\ (t-to) & e^{-k_a}\ (t-to) \end{bmatrix} \qquad (8.9)$$

Measurement Scheme.

Following the presentation in Chapter V, the on-line measurement of TOC and DO monitored at a station x_m and having a sampling period T may be represented as

$$\underline{y}\ (x_{m,}\ i\ T) = \underline{H}\ (i\ T)\ \underline{V}\ (x_{m,}\ i\ T) + \underline{\xi}\ (i\ T) \tag{8.10}$$

$$i = 0,\ 1,\ 2,\ ---$$

The set of delayed measurements consisting of off-line discrete BOD and DO readings, taken at another station x_D and available after a fixed-time delay T_D, are projected to an on-line estimation point $(x_{m,} j\ T_1)$ and represented as

$$\underline{Z}\ (x_{m,} j\ T_1) = \underline{M}\ (j\ T_1)\ \underline{V}\ (x_{m,} j\ T_1) + \underline{o}\ (j\ T_1) \tag{8.11}$$

$$\text{for } j\ T_1 > T_D; \quad j = 0,\ 1,\ 2$$

It is computationally convenient for this stream example with negligible dispersion to choose x_D such that

$$x_m = x_D + U\ T_D \tag{8.12}$$

The optimum location of the station x_m is treated later in the chapter.

Both measurement noises are considered zero-mean and statistically independent with respective variance matrixes written as

$$E\left\{\underline{\xi}\ (iT)\ \underline{\xi}^T(iT)\right\} = \underline{R}\ (iT) = \begin{bmatrix} r_{11}(iT) & 0 \\ 0 & r_{22}(iT) \end{bmatrix}$$

$$E\left\{\underline{\rho}(jT_1)\,\underline{\rho}^T(jT_1)\right\} = \underline{L}(jT_1) = \begin{bmatrix} l_{11}(jT_1) & 0 \\ 0 & l_{22}(jT_1) \end{bmatrix}$$

For simplicity, the sampling period ratio T_1/T is chosen as a fixed integer N such that

$$T_1 = N\,T \tag{8.13}$$

Cost function.

Let the error between the true state profile $\underline{V}(x,t)$ and the estimated profile $\hat{\underline{V}}(x,t)$ be represented by

$$\tilde{\underline{V}}(x,t) = \underline{V}(x,t) - \hat{\underline{V}}(x,t) \tag{8.14}$$

The cost function to be optimized consists of the variance of any linear function of the estimate errors and is formulated as

$$\underline{P}(x,iT) = E\left\{\underline{\lambda}^T(x)\,\tilde{\underline{V}}(x,iT^+)\right\}^2 \tag{8.15}$$

where $\underline{\lambda}(..)$ is specified vector cost factor and iT^- and iT^+ represent instances of time immediately before and after measurements are taken at time iT.

The objective is to obtain the optimum estimates of the state profile $\hat{\underline{V}}(x,t)$ based on all available measurements by deriving algorithms for sequential filters which minimize the specified cost-function.

Derivation of Filter Algorithms

The optimum estimated state profile $\hat{\underline{V}}(x,t)$ based on the multiple measurements (8.10), (8.11) are desired.

By analogy to the approach in [20] two important assumptions are made. Firstly, for $\hat{\underline{V}}(x,t)$ to be an unbaised estimate of $\underline{V}(x,t)$, it is evident from taking the ensemble average of (8.3) that the filtered estimate propagates between sampling as

$$\frac{\partial\hat{\underline{V}}(x,t)}{\partial t} + \frac{U\partial\hat{\underline{V}}(x,t)}{\partial x} = -\underline{k}\,\hat{\underline{V}}(x,t) + \underline{S}(x,t) \qquad (8.16)$$

for $(i-1)\,T < t < iT$

Applying the solutions in (8.7) and (8.8) to (8.3) and (8.16), the true and estimated profiles between sampling then become

$$\underline{V}\,[x,t;x_o,(i-1)T^+] = \underline{\Phi}\,[t,(i-1)T]\,\underline{V}\left\{x-u\,[t-(i-1)T],\ (i-1)\,T\right\}$$
$$+\int_{(i-1)T}^{t} \underline{\Phi}\,(t,\tau)\left\{\underline{S}\,[x-u(t-\tau),\tau] + \underline{D}\,[x-u\,(t-\tau),\ \tau]\right\}d\tau \qquad (8.17)$$

and

$$\hat{\underline{V}}\,[x,t;\,x_o,\ (i-1)\,T^+] = \underline{\Phi}\,[t,\ (i-1)T]\,\hat{\underline{V}}\left\{x - u\,[t-(i-1)T],(i-1)T^+\right\}$$
$$+\int_{(i-1)T}^{t} \underline{\Phi}\,(t,\tau)\,\underline{S}\,[x-u\,(t-\tau),\ \tau]\,d\tau \qquad (8.18)$$

where the condition

$$0 < u\,[t - (i-1)T] < x-x_o$$

holds for both equations.

Subtracting (8.18) from (8.17) yields

$$\tilde{\underline{V}}[x,t] = \underline{\Phi}[t,(i-1)T]\,\tilde{\underline{V}}\left\{x-u[t-(i-1)T],\,(i-1)T^{+}\right\} + \int_{(i-1)T}^{t} \underline{\Phi}(t,\tau)\,\underline{D}[x-u(t-\tau),\tau]\,d\tau \tag{8.19}$$

for $(i-1)T < t < iT$

The covariance matrixes of the estimate error are defined as

$$\underline{Q}(x,y,t) = E\left\{\tilde{\underline{V}}(x,t)\,\tilde{\underline{V}}^{T}(y,t)\right\} \tag{8.20}$$

$$\underline{Q}(x,t) = E\left\{\tilde{\underline{V}}(x,t)\,\tilde{\underline{V}}^{T}(x,t)\right\} \tag{8.21}$$

Applying these definitions to equations (8.19) an noting that $\underline{\omega}(t)$ is a zero mean white noise vector, the dynamics of the covariance matrixes between sampling becomes

$$\underline{Q}(x,t) = \underline{\Phi}[t,(i-1)T]\,\underline{Q}\left\{x-u[t-(i-1)T,\,(i-1)T^{+}]\right\}\underline{\Phi}^{T}[t,(i-1)T] + \int_{(i-1)T}^{t} \underline{\Phi}(t,\tau)\,\underline{F}[x-u(t-\tau),\tau]\,\underline{W}(\tau)\,F^{T}[x-u(t-\tau),\tau]\,\underline{\Phi}^{T}(t,\tau)\,d\tau \tag{8.22}$$

and

$$\underline{Q}(x,x_m,t) = \underline{\Phi}[t,(i-1)]\,\underline{Q}\left\{x-u[t-(i-1)T],\,x_m-u[t-(i-1)T],\,(i-1)T^{+}\right\}\underline{\Phi}[t,(i-1)T]$$

$$+ \int_{(i-1)T}^{t} \underline{\Phi} (t,\tau) \underline{F} [x-u (t-\tau), \tau] \underline{W} (\tau) F^{T} [x_m-u (t-\tau]$$

$$\underline{\Phi}^{T} (t,\tau) d\tau \qquad (8.23)$$

for $\qquad (i-1)T < t < iT$

Equations (8.16), (8.21) and (8.22) provide the algorithms for the dynamics of the filtered estimate and its covariances between sampling.

The second assumption made in this development concerns the formulation of the filtered estimate at sampling. The change in the filtered estimate at sampling is assumed to be a linear operator of all expected errors in measurements. This may be written as

$$\hat{\underline{V}} (x,iT^{+}) - \hat{\underline{V}} (x,iT) = \underline{K}_i [\underline{y} (x_m,iT) - \underline{H} (iT) \hat{\underline{V}} (x_m, iT)]$$

$$+ \sum_{\substack{j=o \\ jNT>TD}}^{\infty} \underline{X}_j \delta (jNT-iT) [\underline{Z} (x_m, jNT) - \underline{M} (jNT) \hat{\underline{V}} (x_m, jNT)]$$

$$(8.24)$$

It is apparent from (8.24) that both sets of measurements are included in the sequential estimation scheme at those time instances when iT = jNT. $\underline{K}_i$, $\underline{X}_j$ are (2x2) matrixes which represent Kalman-type distributed filters. The algorithms for the filters are to be obtained by minimizing the specific cost function given in (8.15).

Since $\underline{P}(x, iT^+)$ may be expanded as

$$\underline{P}(x, iT^+) = \underline{\lambda}^T(x)\, \underline{Q}(x, iT^+)\, \underline{\lambda}(x) \tag{8.25}$$

it follows that the optimum filters may be obtained directly by minimizing the covariance matrix $\underline{Q}(x, iT^+)$

Let

$$\underline{\tilde{V}}(x, iT^+) = \underline{V}(x, iT) - \underline{\hat{V}}(x, iT^+)$$

$$\underline{\tilde{V}}(x, iT^-) = \underline{V}(x, iT) - \underline{\hat{V}}(x, iT^-)$$

Adding and subtracting $\underline{V}(x,iT)$ from the left hand side of (8.24) substituting (8.11) and (8.13) and then collecting terms yields

$$\underline{\tilde{V}}(x, iT^+) = \underline{\tilde{V}}(x, iT^-) - \underline{K}_i\, \underline{H}_i\, \underline{\tilde{V}}(x_m, iT^-)$$

$$- \underline{X}_i\, \underline{M}_i\, \underline{\Delta}_i\, \underline{\tilde{V}}(x_m, iT^-) - \underline{K}_i\, \underline{\xi}(iT) - \underline{X}_i\, \underline{\Delta}_i\, \underline{\rho}(iT) \tag{8.26}$$

where

$$\underline{K}_i = \underline{K}(x, x_m, iT), \quad \underline{H}_i = \underline{H}(iT)$$

$$\underline{X}_i = \underline{X}(x, x_m, iT), \quad \underline{M}_i = \underline{M}(iT)$$

and

$$\underline{\Delta}_i = \sum_{\substack{j=o \\ jNT>T_D}}^{\infty} \delta(jNT - iT)\, \underline{I}$$

It is noted that $\underline{\Delta}i$ is a 2x2 matrix which is either a zero matrix when only one set of measurements is available ($jNT \pm iT$) or a unitary matrix $\underline{I}$, when both sets of measurements are available ($jNT = iT$).

Applying the definition in (8.21) to equation (8.26), the change in the covariance of the filtered estimate may be expressed as

$$\underline{Q}\ (x,\ iT^{+}) = \underline{Q}\ (x,\ iT^{-}) - \underline{N}_i\ Q\ (x_m,\ x,\ iT^{-})$$
$$- \underline{Q}\ (x,\ x_m,\ iT^{-})\ \underline{N}_i^T + \underline{N}_i\ \underline{Q}\ (x_m,\ iT^{-})\ N_i^T$$
$$+ \underline{K}_i\ \underline{R}_i K_i^T + \underline{X}_i\ \underline{\Delta}i\ \underline{L}_i\ \underline{\Delta}_i^T\ \underline{X}_i^T \tag{8.27}$$

where

$$\underline{N}_i = \underline{K}_i\ \underline{H}_i + \underline{X}_i\ \underline{M}_i\ \underline{\Delta}_i$$

Employing differential calculus, by substituting $\underline{K}_i + \Delta K_i$ and $\underline{X}_i + \underline{\Delta X}_i$ into (8.27) and collecting terms, it can be shown that the necessary and sufficient conditions for $\underline{Q}\ (x,\ iT^{+})$ to be minimum are satisfied if the following expressions

$$\underline{H}_i\ \underline{Q}\ (x_m,\ iT^{-})\ \underline{H}_i^T + \underline{R}_i$$

and

$$\underline{M}_i\ \Delta_i\ \underline{Q}\ (x_m,\ iT^{-})\ \underline{\Delta}_i^T\ \underline{M}_i^T + \underline{\Delta}_i\ \underline{L}_i\ \underline{\Delta}_i^T$$

are at least non-negative definite for all i [20]. R_i, L_i and $\underline{Q}\ (x_m,\ o)$ represent measurement and initial errors which are considered non-trivial. If exact initial profile and noiseless measurements are available, there will be no need for filtering.

It follows then that the above expressions are satisfied.

The optimum filters result from equating the coefficient of $\Delta\underline{K}_i$, $\underline{\Delta}X_i$ to zero in the above development. The filter expressions become

$$\underline{K}_i = \underline{Q}(x, x_m, iT^-)\,\underline{B}_i\,[\underline{H}_i\,\underline{Q}(x_m, iT^-)\,\underline{B}_i + \underline{R}_i]^{-1} \tag{8.28}$$

and

$$\underline{X}_i = \left\{\underline{Q}(x, x_m, iT^-)\,\underline{M}_i^T - \underline{K}_i\,[\underline{H}_i\,\underline{Q}(x_m, iT^-)\,\underline{M}_i^T]\right\}\underline{A}_i^{-1} \tag{8.29}$$

where for brevity the following substitutions are made

$$\underline{A}_i = \underline{M}_i\,Q(x_m, iT)\,\underline{M}_i^T + \underline{L}_i \tag{8.30}$$

$$\underline{B}_i = \underline{H}_i^T - \underline{M}_i^T\,\underline{A}_i^{-1}\,\underline{M}_i\,\underline{Q}(x_m, iT^-)\,\underline{H}_i^T \tag{8.31}$$

Equations (8.28) and (8.29) apply at any time iT when both set of measurements are available ($\underline{\Delta}_i = \underline{I}$)

For time iT, when only one set measurement is available [$\underline{\Delta}_i = \underline{o}$] the optimum filter expressions become

$$\underline{K}_i = \underline{Q}(x, x_m, iT^-)\,\underline{H}_i^T\,[\underline{H}_i\,\underline{Q}(x_m, iT^-)\,\underline{H}_i^T + R_i]^{-1} \tag{8.32}$$

and

$$\underline{X}_i = \underline{0}$$

Substituting these expression back into (8.27) yields the change in the covariance $\underline{Q}$ (x, iT$^-$) at sampling

$$\underline{Q}\ (x,\ iT^+) = \underline{Q}\ (x,\ iT^-)\ -\ \underline{N}_i\ \underline{Q}^T\ (x,\ x_m,\ iT^-) \qquad (8.34)$$

Similarly, by putting the filter expressions into (8.24) and employing the definitions in (8.20) and (8.21) yields

$$\underline{Q}\ (x,\ x_m,\ iT^+) = \underline{Q}\ (x,\ x_m,\ iT^-) - \underline{N}_i\ \underline{Q}^T\ (x_m,\ iT^-) \qquad (8.35)$$

The developed multiple measurements filter algorithms are now summarized as follows: Equations (8.16), (8.22) and (8.23) give the dynamics of filtered state estimate at its covariances between sampling [that is, $(i-1)\ T < t < iT$]. They provide the data required in the equations (8.28) (8.29) or (8.32) and (8.33). The optimum filters thus obtained are used in (8.24), (8.34) and (8.35) to compute the changes in the values of the filtered estimates and its covariances at sampling.

It is noteworthy to observe some of the properties of the multiple Kalman filters developed in the precedings. Firstly, it is evident that equations for the multiple filters in (8.28) and (8.29) reduce to (8.32) and (8.33) for the single filter associated with one set of on-line measurements. It may be inferred then that although the single Kalman filter (8.32) is optimum for a single set of on-line measurements, it is sub-optimal when additional forms of measurements are available. This is in fact the case and the proof is given in the following development.

For simplicity, a scalar system is considered and the lower case notations are the scalar reductions from their matrix equivalences in the multivariate case treated above. For a scalar system, the filter equations (8.28), (8.29), (8.32), (8.33) reduce to

$$k_i = \frac{q\ (x,\ x_m,\ iT^-)\ h\ 1}{h^2\ q\ (x_m,\ iT^-)\ 1 + m^2\ q\ (x_m,\ iT^-)\ r + 1\ r} \qquad (8.36)$$

$$x_i = \frac{q\ (x,\ x_m,\ iT^-)\ m\ r}{h^2\ q\ (x_m,\ iT^-)\ 1 + m^2\ q\ (x_m,\ iT^-)\ r + 1\ r} \qquad (8.7)$$

for the multiple sets of measurements

and

$$k_i = \frac{q\ (x,\ x_m,\ iT^-)\ h}{h^2\ q\ (x_m,\ iT^-) + r} \qquad (8.38)$$

$$k_i = 0 \qquad (8.39)$$

for single set of measurements.

It is noted that whenever both sets of measurements are available, the values of the filters are inversely proportional to the level of the measurement noises.

The estimate error covariance (8.34) reduce to

$$q\ (x,\ iT^{+}) = q\ (x,\ iT^{-}) - \frac{h^2\ q^2\ (x,\ x_m,\ iT^{-})}{h^2\ q\ (x_m,\ iT^{-}) + r} \tag{8.40}$$

for single measurements and

$$q\ (x,\ iT^{+}) = q\ (x,\ iT^{-}) - \frac{(h^2\ 1 + m^2 r)\ q^2\ (x,\ x_m,\ iT^{-})}{h^2\ q\ (x_m,\ iT^{-})\ 1 + m^2\ q\ (x_m,\ iT^{-})\ r + 1\ r} \tag{8.41}$$

for multiple measurements. The relative improvement in estimation measured by the reduction in estimate error variance for each case is written from (8.40) and (8.41) as

$$I\ \text{single} = \frac{h^2\ q^2}{h^2\ q^2 + r}$$

$$I\ \text{multiple} = \frac{(h^2\ 1 + m^2\ r)\ q^2}{h^2\ q^2\ 1 + m^2\ q\ r + 1\ r}$$

It is evident that I multiple is a monotonic function of L with values

$$I \text{ multiple} = \begin{cases} q & \text{for } l = 0 \\ \dfrac{h^2 q}{h^2 q^2 + r} & \text{for } l = \infty \end{cases}$$

and I multiple > I single for $0 < l < \infty$

It follows that whenever any other set of measurements with finite measurement error variances ($l \neq \infty$) are available, multiple Kalman-type filters of the type developed above provide improved state estimates.

Another property of the filters, used later in Chapter IX is further presented here. If only one component (y_1) of the on-line measurement vector in (8.10) is available, the measurement may be represented as

$$y_1 (x_m, iT) = h_{11} (iT) V_1 (x_m, iT) + \xi (iT) \qquad (8.42)$$

Following the same analysis used in the foregoing development and considering for the sake of illustration only on-line estimation time $iT \pm jNT$, the expression for the optimum filter associated with the scalar on-line measurement is readily derived as

$$\underline{K}_i = \underline{\psi} (x, x_m, iT^-) \frac{[h_{11} (iT)}{h_{11}^2 (iT) Q_{11} (x_m, iT^-) + r_{11}} \qquad (8.43)$$

where $\underline{K}_i$ here is a 2x1 vector and the (2x1) covariance vector $\underline{\psi}(x, x_m, iT^-)$ is defined as

$$\underline{\psi}(x, x_m, iT^-) = E\left\{\underline{\tilde{V}}(x, iT^-)\, V_1(x_m, iT)\right\} \qquad (8.45)$$

Also, expressions similar to (8.34), (8.35) are obtained for the changes in the covariance matrix $\underline{Q}(x, iT)$ at sampling with vectors $\underline{K}_i$, $\underline{\psi}$ replacing matrixes $\underline{K}_i$ and $\underline{Q}(x, x_m, iT)$.

It may be observed that identical results are obtained by directly substituting an infinite value for the measurement error variance associated with the unknown measurement component $[r_{22}(iT) = \infty]$, in equations (8.32), (8.34) and (8.35). It follows then that when only one component of a measurement vector is available, a vector formulation such as in (8.10) may still be used, with the measurement error variance of the unknown vector set to infinity. This property enables the consideration of a specific number M, of monitoring stations for both components of the state vector even though the results in Chapter VI show that optimum monitoring stations may vary for each state variable.

Optimum Measurements Stations

The relative monitoring locations, for the on-line and off-line measurements have already been established in equation (8.12). The choice of the on-line estimation station x_m is made to satisfy the observability condition in a deterministic steady state stream. The steady state solution of the noise-free system (8.1) and (8.2) may be written as

$$L(x) = L(o)\, e^{-k_r \frac{x}{u}} \qquad (8.46)$$

$$C(x) = \frac{-k_d L_o}{ka-kr}\left[e^{-k_r \frac{x}{u}} - e^{-k_a \frac{x}{u}}\right] + Co\, e^{-k_a \frac{x}{u}}$$

$$+ \frac{S_2}{ka}\left(1 - e^{\frac{-k_a x}{u}}\right) \qquad (8.47)$$

where $S_2 = K_a C_s + \overline{P} - \overline{R} - \overline{B}$

Following the assumption in this chapter that the stream parameters are known, the only unknowns are the boundary conditions L (o), C (o). Observability of equation (8.46) and (8.47) are satisfied if L (o) and C (o) are derivable from measurements of L (x) and C (x) at any point x in the spatial domain. Following the development in Chapter VI, for the simple stream model considered here, an analytical solution of the optimum measurement locations is possible. The sensitivity coefficient

$$\left[\frac{\partial C(x)}{\partial L(o)}\right]^2$$

is maximum at $x = \frac{1}{ka-kr} \ln \frac{ka}{kr}$ and this point is chosen as the measurement station x_M. For values of u, kr and ka typical of streams as in the case of the numerical example in the next section, the point x_D, $(x_D = x_m - UT_D)$ where the delayed measurements are taken may fall upstream of the boundary. In that case, the measurements may be taken at the upstream boundary where the sensitivity coefficient

$$\left[\frac{\partial L(x)}{\partial L(o)}\right]^2 \quad \text{is maximum.}$$

The theory of multiple measurements for optimum state estimation in a class of distributed parameter systems representable by a stream model has been presented in the preceding sections. The implementation of the algorithms are shown in the following numerical examples.

Numerical Examples

In the two numerical examples, time-invariant systems with the following parameter values are considered.

$K_r = 0.164,\ K_d = 0.164,\ K_a = 0.658,\ C_s = 9.062$

$U = 0.75,\ \overline{P} - \overline{R} = 0.921,\ \overline{B} = 0.0$

$E_1 = 1.0,\ E_2 = 1.0,\ W_1 = 0.25,\ W_2 = 0.25$

$T1/T = N = 24$

$H_1 = 2.5,\ H_2 = 1.0$ for all iT

$\lambda_1 = 1.0,\ \lambda_2 = 5.0$ for all x.

The stream is initially at a steady-state condition long enough to enable DO and BOD measurements of initial values. Subsequent transient condition is caused by an additional dumping of BOD (V_1 (o,t) = 30 mg/l)at the upstream boundary at t = o. For the following examples, measurements are simulated by adding a generated random number to an expected measurement value as in equation (8.10)

Constant measurement error variances and zero observation costs.

For this example

$R_1 = 25, \quad R_2 = 1.0$

$N_1 = 1.0, N_2 = 1.0$ for all iT

$X_D = 0.0, X_M = 1.5$ miles

Based on the noisy measurements taking, figure VIII-1 shows the improvement in estimation at the critical DO sag point due to multiple measurements, and also the parts of the variances of the estimate errors.

Measurement error variances which are fixed ratios of the expected values.

This approach is characteristic of measuring instruments with specified accuracies. Again, zero observation costs are considered, along with the following

Standard deviation of TOC measurement = 10% of expected value

Standard deviation of DO measurement = 5% of expected value

Standard deviation of BOD measurement = 5% of expected value

$X_D = 0.0$ and $X_m = 1.5$ miles.

Figure VIII-2 again shows the improvement in estimation at the DO sag point due to multiple measurements and also the new steady-state profiles.

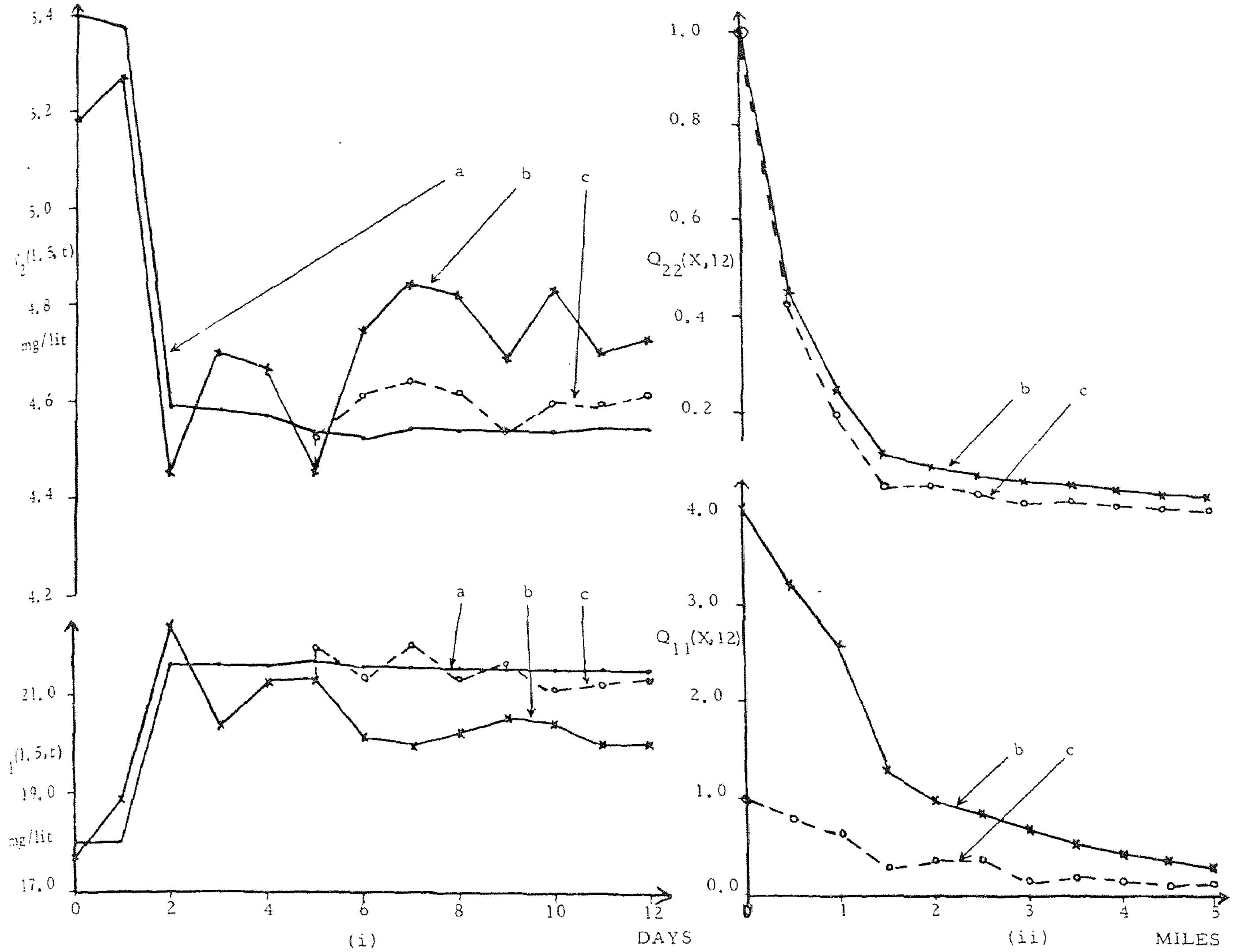


FIGURE VIII-1. Filtering with Constant Observation Error Variances and No Observation Costs.
Temporal Profiles of Estimates of DO and BOD (i) and Spatial Profiles of Estimate Error Variances (ii) Based on;

a) True values
b) Noisy measurements of TOC and DO
c) Noisy multiple measurements of TOC, BOD and DO.

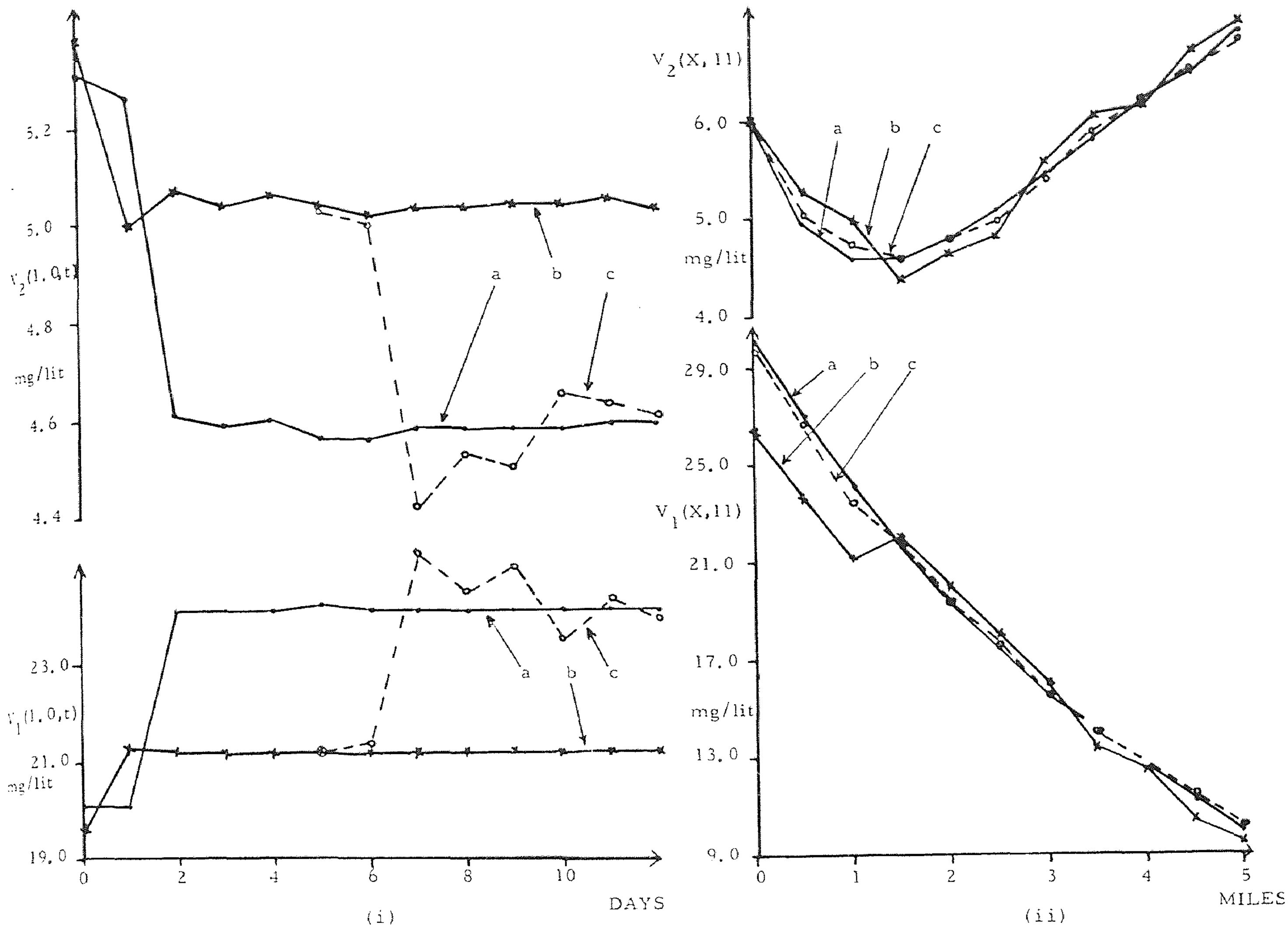


FIGURE VIII-2. Filtering with Constant Observation Error Variance-to-Signal Ratio and No Observation Costs. Estimates of Temporal (i) and spacial (ii) profiles of DO and BOD based on

a) True values.
b) Noisy Measurements of TOC and DO.
c) Noisy Multiple Measurements of TOC, BOD and DO.

Algorithms have been derived in this chapter for multiple distributed Kalman filters for estimation of stream water quality state profiles, based on measurements at different stations and with different sampling rates. The results of Chapter V have been applied to optimally utilize the off-line measurements in the on-line estimation. Also, the results of Chapter VI have been applied to establish the optimum measurement station where estimation may be done sequential. Estimates based on typical stream parameters and measured values have been presented in the numerical examples. Figures VIII-1 and VIII-2 are typical of other results accumulated for various other conditions of the stream model studied in this chapter. The results demonstrate the consistent superiority of the multiple measurements technique and encourage the use of on-line TOC measurement in water monitoring and control. Cost considerations have been omitted in the preceding developments, and reserved for treatment in Chapter X.

CHAPTER IX

MULTIPLE KALMAN FILTERING IN ESTUARIES WITH UNKNOWN PARAMETERS

The theory of Multiple Kalman-type filtering developed for a stream system in Chapter VIII is now extended for optimum estimation of BOD and DO profiles in polluted estuaries. Specific examples of estuary conditions considered include

(i) a one-dimensional tidal river with steady flow

(ii) a one-dimensional non-saline estuary with tidal oscillatory flow

(iii) a two-dimensional saline estuary with spatially varying tidal velocity.

In the cases treated, dispersion terms, reaction decay rates and the amplitudes of tidal velocities are assumed to be constants but unkn wn a priori. The stochastic approximation techniques discussed in Chapter VII are utilized for on-line identification of these parameters.

Estimation is based on multiple sets of on-line and off-line noisy measurements taken at various stations. The optimum locations of monitoring stations within the spatial domain of a specific estuary system have already been studied in Chapter VI. A similar method of projecting delayed measurements to the points of on-line estimation employed earlier for the stream system is used. However, the projection equations based on the impulsive responses of the estuary systems are more complex as evidenced by comparing equations (4.12) and (4.14) with (4.10).

Because analytical solutions of the differential equations describing estuary conditions are complicated and in several cases unavailable, the developments in the sequel are based on explicit finite difference approximations. The multiple filters derived in these examples are suboptimal to the extent that the above and other necessary approximations are made to simplify the analysis and to obtain numerical results pertinent to the scope of this study. When there is no limitation to the computer time and size available to the researcher, procedures for obtaining optimal filters for these specific estuary cases are discussed.

Again, a cost function consisting of only the variance matrix of the estimate errors is optimized. The more general cost function that includes observation cost is treated in the next chapter. Some of the numerical results obtained for the cases studied here also are presented.

One-Dimensional Tidal River With Steady Flow

Problem formulation.

The mathematical model for a one-dimensional estuary has been presented in equations (2.11) and (2.12). Under uniform cross section, constant parameter and steady flow conditions, these equations reduce to

$$\frac{\partial L(x,t)}{\partial t} = E \frac{\partial^2 L}{\partial x^2} - U \frac{\partial L}{\partial x} - K_r L + L_a \tag{9.1}$$

$$\frac{\partial C(x,t)}{\partial t} = E \frac{\partial^2 C}{\partial x^2} = U \frac{\partial C}{\partial x} - K_d L - K_a C + K_a C_s + P(x,t) - R(x,t) - B(x,t) \tag{9.2}$$

Definitions of the variables and parameters are analogons to those in Chapter VIII with additional terms E donating longitudinal dispersion coefficient (sq mi/day) and L_a, the rate of BOD increase resulting from urban runoff (mg/l - day).

For brevity, (9.1) and (9.2) are written in a vector form as

$$\frac{\partial \underline{V}(x,t)}{\partial t} = E \frac{\partial^2 \underline{V}}{\partial x^2} - U \frac{\partial \underline{V}}{\partial x} - \underline{K}\ \underline{V} + S(x,t) \tag{9.3}$$

Usually, only estimates of the parameters E, U, $\underline{K}$ and $\underline{S}$ determined from previous measurements or analysis are known a priori. The stochastic approximation techniques applied to a water quality stream model in Chapter VII may be employed in a sequential fashion to update the numerical values of the parameter estimates from available measurements. If parameter estimate errors may be assumed small and E, for instance, is written as

$$E = \hat{E} + \Delta E$$

the equation (9.3) may be written in terms of current values of the parameter estimates as

$$\frac{\partial \underline{V}(x,t)}{\partial t} = \hat{E}\,\frac{\partial^2 \underline{V}}{\partial x^2} - \hat{U}\,\frac{\partial \underline{V}}{\partial x} - \hat{\underline{K}}\,\underline{V} + \hat{\underline{S}}(x,t) + \underline{F}(x,t)\,\underline{\omega}(t)$$

where the effects of the estimate errors have been lumped into a driving function noise vector $\underline{\omega}(t)$, and $\underline{F}(x,t)$ is the distribution matrix. In general, the dynamic error thus formulated may be zero-mean but state-correlated because the parameter estimates are based on past estimates of the state profile. In that case filtering methods such as in [17] may be used. Without loss of generality, the dynamic error in the development is represented as a zero-mean gaussian white noise vector having a variance term typified by equation (8.4).

The measurement representations to be used in the sequel differ from those in Chapter VIII only to the extent that an arbitrary number M of on-line measurement stations are assumed here. Following the development in Chapter VI, the optimum number and locations of the monitoring stations vary with the number of parameters to be updated on-line. In addition, although both components of the state vector may not be monitored at a specific station, the scalar measurement may still be formulated in a vector form and the measurement error variance associated with the unknown component is then represented by an infinite value as shown in Chapter VIII.

With the preceding in perspective, the multiple measurements are represented as

$$\underline{y}(x_m, iT) = \underline{H}(iT)\ \underline{V}(x_m, iT) + \underline{\xi}(x_m, iT) \qquad (9.5)$$

$$i = 0,1,2\ ---$$

and

$$\underline{z}(x_m, jT_1) = \underline{M}(jT_1)\ \underline{V}(x_m, jT_1) + \underline{\rho}(x_m, jT_1) \qquad (9.6)$$

$$j = 0,1,2\ ---;\ jT_1 > T_D$$

The second component of $\underline{z}\ (x_m, jT_1)$ is actually an on-line DO readirg included for a symmetric vector representation. Following the development in equations (5.14), (5.15) and (5.16)

$$\rho_1\ (jT_1) = U\ \phi\ \eta_1\ (x_D,\ jT_1 - T_D)$$

$$E\ [\ \rho_1^2\ (jT_1)] = U^2\ \phi^2\ N_1\ (x_D,\ jT_1 - T_D)$$

where us'ng (5.12)

$$\phi = \frac{1}{\sqrt{4\pi E T_D}} \quad \exp\left\{-\frac{[(x_m - x_D) - U\ T_D]^2}{4ET_D} - K_r\ T_D\right\} \qquad (9.7)$$

and N_1 is the variance of the delayed off-line BOD reading taken at $(x_D,\ jT_1 - T_D)$.

By analogy to equation (8.25), the objective here is to obtain the optimum estimate of $\hat{\underline{V}}\ (x,t)$ based on measurements (9.5) and (9.6) by deriving algorithms for sequential filters which minimize the variance matrix of the estimate error

$$Q(x, iT^{+}) = E\left\{\underline{\tilde{V}}(x, iT^{+})\, \underline{\tilde{V}}^{T}(x, iT^{+})\right\} \tag{9.7}$$

Derivation of filter algorithms.

Again for $\underline{\hat{V}}(x,t)$ to be an unbaised estimate of $\underline{V}(x,t)$, it follows from (9.4) that the filtered state estimate propagates between sampling as

$$\frac{\partial \underline{\hat{V}}}{\partial t}(x,t) = \hat{E}\frac{\partial \underline{\hat{V}}}{\partial x^{2}} - \hat{U}\frac{\partial \underline{\hat{V}}}{\partial x} - \underline{\hat{K}}\,\underline{V} + \underline{\hat{S}}(x,t) \tag{9.8}$$

By subtracting (9.8) from (9.4), the dynamics of the state estimate error between sampling becomes

$$\frac{\partial \underline{\tilde{V}}}{\partial t}(x,t) = \hat{E}\frac{\partial^{2} \underline{\tilde{V}}}{\partial x^{2}} - \hat{U}\frac{\partial \underline{\tilde{V}}}{\partial x} - \underline{\hat{K}}\,\underline{\tilde{V}} + \underline{F}\,\underline{\omega}(t) \tag{9.9}$$

$$\text{for } (i-1)T < t < iT$$

The analytical solution of (9.9) for general initial and boundary conditions is unavailable. Instead, the explicit finite difference solution between sampling is written as

$$\begin{aligned}
\underline{\tilde{V}}_{x,\, iT^{-}} = {} & \frac{\hat{E}}{(\Delta X)^{2}}\left[\underline{\tilde{V}}_{x+1,(i-1)T^{+}} - 2\underline{\tilde{V}}_{x,(i-1)T^{+}} + \tilde{V}_{x-1,(i-1)T^{+}}\right] \\
& - \hat{U}\frac{\Delta t}{2\Delta x}\left[\underline{\tilde{V}}_{x+1,(i-1)T^{+}} - \underline{\tilde{V}}_{x-1,(i-1)T^{+}}\right] \\
& - \Delta t\, \underline{\hat{K}}\, \underline{\tilde{V}}_{x,(i-1)T^{+}} + \underline{\tilde{V}}_{x,(i-1)T^{+}} \\
& + \Delta t\, F_{x,(i-1)T^{+}}\, \underline{\omega}_{(i-1)T^{+}}
\end{aligned} \tag{9.10}$$

Collecting terms in (9.10) results in

$$\underline{\tilde{V}}_{x,iT^-} = \hat{a}_{x+1}\, \underline{\tilde{V}}_{x+1} + \hat{\underline{b}}_x\, \underline{\tilde{V}}_x$$

$$+ \hat{c}_{x-1}\, \underline{\tilde{V}}_{x-1} + \Delta t\, F_{x,(i-1)T^+} \;\; \underline{\omega}_{(i-1)T^+} \qquad (9.11)$$

where

$$\hat{a}_{x+1} = \frac{\hat{E}\,\Delta t}{(\Delta x)^2} - \frac{\hat{U}\,\Delta t}{2\Delta x} \qquad (9.12)$$

$$\hat{\underline{b}}_x = \left(\frac{-2\,\hat{E}\,\Delta t}{(\Delta x)^2} + 1\right) \underline{I} - \Delta t\, \hat{\underline{K}} \qquad (9.13)$$

$$\hat{c}_{x-1} = \frac{\hat{E}\,\Delta t}{(\Delta x)^2} + \frac{\hat{U}\,\Delta t}{2\Delta x} \qquad (9.14)$$

The spatial increment is

$$\Delta x = (x+1) - x$$

The dynamics of the error covariance matrix for any two spatial points (x,y) between sampling is obtained by postmultiplying (9.11) by its own transpose and taking the ensemble average. This results in

$$\underline{Q}\,(x,t,iT^-) = a_{x+1}\, \underline{Q}\,(x+1,y+1)\, a_{y+1} + \underline{b}_x\, \underline{Q}\,(x,y+1)\, a_{y+1}$$

$$+ c_{x-1}\, \underline{Q}\,(x-1,y+1)\, a_{y+1} + a_{x+1}\, Q\,(x+1,y)\, \underline{b}_y^T\, b_x\, \underline{Q}(x,y)\, \underline{b}_y^T$$

$$+ \underline{b}_x\, \underline{Q}\,(x,y-1)\, c_{y-1} + c_{x-1}\, \underline{Q}\,(x-1,y-1)\, c_{y-1}$$

$$+ \Delta t^2 \underline{F}_x \; \underline{W} \; \underline{F}_y^T \qquad (9.15)$$

for $(i-1)\,T^+ < t < iT^-$

Subscripts $(i-1)T^+$ in (9.11) and $(i-1)T^-$ and $\wedge$ in (9.15) have been dropped for clearity.

Explicit finite difference solutions of (9.8) and equation (9.15) then represent the propagation of the filtered estimate and its covariance between sampling time $(i-1)T^+$ and iT. They are analogous to (8.16) and 8.23).

To complete the development, it is now desired to derive the optimum filters from the available measurements at sampling. By analogy to equation (8.24), the change in the filtered estimate at sampling is formulated as

$$\hat{\underline{V}}(x,iT^+) - \hat{\underline{V}}(x,iT^-) = \sum_{m=1}^{M} Km,i\,[\underline{y}(x_m,iT) - \underline{H}(it)\,\hat{\underline{V}}(x_m,iT^-)]$$
$$+ \sum_{m=1}^{M} \sum_{\substack{j=o \\ jNT>T_D}}^{\infty} \underline{X}_{m,j}\,\delta\,(jNT-iT)\,[z(x_m,jNT) - M(jNT)\,\hat{\underline{V}}(x_m,jNT^-)] \qquad (9.16)$$

where

$$\underline{K}_{m,i} = \underline{K}\,(x,x_m,iT)$$

$$\underline{X}_{m,j} = \underline{X}\,(x,x_m,jNT)$$

are the multiple Kalman-type filters to be derived by minimizing the covariance matrix (9.7).

Following a similar procedure as in (8.26) and (8.27) the covariance matrix becomes

$$\underline{Q}\ (x, iT^{+}) = \underline{Q}\ (x) - \sum_{m=1}^{M} \underline{N}m\ \underline{Q}\ (x_m, x) - \sum_{m=1}^{M} \underline{Q}\ (x, x_m)\ \underline{N}_m^T$$

$$+ \sum_{m=1}^{M} \sum_{n=1}^{M} \underline{N}m\ \underline{Q}\ (x_m,\ x_n)\ \underline{N}_m^T + \sum_{m=1}^{M} \underline{K}m\ \underline{R}m\ \underline{K}_m^T$$

$$+ \sum_{m=1}^{M} Xm\ \underline{\Delta}\ \underline{L}_m\ \underline{\Delta}^T\ \underline{X}_m^T \qquad (9.17)$$

and

$$\underline{N}m = \underline{K}m\ H + Xm\ \underline{M}\ \underline{\Delta} \qquad (9.18)$$

where all expressions on the right hand side of (9.17) and (9.18) are evaluated at iT^{-}.

Using differential calculus to minimize $\underline{Q}\ (x, iT^{+})$ by substituting ($\underline{K}m + \Delta\underline{K}m$) and ($\underline{X}m + \Delta\underline{X}m$) into (9.17) and collecting terms for the coefficients of $\Delta\underline{K}_m^T$ and $\Delta\underline{X}_m^T$, yields necessary and sufficient conditions of optimization [20]

$$- \underline{Q}\ (x, x_m)\ \underline{H}^T + \sum_{m=1}^{M} \underline{N}_n\ \underline{Q}\ (x_n,\ x_m)\ H^T + \underline{K}_m\ \underline{R}_m = \underline{0} \qquad (9.19)$$

$$- \underline{Q}\ (x, x_m)\ \underline{\Delta}^T\ \underline{M}^T + \sum_{m=1}^{M} \underline{N}_m\ \underline{Q}\ (x_n,\ x_m)\ \underline{\Delta}^T\ \underline{M}^T$$

$$+ \underline{X}_m\ \underline{\Delta}\ \underline{L}_m = 0 \qquad (9.20)$$

for

$m = 1, 2 --- M.$

The true optimum multiple Kalman filter are the solutions of the simultaneous equations of matrixes (9.19) and (9.20). Although, very complicated, a solution does exist. For example, for $\underline{\Delta} = \underline{0}$ (single set of measurements) and with two on-line monitoring stations (M=2), it can be readily shown that

$$\underline{K}_2 = \left\{\underline{Q}\ (x,x_2)\ \underline{H}^T - \underline{K}_1\ \underline{H}\ \underline{Q}\ (x_1,x_2)\ \underline{H}^T\right\} \left\{\underline{H}\ \underline{Q}\ (x_2)\ \underline{H}^T + \underline{R}_2\right\}^{-1} \tag{9.21}$$

and

$$K_1 = \left\{\underline{Q}\ (x,x_1)\ H^T - \underline{Q}\ (x,x_2)\ H^T\ \underline{B}\right\} \left\{\underline{H}\ \underline{Q}\ (x_1)\ \underline{H}^T + \underline{R}_1) + \underline{H}\ \underline{Q}\ (x_1,x_2)\ \underline{H}^T\ \underline{B}\right\}^{-1} \tag{9.22}$$

where

$$\underline{B} = (\underline{H}\ \underline{Q}\ (x_2)\ \underline{H}^T + \underline{R}_2)^{-1}\ \ \underline{H}\ \underline{Q}\ (x_2,\ x_1)\ \underline{H}^T$$

Even for this simplified case, the matrix manipulation is enormous. For a two-dimensional estuary where up to six monitoring stations are considered as in a later example, the matrix manipulation becomes excessive. This motivates the derivation of a simpler but suboptimal filter.

The suboptimal filters developed in the following derivations are based on an assumption that there is little correlation between estimate errors at any two independent measurement stations.

$$\underline{Q}\ (x_m, x_n) = \underline{0} \text{ for } m \neq n \tag{9.23}$$

This assumption is valid in the limit as the measurement error goes to zero. Substituting (9.23) into (9.19) and (9.20) yields

$$\underline{K}_m\ [\underline{H}\ \underline{Q}\ (x_m)\ \underline{H}^T + \underline{R}_m] + \underline{X}_m\ \underline{M}\ \underline{\Delta}\ \underline{Q}\ (x_m)\ \underline{H}^T = \underline{Q}\ (x, x_m)\ \underline{H}^T \tag{9.24}$$

$$\underline{K}_m\ \underline{H}\ Q\ (x_m)\ \underline{\Delta}^T\ \underline{M}^T + \underline{X}_m\ [\ \underline{M}\ \underline{\Delta}\ \underline{Q}\ (x_m)\ \underline{\Delta}^T\ \underline{M}^T + \Delta\ \underline{L}_m]$$
$$= \underline{Q}\ (x, x_m)\ \underline{\Delta}^T\ M^T \tag{9.25}$$

for $m = 1, 2 --- M$.

The solutions of (9.24) and (9.25) yield the suboptimal multiple filters $\underline{K}\ (x, x_m, iT)$, $\underline{X}\ (x, x_m, iT)$, $i = 1, 2 --- M$ with expressions identical with equations (8.28) and (8.29) for time $iT = jNT$ when both sets of measurements are available. At $iT \neq jNT$, when only one set of measurements is available the solutions of (9.24) and (9.25) reduce to (8.32) and (8.33).

Substituting the filter algorithms back into (9.17) results in the algorithm for the change in covariance matrixes $Q\ (x,t)$, $Q\ (x, x_m, t)$ at sampling

$$\underline{Q}\ (x, iT^+) = \underline{Q}\ (x, iT^-) - \sum_{m=1}^{M} \underline{N}\ (x, x_m, iT)\ \underline{Q}^T\ (x, x_m, iT^-) \tag{9.26}$$

and

$$\underline{Q} (x,x_m,iT^+) = \underline{Q} (x,x_m iT^-) - \sum_{m=1}^{M} \underline{N} (x,x_m,iT) \underline{Q}^T (x_m,iT^-) \tag{9.27}$$

In summary, algorithms (9.8), (9.15) are used to compute the values of the filtered state profile and its covariances between sampling. They provide the data at iT^- to compute the filters from (9.24) and (9.26). The resulting filter expressions are then used in (9.16), (9.26) and (9.27) to obtain the corrections to be applied to the filtered state estimate and its covariances at sampling. In addition, stochastic approximation method developed in Chapter VII are applied to update the parameters based on the available measurements at sampling.

One-Dimensional Tidal River With Oscillatory Flow

The filtering problem here differs from the preceding only to the extent that the tidal velocity term in (9.1) and (9.2) is not a constant but represented as

$$U (x,t) = U_F + U_T \operatorname{Sin} \omega t$$

In addition, the corresponding projected off-line BOD measurements error becomes

$$\varrho_1 (j T_1) = U_F \phi \eta_1 (x_D, jT_1 - T_D)$$

$$E [\varrho_1^2 (j T_1)] = U_F^2 \phi^2 N_1 (x_D, jT_1 - T_D)$$

and from (4.12)

$$\phi = \frac{1}{\sqrt{4\pi T_D}} \exp \left\{ \frac{-\left[(x_m - x_D) - U_F T_D + \frac{U_T}{\omega} \left(\cos\omega j T_1 - \cos\omega (jT_1 - T_D) \right) \right]^2}{4\, E\, T_D} - K_r T_D \right\}$$

With these modifications, the algorithms derived for optimum filtering in the preceding section apply to this example of a one-dimensional estuary with oscillatory flow.

Two-Dimensional Estuary With Salinity Intrusion

The development here follows very closely to that of the one-dimensional estuary; the major difference is the increased number of terms resulting from the additional spatial dimension. Figure IX-1 shows the comparison between the number of elements of the profiles from the previous time-step required for the computation of the current profile for both one-dimensional and two-dimensional cases.

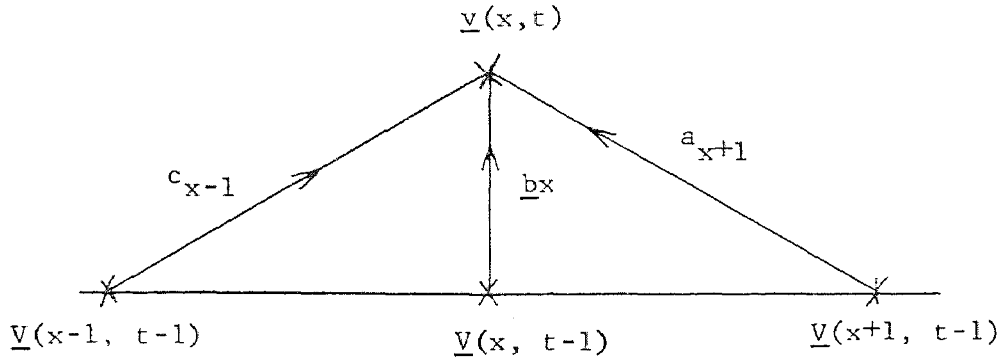
Problem Formulation.

The system considered here is represented as

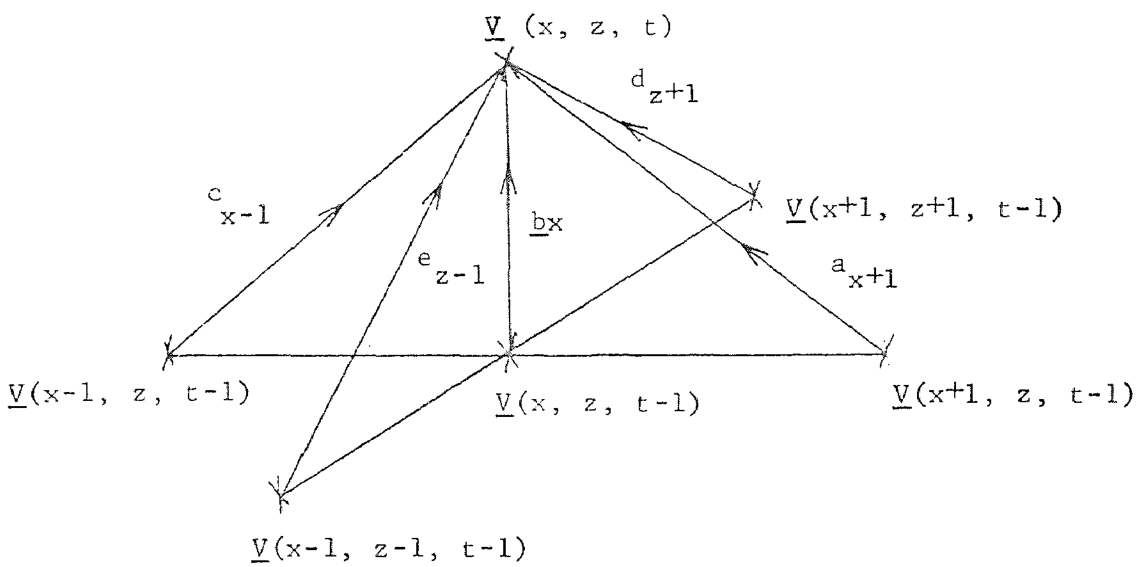
$$\frac{\partial L(x,z,t)}{\partial t} = Ex \frac{\partial^2 L}{\partial x^2} + Ez \frac{\partial^2 L}{\partial z^2} - U \frac{\partial L}{\partial x} - Kr\, L + La \qquad (9.28)$$

$$\frac{\partial C(x,z,t)}{\partial t} = Ex \frac{\partial^2 C}{\partial x^2} + Ez \frac{\partial^2 C}{\partial z^2} - U \frac{\partial C}{\partial x} - Kd\, L - Ka\, C$$

$$+ K_a C_s + P - R - B \qquad (9.29)$$



(i) One Dimensional Estuary



(ii) Two Dimensional Estuary

FIGURE IX-1. Profile Computation in Estuary Systems by Explicit Finite Difference Method

A one-dimensional advective flow in the horizontal direction is assumed and the additional term Ez represents eddy diffusion in the vertical direction. The time-averaged component of the tidal velocity is formulated as

$$U_a (x,z,t) = U_F \left[1 + 2 \left(\frac{z}{zo} - 1\right) \frac{x}{xo}\right] \tag{9.30}$$

to approximate the logarithmic vertical profile that has been observed to result from salinity intrusion in an estuary [52]. In addition, a linear approximation of the results in [123] is employed in formulating the time-varying component

$$U_v (x,z,t) = U_T \frac{x}{xo} \text{Sin}\, \omega_T t.$$

The tidal velocity term used in the following example is then written as

$$U (x,z,t) = U_a (x,z,t) + U_v (x,z,t) \tag{9.32}$$

The preceding approximations are made to incorporate realistic estuary conditions and yet maintain computational simplicity in the development.

Estimation is based on multiple sets of measurements

$$\underline{Y} (x_m, z_m, iT) = \underline{H} (iT) \underline{V} (x_m, z_m, iT) + \underline{\xi} (x_m, z_m, iT)$$

$$\underline{z}\ (x_m, z_m, jT_1) = \underline{M}\ (jT_1)\ \underline{V}\ (x_m, z_m, iT) + \underline{\rho}\ (x_m, z_m, iT)$$

for $m = 1, 2 \text{ --- } M$

The projected off-line BOD measurement error is again represented as

$$\rho_1\ (x_m, z_m, jT_1) = U_F\ \phi\ \eta_1\ (x_D, z_D, jT_1)$$

$$E\ [\rho_1^2\ (x_m, z_m, jT_1)\ ] = U_F^2\ \phi^2\ N_1\ (x_D,\ z_D,\ jT_1 - T_D)$$

where by using equation (4.14)

$$\phi = \frac{1}{4\pi T_D\sqrt{Ex\ Ez}}\ \exp\left\{-\frac{[\,(x_m - x_D) - U_F T_D + \frac{U_T}{\omega}\left(\cos\omega t - \cos\omega\ (jT_1 - T_D)\right)]^2}{4\ E_x\ T_D} - \frac{[z_m - z_D]^2}{4E_z T_D} - K_r\ T_D\right\}$$

Again, a variance matrix cost function

$$Q\ (x,z,iT^+) = E\left\{\ \underline{\tilde{V}}\ (x,z,iT^+)\ \underline{\tilde{V}}^T(x,z,iT^+)\right\}$$

is to be optimized.

<u>Derivation of filter algorithms</u>.

By analogy to (9.8), the filtered estimate propagates between sampling as

$$\frac{\partial \hat{\underline{V}}}{\partial t}(x,z,t) = Ex \frac{\partial^2 \hat{\underline{V}}}{\partial x^2} + Ez \frac{\partial^2 \hat{\underline{V}}}{\partial z^2} - \hat{U} \frac{\partial \underline{V}}{\partial x} - \hat{\underline{K}}\, \underline{V} + \hat{\underline{S}}(x,z,t) \tag{9.33}$$

Following earlier developments, the estimate error dynamics between sampling becomes

$$\tilde{\underline{V}}_{x,z,iT^-} = a_{x+1}\, \tilde{\underline{V}}_{x+1,z} + \underline{b}_x\, \tilde{\underline{V}}_{x,z} + c_{x-1}\, \tilde{\underline{V}}_{x-1,z} + d_{z+1}\, \tilde{\underline{V}}_{x,z+1} + e_{z-1}\, \tilde{\underline{V}}_{x,z-1} + \Delta t\, \underline{F}_{x,z,(i-1)T^+}\ \underline{W}_{(i-1)T^+} \tag{9.34}$$

where

$$a_{x+1} = \left[\frac{\hat{E}x\, \Delta t}{\Delta x^2} + \frac{\hat{U}\, \Delta t}{2\Delta x} \right]$$

$$\underline{b}_x = \left[-2\, \frac{\hat{E}x\, \Delta t}{\Delta x^2} - 2\, \frac{\hat{E}z\, \Delta t}{\Delta z^2} + 1 \right] \underline{I} + \Delta t\, \hat{\underline{K}}$$

$$c_{x-1} = \left[\frac{\hat{E}x\, \Delta t}{\Delta x^2} - \frac{\hat{U}\, \Delta t}{2\Delta x} \right]$$

$$d_{z+1} = \frac{\hat{E}z\, \Delta t}{\Delta z^2}$$

$$e_{z-1} = \frac{\hat{E}z\, \Delta t}{\Delta z^2}$$

The resulting dynamics of the covariance matrix between sampling is straight forward from equation (9.15). It contains 25 combinations of covariance terms of the type

$$a_{x+1,z}\ \underline{Q}\ (x+1,z;\ y,s,\ \ iT^{+})\ \underline{b}^{T}\ y,s$$

and a term $\Delta t^2\ \underline{F}_{x,z}\ \underline{W}\ \underline{F}^{T}_{x,z}$ which is the propagation of the error dynamics. The term $\underline{Q}$ $(x+1,z;\ y,s;\ \ iT^{+})$ is the covariance between the estimate errors at any two spatial points $(x+1,z)$ and (y,s). The algorithms for the filters in (9.24), (9.25), (9.26) and (9.27) are modified only by the additional dimension for this two-dimensional estuary case.

The implementation of these equations on a digital computer is straight-forward. Because, the estimation is done sequentially, memory storage is needed only for the current values of the state estimate profile and its covariances. However, for a large grid size, storage may become a critical problem. Unfortunately, the grid size cannot be reduced arbitrarily because this might violate the stability conditions.

Numerical Example

For the following numerical example, a two-dimensional saline-estuary conditin of the type treated in the preceding section is considered. Numerical values for the estuary parameters are as follows

(i) physical parameters

estuary length ss = 5 miles

estuary depth zz = 30 ft.

(ii) hydrodynamic parameters

longitudinal dispersion in x - direction $E_x = .12\ mi^2/d$

vertical eddy diffusion $Ez = 5 \times 10^{-4}\ ft^2/sec$

fresh water flow at upstream boundary $U_F = .25$ mi/d

maximum tidal velocity $U_T = 0.1$ mi/d.

A non-linear distributed tidal velocity of the form

$$U\ (x,z,t) = U_F\ [1 + 2\frac{x}{ss}\ (2\frac{z}{zz} - 1)]$$

$$+ U_T\ \frac{x}{xo}\ \text{Sin}\ \omega_T\ t$$

is used

where the tidal period $TT = \frac{2\pi}{\omega_T} = 12.4$ hrs.

(iii) biochemical parameters

$K_r = 0.25$ /day

$K_d = 0.25$ /day

$K_a = 0.65$ /day

$C_s = 9.5$ mg/l

$P - R - B = 0$

(iv) the system is assumed to be at steady state initially with up-stream boundary conditions

$V_1\ (o,z,0^-) = 20$ mg/l

$V_2\ (o,z,0^-) = 6.5$ mg/l

(v) transient conditions are generated by an additional BOD dumping at the upstream boundary

$$V_1\ (o,z,0^+) = 30\ mg/l$$

$$V_2\ (o,z,0^+) = 6.5\ mg/l$$

Multiple measurements of the type discussed in the text are used in the simulation. On-line measurements of DO and TOC are taken every two hours

MT = 2 hours

and the off-line BOD measurements are taken every six hours with a five-day delay

MB = 6 hours

TD = 5 days

The standard deviation associated with the measurements are

standard deviation for TOC measurements VT = 5.0 mg/l

standard deviation for DO measurements VC = 1.0 mg/l

standard deviation for BOD measurements VL = 1.0 mg/l

A linear function assumed for TOC and BOD values is

TOC = TG x BOD + TIN

where

TG = 2.5

TIN = 0.

The parameters updated on-line in the simulation are E_x, E_z, U_F, U_T, K_r and K_a. The values of the initial parameter estimates used are

$$EE_x = 0.15 \text{ mi}^2/\text{d}$$

$$EE_z = 8 \times 10^{-4} \text{ ft}^2/\text{sec}$$

$$EU_F = 0.4 \text{ mi/day}$$

$$EU_T = 0.15 \text{ mi/day}$$

$$EK_r = 0.5/\text{day}$$

$$EK_a = 0.25/\text{day}$$

For initial conditions of the state profile estimate, values consisting of the true state profile and additive simulated noise are used with variances

$$\underline{Q}(x,z,0^+) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and $Q(x,z;y,s) = \underline{0}$, for $x \neq y$ or $z \neq s$

Initially, five BOD and TOC measurement stations and six DO measurement stations located at equal interval along the center line of the estuary are assumed. The subsequent locations of the measurement stations are obtained using the algorithms developed in Chapter VI for optimum monitoring locations.

A spatial grid increment Dx = 0.2 miles and a temporal grid increment DT = 1 hour were found to provide marginal stable solutions. The results obtained by applying the distributed multiple Kalman filtering algorithms developed in the text, to this specific numerical example are shown in Tables IX-1 and IX-2.

Table IX-1 shows the true BOD state profile and the estimated state profile, with the corresponding estimate error variance after eight days of estimation.

Similarly, Table IX-2 shows the true DO state profile and the corresponding state extimate and error variance after eight days of iteration. In addition, the optimum monitoring locations compared with the uniform intervals originally assumed are

optimum DO monitoring stations (x_1, z_1) = (.8 mile, 18 ft)

(x_2, z_2) = (1.6 mile, 18 ft)

(x_3, z_3) = (3.2 mile, 18 ft)

(x_4, z_4) = (4.8 mile, 30 ft)

(x_5, z_5) = (4.8 mile, 18 ft)

(x_6, z_6) = (2.4 mile, 18 ft)

Z ft. \ X miles	0			1			2			3			4			5		
	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c
0	30	28.7	.32	6.6	6.6	.32	2.2	2.1	.32	1.1	1.1	.32	.23	.25	.32	.04	.01	.32
6	30	29.0	.32	6.8	6.4	.32	2.9	3.0	.32	1.1	1.3	.32	.27	.28	.32	.03	.05	.32
12	30	31.2	.32	6.9	6.7	.32	2.6	2.4	.32	1.1	1.6	.32	.12	.11	.32	.15	.17	.32
18	30	30.0	.32	7.4	7.8	.32	2.3	2.7	.32	1.2	1.0	.32	.23	.20	.32	.17	.17	.32
24	30	30.0	.32	7.4	7.2	.32	2.6	2.6	.32	1.5	1.4	.32	.48	.51	.32	.32	.28	.32
30	30	28.9	.32	7.4	7.2	.32	2.8	3.0	.32	1.9	2.2	.32	.60	.62	.32	.41	.45	.32

Table IX - 1 Multiple Kalman Filtering in Stratified Estuary with Constant Observation Error Variances - BOD Profile

a) True BOD Profile
b) Estimated BOD Profile based on Multiple Measurements
c) Estimate Error Variance

z ft. \ X miles	0			1			2			3			4			5		
	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c
0	6.5	6.3	.27	6.0	6.2	.27	6.7	6.3	.27	8.1	8.4	.27	9.0	8.9	.27	9.4	9.3	.27
6	6.5	6.2	.27	5.9	6.0	.27	7.9	8.2	.27	8.6	8.4	.27	8.7	8.5	.27	9.0	8.8	.27
12	6.5	6.3	.27	4.9	4.7	.27	8.0	7.7	.27	9.0	9.0	.27	8.3	8.8	.27	8.5	8.8	.27
18	6.5	6.7	.27	4.7	4.3	.27	8.2	7.6	.27	8.4	8.8	.27	7.8	7.9	.27	8.8	8.4	.27
24	6.5	6.2	.27	6.4	6.7	.27	7.6	7.6	.27	9.0	9.0	.27	8.6	8.7	.27	8.6	8.7	.27
30	6.5	6.6	.27	6.7	6.3	.27	7.4	7.3	.27	7.4	6.9	.27	7.6	7.9	.27	8.4	7.9	.27

Table IX - 2 Multiple Kalman Filtering in a Stratified Estuary with Constant Observation Error Variances - DO Profile

a) True DO Profile
b) Estimated DO Profile Based on Multiple Measurements
c) Estimate Error Variance

optimum BOD and TOC monitoring stations

$$(x_1, z_1) = (4.8 \text{ mile}, 30 \text{ ft})$$

$$(x_2, z_2) = (4.8 \text{ mile}, 30 \text{ ft})$$

$$(x_3, z_3) = (3.2 \text{ mile}, 18 \text{ ft})$$

$$(x_4, z_4) = (2.4 \text{ mile}, 18 \text{ ft})$$

$$(x_5, z_5) = (4.8 \text{ mile}, 30 \text{ ft})$$

A multiple measurements technique for optimum state estimation in a class of non-linear dynamic distributed parameter systems has been presented in this chapter. Algorithms for Kalman type filters for both off-line and on-line measurements have been developed. The development is based on the finite difference representation of the state differential equations. The off-line measurement projection method and the theory of optimum spatial monitoring stations developed in earlier chapters have been applied along with the filter algorithms in this chapter to a realistic saline estuary model with non-linear tidal velocity distribution. The results show improvement in estimate based on multiple measurements. In addition, as it may be observed from the BOD monitoring stations, the optimum locations are not necessarily spaced at equal intervals.

CHAPTER X

COST CONSIDERATIONS AND THE OPTIMUM ESTIMATOR INDICATOR

Optimization may be defined, in a broad sense, as a procedure by which a specified goal is realized with the minimum amount of effort possible. Thus, an optimization criterion, to be realistic, should include both the penalty associated with any deviation from the desired goal and the costs of the efforts expended. This approach has found wide application in control theory where often, the problem is to obtain the optimum strategy for the control effort.

As part of the contribution of this study, a realistic cost function is applied to the problem of optimum estimation in water quality systems. The various factors that may contribute to the uncertainty of the estimated value of a water quality variable, have already been presented in the previous chapters. These factors include modeling approximation errors, instrument noises and other errors that may result from the various empirical procedures by which some water quality parameters are evaluated. The cost of uncertainties in estimates, thus constitutes one part of the cost function treated in this chapter. It represents the possible damage to the water resource, that may result from management and control policies based on uncertain information.

Furthermore, as it is the case in practical engineering problems, significant costs may be associated with the acquisition of data on shich the analysis of a system is based. Observation costs, which for water quality systems, often include the costs of laboratory apparatus, instruments and operational costs, constitute the other part of the cost function considered in this study.

The formulation of the cost function as described above implies a knowledge of the explicit significance of each cost component. The determination of the observation costs can readily be based, among other factors, on the wages of the laboratory personnel, the price quotations and life expectancy of the instruments [8, 48, 63].

However, the determination of the cost of uncertainties in estimates presumes an explicit knowledge of the complete asset of the water resource. The latter is a formidable problem that has received considerable political, social and economic attention in recent years, particularly because of the multipurpose use of water resources. Extensive studies have been made on cost benefit analysis [59, 16], to evaluate the asset of natural water systems to assimilate wastes, and the detrimental effect of water pollution on such benefits as drinking water supply, aquatic life and contact recreation.

Alternatively, the cost of uncertainties in estimates may be evaluated from the viewpoint of enforcement where a penalty is imposed whenever a plant's effluent exceeds an allowable BOD load limit. In addition, the costs of the improvement in treatment facilities, artificial aeration and so on, which may be necessary to maintain acceptable water quality conditions may be considered [152].

The scope of this study is limited to an assumption that the various pertinent cost factors discussed in the precedings, are available. The contribution here is the application of these factors to obtain an optimum observation strategy for monitoring water quality systems. An algorithm is derived for an estimation indicator whose optimum values dictate the optimum number of observations and their temporal spacing. This, along with the development in Chapter VI for the optimum spatial measurement stations, thus provide a comprehensive monitoring policy for the analysis and control of water quality systems.

The implementation of the estimator indicator algorithm is given in a numerical example and the results demonstrate that improved estimation based on fewer samples may be obtained.

Cost Function

The definition of the various terms included in the general cost formulation given in equation (5.17) are now presented. The cost function includes the spatial integral of the mean square of a linear function of the state estimate errors and the costs of all observations.

$$P\ (x, iT^+) = \int_{x_o}^{x_f} E \left\{ [\underline{\lambda}^T\ (x)\quad V\ (x, iT^+)\ ]^2 \right\}\ dx$$

$$+ \sum_{x_m, x_D} e\ (x_m, iT)\ [\delta\ (iT - jT_1)\ \underline{\beta}^T\ C_D\ (x_D)$$

$$+ \underline{\alpha}^T\ \underline{C}\ (x_m)\ ] \qquad (10.1)$$

The variance term represents the cost of uncertainties in estimates, and the second term on the right hand side of (10.1) includes all costs of the on-line and off-line observations. $\underline{C}\ (x_m)$ is the average observation cost vector for the on-line TOC and DO measurements monitored at station x_m, while $\underline{C}_D\ (x_D)$ represents the observation cost vector of the off-line delayed BOD and DO at x_D. Numerical values for $\underline{C}\ (x_m)$ and $\underline{C}_D\ (x_D)$ may be established from wages and instrument prices. As done in previous chapters, the kronecker delta $\delta\ (iT - jT_1)$ is included to incorporate the costs of the delayed measurements at times $(iT - jT_1)$ when they become available.

The estimator indicator $e\ (x_m,\ iT)$, whose optimum values indicates whether an observation should or should not be taken is discussed further in the next section. $\underline{\lambda}(x)$, $\underline{\alpha}$, and $\underline{\beta}$ are specified cost factors which establish the relative significance of each cost component. Because these parameters are relative weights the following discussion is limited only to $\underline{\lambda}$ (x), with an understanding that numerical values of $\underline{\alpha}$ and $\underline{\beta}$ can be readily based on $\underline{\lambda}$ (x).

Evaluation of cost factor.

In the preceding chapter, the estimation problems have been based only on the minimization of the estimate error covariance. The results have provided a state estimate profile $\hat{\underline{V}}$ (x,iT) which is unbiased (E $\{\hat{\underline{V}}$ (x,iT)$\}$ = $\underline{V}$ (x,iT) and has an associated measure of uncertainty in the form of a covariance $\underline{Q}$ (x,iT). To properly illustrate the significance of these results in the following development, an example of the scalar components are employed. Hence, V_2 (x,iT) may represent the true DO profile at time iT, $\hat{V}_2$ (x,iT) represents the estimated profile and Q_{22} (x,iT) is the variance of the estimate error.

Because Gaussian white noise type are being considered, the density distribution of the unknown true value V (x,iT), given an estimate $\hat{V}$ (x,iT), is shown as a normal distribution in Figure X-1. A threshold minimum value V_{2S} is assumed to be the standard quality criterion imposed on the stream. Methods of establishing water quality standards are contained in many studies [115].

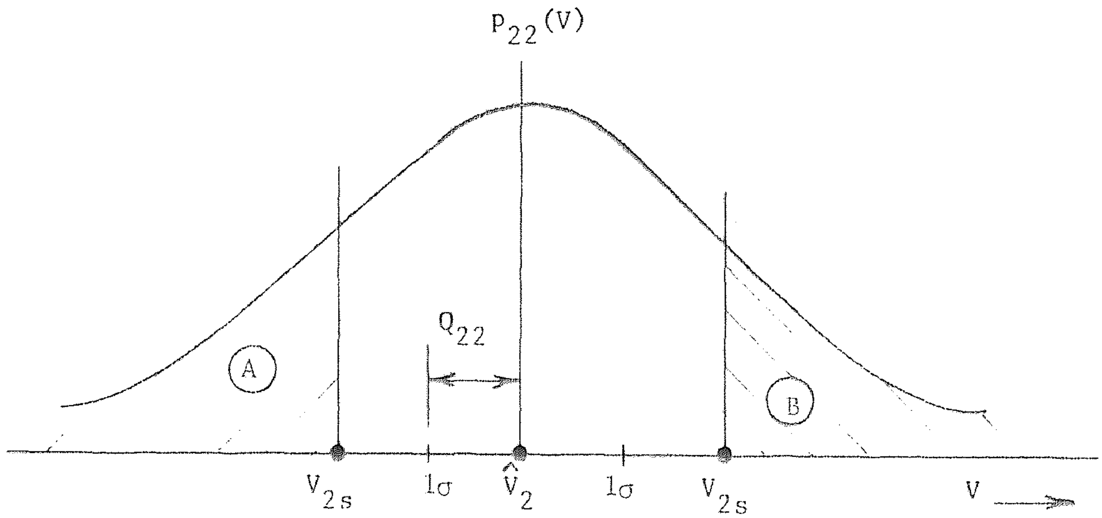


FIGURE X-1. Evaluation of the Cost Factor

The fact that an estimate $\hat{V}_2$ (x,iT) is greater that V_{2S}, does not imply conclusively that the true value V_2 (x,iT) is also greater that V_{2S}. In fact, the shaded area A in the figure represents the probability that the true value V_2 (x,iT) indeed violates the stream standard. This probability value is written as

$$\text{Prob}_D\ (V_{2S})\ \int_{-\infty}^{V_{2S}} P_{22}\ (v)\ dV \qquad (10.2)$$

$$\text{for } \hat{V}_2 > V_{2S}$$

where

$$P_{22}\ (V) = \frac{1}{\sqrt{2\pi Q_{22}(x,iT)}} \quad \exp - \left[\frac{(V - \hat{V}_2)^2}{2Q_{22}(x,iT)}\right] \qquad (10.3)$$

Prob_D represents the condition under which the stream is actually being degraded, but no correction policy is initiated because of the incertainty in the estimate. It may also be viewed as the cost associated with aeration that may later be necessary to restore the stream to a standard level. [152].

Similarly, if an estimate $\hat{V}_2$ (x,iT) < V_{2S}, it is not conclusive that V_2 (x,iT) is less than V_{2S}. The expression

$$\text{Prob}_U\ (\hat{V}_2,\ V_{2S}) = \int_{V_{2S}}^{\infty} P_{22}\ (V)\ dV \qquad \text{for } V_2 < V_{2S}$$

represents the probability that the stream condition might already have met the standard. Any costs of the correction measures based on the apparent deficiency (V_{2S} - $\hat{V}_2$) may be considered as unwarranted. $Prob_U$ is shown as the shaded area B on Figure X-1.

The preceding arguments are tendered only to give an insight into the application of the results here; the basis for the arguments are subject to debate based on the interest of the user. (e.g. a treatment plant manager who seaks to minimize his plant upgrading cost versus an environmentalist whose goal is to restore the stream to its natural form at all cost).

However, it is assumed here that the total cost to be minimized is a judicious weighted sum of $Prob_D$ and $Prob_U$, from which the cost factor λ (x) may be established. The actual determination of λ (x) is beyond the scope of this dissertation.

It is now desired to develop an observation strategy to optimize the sampling rates of observations with respect to the observation cost.

Estimation Indicator

The problem of observation cost has been studied for some control systems [88, 25, 4] in which dynamic programming was used. Because a sequential filtering algorithm is developed here, a different and simpler approach is used.

The resulting change in the variance matrix $\underline{Q}$ (x,iT) is repeated here from equation (9.34)

$$\underline{Q}\ (x,iT) = \underline{Q}\ (x,iT^-) - [\underline{K}_i\ \underline{H}_i + \underline{X}_i\ \underline{M}_i\ \underline{\Delta}_i\ ]\ \underline{Q}^T\ (x,x_m,iT^-) \qquad (10.4)$$

substituting (10.4) into (8.25) yields

$$P\ (x,iT^+) = P\ (x,iT^-) - \int_{X_o}^{X_f} \underline{\lambda}^T(x)\ [\underline{K}_i\ \underline{H}_i + X_i\ M_i\ \Delta_i)\ Q^T\ (x,x_m,iT)$$

$$\underline{\lambda}\ (x)]dx \qquad (10.5)$$

The expected decrease (improvement) in the total cost function if measurements are taken at iT is

$$E\ (x_m,iT) = \int_{X_o}^{X_f} \underline{\lambda}^T\ (x)\ [K_i\ H_i + X_i\ M_i\ \Delta_i]\ Q^T\ (x,x_m,\ iT^-)\ \underline{\lambda}\ (x)\ dx$$

This improvement must be weighed against the additional cost of making measurements. If the expected improvement in estimates outweighs the addition observation cost then, an observation is taken [e $(x_m,iT) = 1$]. Conversely, if the expected improvement is marginal or significantly less than the cost, observation, then no measurements are taken [e $(x_m,iT) = 0$]. The algorithms for the estimator indicator e $(x_m,$ iT) in (5.17) becomes

$$e\ (x_m,iT) = \begin{cases} 1 & \text{if} \quad E\ (x_m,iT) > \delta\ (jNT - iT)\ \underline{\beta}\ C_D + \underline{\alpha}\ \underline{C}\ (m) \\ 0 & \text{if} \quad E\ (x_m,iT) \le \delta\ (jNT - iT)\ \underline{\beta}\ C_D + \underline{\alpha}\ \underline{C} \end{cases}$$

The results in the following presentation are applied to the following numerical example.

Numerical Example

The algorithm for the estimator indicator was incorporated into the numerical example for the stream system in Chapter VIII. The same parameters are used in addition to the cost factors

$$\underline{\alpha}^T \underline{C} (m) = 0.008$$

$$\underline{\beta}^T \underline{C}_D = 0.075$$

The assumption here is that the cost for one analytical BOD test is about ten times the cost per on-line TOC reading.

Figure X-2, (ii) and (iii) show the improvement in the state estimate profiles based on the multiple measurements. However, a particularly interesting result is that these improved estimates are based on fewer samples than the single measurments.

Because the algorithm of the estimator indicator is based on the variances of the measurement errors and not the measured values themselves, the observation strategy may be developed off-line. That is the number and temporal spacing of observations may be planned before the measurements are taken. In some practical cases, however, where the noise variances are not known a priori, approximate expressions of the type presented in [15] based on measured values, may be used.

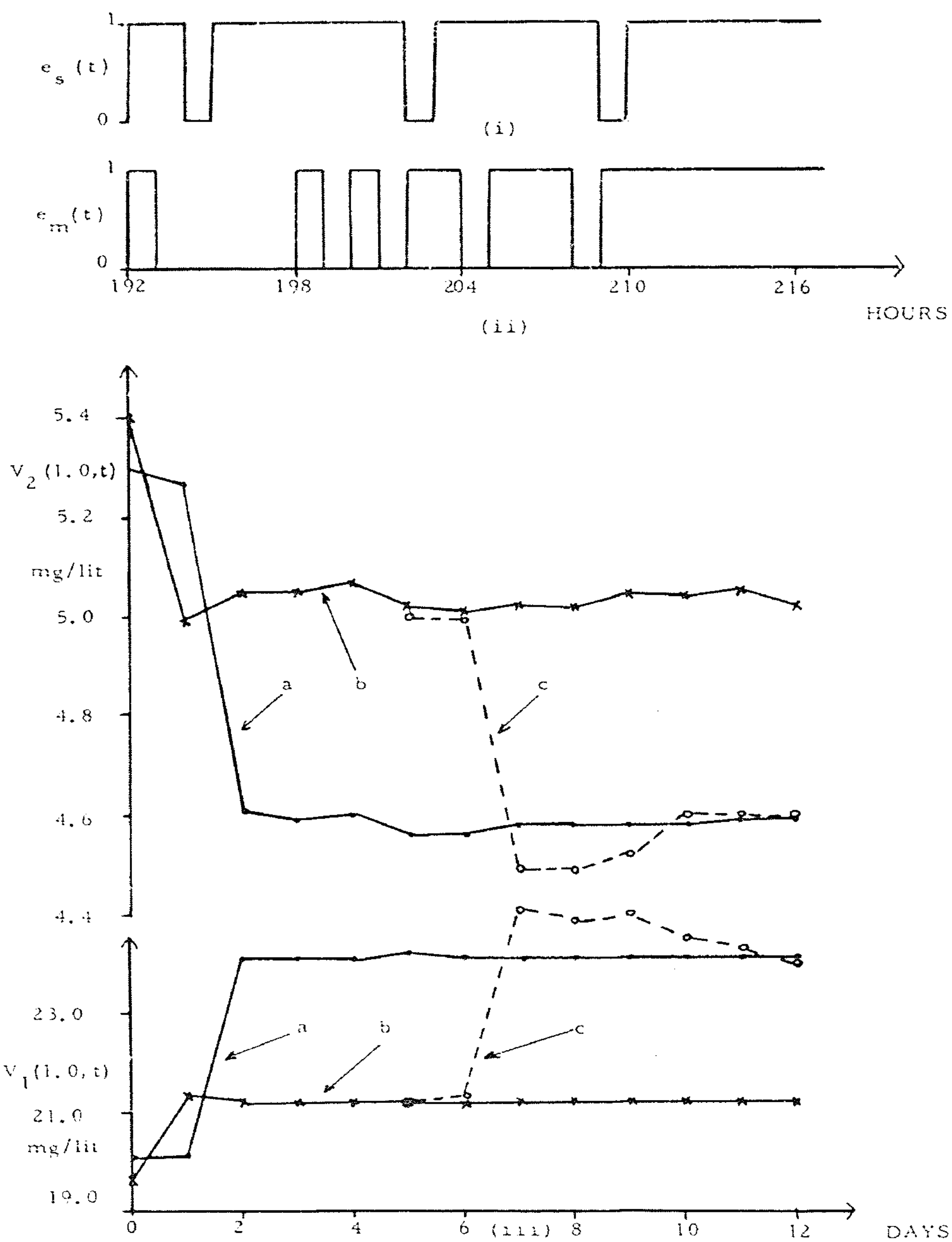


FIGURE X-2. Filtering with Constant Observation Error Variance-to-Signal Ratio and Observation Costs. Typical Observation Strategies for Noisy (i) TOC, (ii) TOC, BOD and DO Measurements (iii) Estimates of Temporal DO and BOD Profiles.

a) True values
b) Noisy measurements of TOC and DO
c) Noisy multiple Measurements of TOC BOD and DO

The observation strategy developed in this chapter along with the optimum spatial measurement stations in Chapter VI, thus represents a comprehensive optimum monitoring policy for estimation and control of distributed parameter systems. The results have demonstrated that fewer samples of multiple measurements when taken and applied properly may produce better estimates of the state and parameter in the class of distributed parameter systems treated in this study.

CHAPTER XI

CONCLUSIONS

The overall objective of this study which was to develop a comprehensive multiple measurements theory for the on-line optimum state and parameter estimation in distributed systems has been accomplished. The specific contributions have been:

(a) The development of a measurement projection method to optimally utilize off-line delayed measurements for on-line estimation and control.

(b) The development of a comprehensive measurement policy that includes the optimum spatial monitoring stations and an observation strategy for the optimum number and temporal intervals of measurements.

(c) The development of Kalman type distributed filters for optimum state estimation based on all available types of off-line and on-line measurements.

(d) The successful application of the techniques developed to numerical examples which typify realistic engineering problems.

(e) The presentation of the multiple measurements algorithms which demonstrated considerable improvement over existing estimation and monitoring methods for the class of problems treated.

The organization of the text was made to underscore the sequence of the problems in monitoring, estimation and control of a class distributed systems. The development of the class of water quality models to be studied was presented and the features and significance of each variable were discussed. The state-of-the-art methods of measurements and evaluation of the critical parameters with particular emphasis on their limitations were presented. The relationship among the multiple forms of oxygen demands were explored.

Recognizing that closed-form solutions are often not available for practical dynamic distributed models, the explicit finite difference techniques applicable to the specific systems under consideration were presented. The associated criteria for stability and boundary conditions which are necessary for the useful application of the solution techniques on a digital computer program were given.

A unique method of projecting off-line measurements for optimal utilization in an on-line process was developed. The development was based on the implusive responses which are readily obtained by analytical or experimental methods for many distributed models.

An optimal measurement strategy for spatial monitoring stations based on statistical experimental design techniques was developed. Two theorems were given for the optimum number of spatial locations of monitoring stations.

The applicability of the multiple measurements techniques for parameter identification in constant parameter systems was demonstrated. The rates of convergence and the final accuracy of the estimates obtained for multiple measurements were found to be consistently superior to those obtained from single sets of measurements. In addition, the multiple measurements techniques were applied to track time-varying parameters, and again improved results were obtained.

The results obtained from the application of the multiple measurement techniques to state profile estimation also demonstrated the superiority over Kalman type filters based on single sets of measurements. The possible applications of the results from this study in real engineering problems were also discussed.

CHAPTER XII

RECOMMENDATIONS

The applicability of the multiple measurements techniques developed in this study has been demonstrated for practical simulated numerical examples. It is of interest in future work to incorporate these techniques into real engineering problems of monitoring and control of water quality systems. The extension of the results of this study to other classes of distributed systems is relatively straight forward. A representative mathematical model and a realistic understanding of the measurement methods available are required.

Care needs to be exercised in the representation of initial and boundary conditions as these greatly affect the stability and reliability of solutions.

The sequential development of the algorithms facilitates a minimum requirement of computer time and memory. As larger and more complex systems are considered, the computer cost may become very significant.

The techniques developed here can readily be integrated along with the necessary hardware, for useful applications in the monitoring and control of distributed parameter systems.

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