

DISSERTATION

SELECTION OF MODELING AND MONITORING STRATEGIES FOR
ESTUARINE WATER QUALITY MANAGEMENT

Submitted by

Kumaraswamy Sivakumaran

Civil Engineering Department

In partial fulfillment of the requirements

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Colorado State University

Fort Collins, Colorado

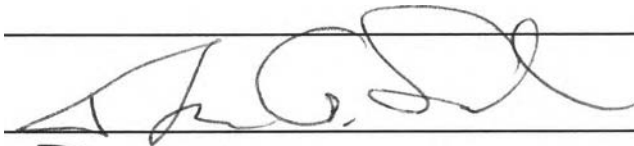
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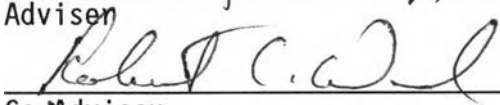
WE HEREBY RECOMMEND THAT THE DISSERTATION PREPARED UNDER OUR SUPERVISION BY KUMARASWAMY SIVAKUMARAN ENTITLED SELECTION OF MODELING AND MONITORING STRATEGIES FOR ESTUARINE WATER QUALITY MANAGEMENT BE ACCEPTED AS FULFILLING IN PART REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY.


Committee on Graduate Work



Daniel S. Fontane

N. J. Nriagu

Adviser


Co-Adviser


Department Head

ABSTRACT OF DISSERTATION

SELECTION OF MODELING AND MONITORING STRATEGIES FOR ESTUARINE WATER QUALITY MANAGEMENT

Estuarine water quality management is challenging owing to the complex hydrodynamics, water quality kinetics, international and domestic legislation, and human impact that take place in an estuarine environment. Scientists respond to this challenge by 'observing, hypothesizing and predicting' the behavior of the estuary. This is accomplished via developing water quality models which are idealizations of the behavior and by water quality monitoring.

As most of the water quality models were developed for research, they did not serve the purposes of management. Because scientific methods were not widely known, the direction by Congress to collect water quality data led to non-scientific methods of collecting data.

The research (with the objective of using water quality models effectively) embarked on designing a water quality monitoring system using a model. A model based on the hypothesis of conservation of mass was expressed as a one dimensional convective diffusion equation. The convective-diffusion equation was then solved recursively. Field observations from the Potomac estuary were obtained from government agencies and reports. An algorithm developed by Kalman was used to combine the model predictions and field measurements.

In order to design the monitoring system the term 'TRACE OF ESTUARY' (TOE) was defined. The relative value of TOE determined the

optimum number of sampling locations for an ongoing water quality monitoring program.

The approach resulted in the reduction of sampling locations in the Potomac estuary from 12 to 5. It also showed that water quality data must be representative of similar sized segments. The concept of using the physical behavior of the system to design a water quality monitoring network was established. It was further established that the use of "better and accurate" models (not necessarily complex models) will reduce the number of sampling points.

The significance of the research is that:

- (i) modeling and monitoring are used in an integrated fashion;
- (ii) a scientific approach is used to determine the number of sampling locations; and
- (iii) an accurate model will lead to a reduction in the sampling locations necessary for water quality management.

Kumaraswamy Sivakumaran
Civil Engineering Department
Colorado State University
Fort Collins, CO 80523
Summer 1989

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CHAPTER 1

INTRODUCTION

1.1 General

Water quality models have been developed for many years to assist in managing water quality. These models are often developed in a research context and not related to on-going management decision making. Literature pertaining to four hundred water quality models was reviewed by Orlob [11], and his conclusion was that most of them were research oriented. The International Hydrology Program of UNESCO embarked on a project entitled "Effectiveness of estuarine water quality models on policy analysis and decisionmaking." Gunnerson [13] in 1966, reported that water quality managers are going to be immersed with water quality data. Ward et al. [14], twenty years later report the "Data rich but information poor syndrome." All these lead us to believe that there is a proliferation of water quality models and water quality data. Or in other words, there is a problem of too many water quality models and too much water quality data. This is true for the estuarine environment too. The present chapter briefly explains what an estuary is, its uses, and how the above problem can be solved for an estuarine environment.

1.2 Estuaries and Their Use

An estuary is the region where the fresh water from the river mixes with sea water. Owing to the geologic formation, fresh water

flows, circulation patterns, tides and ocean currents, there is no fixed boundary for an estuary and it is always in a dynamic state. Some estuaries are short (Duck river, Australia, 6.5 km) [1], while others are long (Delaware estuary, USA, 214 km). In the US, 70 % of the population lives in coastal states [2]. Estuaries provide water for this population and industries; allow ships and boats to navigate; receive wastes; and are a place for recreation such as boating and fishing. A schematic view of an estuary is illustrated in Figure 1.1. These activities indicate a conflicting interest in the use of water from the estuary. They also indicate that the estuary is subjected to an enormous stress. If all these needs are to be met, the quality of water in an estuary must be maintained.

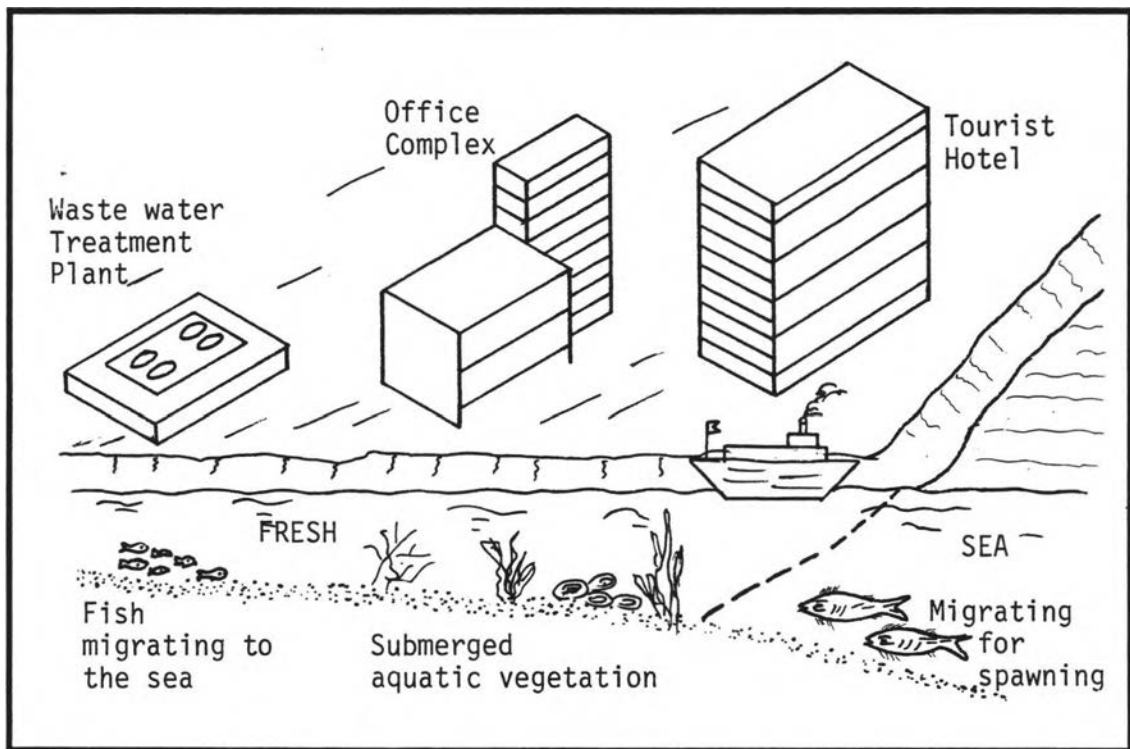


Figure 1.1. A Schematic View - Estuary.

1.3 Managing Estuarine Water Quality

In order to maintain the quality of water in an estuary a two pronged attack is necessary. At the government level, laws have to be enacted, implemented and upheld by the courts of law of a country. Then sufficient research has to be done at the scientific level so that the necessary information is provided for those at the government level to take up appropriate actions and decisions.

The laws of a country reflect the desires of the society. As the desires of the society change the laws change; the interpretation of the statutes in the courts of law change. During the latter half of the 19th century, and in the early part of the 20th century, economic development was critical in the U. S. The courts of law paid little attention to economic activities that were detrimental to the environment. "The federal government ... adopted acts ... as inducements to engage its citizens in the exploration and development of its mineral resources. In fact the development of mineral resources ... is the settled policy of the state and the nation ..." [3]. However in the nineteen sixties, environmental degradation was a major concern. In the case of United States vs. Joseph G. Moretti Inc. [4], the defendant had to give up the construction of mobile home parks near Florida bay, and had to restore the bay to its original condition. Further, he was prevented from either leasing or selling the property until it was brought back to its initial state.

In the U. S., the Congress is concerned about pollution in estuaries and coastal zones. In order to manage the coastal zones which include the estuaries, the Coastal Zone Management Act was enacted in 1972. It was then revised three times; 1976, 1978 and 1980

[5]. In 1976, the Congress was so concerned about pollution in the Chesapeake Bay that it directed the Environmental Protection Agency (EPA) to conduct a study of the Bay. The outcome of the study was the "Chesapeake Bay Agreement of 1983," signed by the Commonwealths of Pennsylvania and Virginia, the state of Maryland, the District of Columbia, the Chesapeake Bay Commission and the U. S. Environmental Protection Agency on December 9, 1983 [6]. The commitment by all these agencies resulted in the "Chesapeake Bay - Restoration and Protection Plan." A coordinated monitoring plan was developed for the Chesapeake Bay and monitoring reports are published annually [7]. The U. S. Corps of Engineers was about to develop a three dimensional, time varying water quality model for the Chesapeake Bay [8]. A further boost to the Chesapeake Bay Program was given in 1987, when the Congress authorized grants to states which were involved in interstate management plans developed in accordance with the Bay Program [9].

The Congress established a "National Estuary Program" under the Water Quality Act of 1987, and encouraged the preparation of management plans. It gave priorities to the following estuaries and harbors in the U. S.: Long Island Sound, Narragansett Bay, Buzzards Bay, Puget Sound, New York-New Jersey Harbor, Delaware Bay, Delaware Inland bays, Albermale Sound, Sarasota Bay, San Francisco Bay and Galveston Bay.

The characteristics of the estuary are a puzzling phenomena to scientists, and even a proper classification system does not exist. However, estuaries can be classified into four categories based on topography; Coastal Plain estuary (Drowned river valley), Fjord like estuaries, bar built estuaries and tectonic process estuaries. If the physical processes are taken into account, stratified, well mixed and

partially mixed are three categories of estuaries. In the sixties, Hansen and Rattray [10], assuming that the estuaries elongate in a form such that lateral variations are relatively insignificant, proposed a classification system based on two parameters; stratification parameter and circulation parameter. This method is still considered valid for water quality assessment.

At the scientific level, physical, chemical and biological variables are used to measure the quality of water. The dynamic nature of the estuary makes the determination of the values for these variables an arduous and challenging task. Scientists approach these problems based on three factors, observation, hypothesis and prediction. In water quality management of estuaries this reduces to water quality modeling and water quality monitoring. Water quality models for estuaries are mathematical approximations of the behavior of the estuary. Although several hundred models are in existence, very few are used for water quality management. This is because most of the models were used for basic research and are of little use for management [11]. You hardly find literature describing a scientific method of monitoring estuaries. Field measurements or observations have been taken for years and stacked in files, disks and tapes. These have been collected over several years, using different methods and are of little use for scientific analysis [12].

1.4 Objective

The first step in a scientific approach to the solution of a problem is to observe and take measurements. Based on the observations, we hypothesize the characteristics of the problem and formulate a mathematical model. If the mathematical model is an ideal

one, it will be able to predict the expected observations, accurately. If the observations can be predicted accurately using a mathematical model, field measurements are unnecessary. However, in reality neither the model predictions, nor the field measurements are accurate. Model predictions are inaccurate due to inevitable assumptions made in the formulation of the model. Errors in measurements are due to human, instrumentation and other sources. As we can never achieve an ideal model which will eliminate the need for measurements, we should be able to arrive at an optimum number of observations, based on the near ideal formulation of the behavior of the water body, the model, for a predetermined deviation from the ideal state. This will lead us to estimate the state as accurately as possible.

Very little literature exists to show the use of this basic scientific approach to estuarine water quality monitoring and modeling in an integrated fashion. The contribution of this research is using the physical understanding of the estuary as reflected by water quality models to establish the number of sampling locations for a water quality monitoring system in an estuary. Dissolved oxygen (DO) is the water quality variable used for the study. More specifically the study will:

- (i) Develop a theory and formulate hypothesis to show how a water quality model can be used to determine the number of sampling locations in an estuary.
- (ii) Test the theory with real data from the Potomac estuary.
- (iii) Confirm the hypothesis, and
- (iv) Arrive at conclusions.

1.5 Scope of Research

- The physical understanding of the estuary, as reflected by a water quality model is used to determine the optimum number of sampling locations for an estuary, where an ongoing water quality monitoring program exists.
- Linear Kalman Filter (LKF) algorithm, one of the recursive estimation techniques is used to combine the model predictions and field measurements. Estimating the state of the estuary, as represented by the variable dissolved oxygen (DO), is the aim.

The intention of the research is not to develop sophisticated water quality models, but to use simple ones that currently exist to verify the hypothesis. Existing data collected by various government and private agencies will be used in this study, and no new field measurements will be made. The selection of the Potomac estuary is arbitrary, and the results are subject to the various assumptions and approximations described in the latter chapters.

1.6 Organization of the Dissertation

Literature on water quality modeling, monitoring, and the use of Kalman filter in water quality management are reviewed in Chapter 2. Chapter 3 portrays the basic research approach for an estuarine environment. The concepts of modeling, and the theory behind combining the model and the field measurements are described in Chapter 4. A new approach has to be validated by an example case study. Hence, Chapter 5 presents results of data used from the Potomac estuary. Discussion of the results and the various assumptions made were reserved for Chapter 6. The conclusions in Chapter 7, are the closure for the

dissertation. The appendix at the end provides details of data, listings of computer programs, statistical analysis of trends and other information.

CHAPTER 2

A GLIMPSE OF THE PAST

2.1 Introduction

Identifying a research topic is a challenging task. A meticulous, painstaking and careful review of published literature will reveal thought-provoking ideas, which can be used for research. The subject of using 'internally descriptive water quality models to design water quality monitoring networks for estuaries with the aid of Kalman filter algorithm' is the outcome of such an effort.

The amount of literature available on water quality modeling is vast. In the case of water quality monitoring it is limited. The use of Kalman filter in water quality management is even more limited. As it is difficult to list and review every available article, the review is limited to those papers that are relevant to this particular research. The literature review is divided into four major sections; state of the art of modeling, water quality models, water quality monitoring, and the use of Kalman filter in water quality management.

2.2 State of the Art of Modeling

The use of systems analysis in water resources in the USA, over the last two centuries was analyzed, by Burges [1]. Legal constraints and objectives were few 200 years back. Therefore, the systems approach was not practiced in planning. Subsequently, there were technical and financial constraints. At present, there are constraints

on resources. These resource constraints necessitated the use of the systems approach to planning. The use of mixed integer programming and integer dynamic programming have contributed significantly to the systems approach. Burges [1] concluded that, even though the systems analysis approach did not play a major role 200 years back, it is making a significant contribution now.

The Office of Technology Assessment [2] made a study on the use of models in water resources management, planning and policy. They identified 33 water resource issues of which surface water quality comprised 10. They came out with nine major findings. Among these are "models are efficient tools and enable federal requirements to be met; they improve decisionmaking; they must be used by knowledgeable professionals; development is a complex process and requires a lot of funds."

However, Rogers and Fiering [3], narrowly defined models. Their conclusion was restricted to optimization models. According to them, less developed countries had used models more than the US. Models had been used more in operating than in planning.

In England and Wales, the Water Authorities and the Water Research Centre played equal roles in the development of models. At the end of the year 1978, 27 models were in use or used. Planning new treatment works, setting consent standards for discharges and establishing rates for discharges were the major uses. The authors concluded that there is more scope for model use in water quality management [4].

2.3 Water Quality Models

2.3.1 Mathematical Models

2.3.1.1 General Description

Hinwood and Wallis [5], did a world wide survey of 108 models for estuaries. They considered simulation models only. Based on the spatial dimensions, the reference frame used and the degree to which hydrodynamic processes were included, models were categorized as follows:

Spatial dimension : - Zero, One dimensional, Two dimensional
Plan view, Two dimensional Side
elevation and Three dimensional

Reference frame : - Eulerian and Lagrangian

Hydrodynamic process : - Hydrodynamic model, Kinematic model and
Transport model.

The choice of a model will depend on the use for which the model is to be put, resources available for the investigation, the nature of wastes and the characteristics of the estuary and its boundaries.

Having classified the models, they went on to describe the use of each category of models [6]. Zero dimensional models can estimate the seriousness of the waste discharge problem. A one-dimensional Eulerian model predicts well for a well mixed estuary. They are inadequate when tidal flats and embayments are present. One-dimensional transport models predict longitudinal waste concentration well for an estuary having a regular channel. However, estimating effective dispersion is a problem. Two-dimensional transport models (Plan view) have to be used in all real estuaries. These take into account the wind and Coriolis effects, bends, embayments, non uniform cross-sections etc.

The two-dimensional side elevation model is useful for stratified estuaries. The three-dimensional model predicts concentration of the form, $C = C(x,y,z,t)$.

2.3.1.2 One-Dimensional Models

A one-dimensional model was used to study the variation in salinity due to natural and man-made changes [7]. The factors considered were the effects of reservoir regulation and consumptive fresh water withdrawals. It was a one-dimensional model, varying along the length of the estuary. An equation for the calculation of the dispersion coefficient was developed. It was dependent on the vertical stratification of the estuary, salinity gradient, channel irregularities and Taylor type dispersion coefficient. Two new parameters, Densimetric estuary number and Densimetric Froude number were defined. Although, there were limitations in the model, it predicted chloride concentrations with an acceptable accuracy [7].

James [8] mathematically described the DO concentration and nutrients concentration in the Tyne estuary. The tidal and depth averaged salinity varied linearly with distance from the estuary mouth. If S_0 was the salinity at the estuary mouth, the salinity S_x at a distance X from the river mouth was given by, $S_x = S_0 + m X$. The One-D convective-diffusion equation was used to study the DO and BOD variations. A theoretical model having an exponential term was also developed for the build up of nitrogen in the North Sea.

A one-dimensional model was used by the Northumbrian Water authority [9] to study the pollution due to coke-oven effluents and ammonium - nitrogen in the estuary. Three major targets were set and the model was used to evaluate the costs of meeting these targets. A

consensus was reached by all the parties concerned as to which target should be met and when.

Najarian and Harleman [10] used a one-dimensional model and demonstrated that mixing, biochemical transformation and intratidal cycle transport processes in an estuary were coupled. They recommended that traditional methods of field data collection had to be changed if useful information was to be gained from models.

A nitrogen cycle model was calibrated and verified [11]. It contained seven non-linear, partial differential equations describing the transient changes in the concentration of elemental nitrogen. The ecological model structure contained two trophic levels. The authors concluded that the periodicity of nitrogen concentrations in the Manasquan estuary was due to the phase difference between the tides at open boundary. They also opined that tide induced circulation must be considered when fresh water input is small.

A one-dimensional model FLUSS was used to study the effect of material transport and load in the Elbe estuary, West Germany [12]. Flocculation, remobilization, adsorption or other chemical exchange processes were not considered. Particles settled around slack water. When strong currents were present sediments were eroded. Settling velocity of the sediments varied from 0.003 cm/s to 0.3 cm/s. A regression analysis showed that the concentration 'c' was proportional to w^2 , where 'w' was the settling velocity. The authors also found that Fe and Pb were quantitatively bound to suspended matter.

The purpose of the one-dimensional model was to describe theoretically, the changes that take place to the organic content of the sediment and the rate of sediment turnover [13]. The model was one

dimensional in the vertical direction, and was developed to study the effects of dredging in estuaries. The assumptions made were described. Finite difference approach was used to develop a computer program to solve the equations. Free sulphides in sediment depended on the organic contents and the rate of sediment turnover. If there was a high turnover rate in the sediments, pyrite will be formed and sulphide capacity will be lost.

The Water Research Centre in England developed a one-dimensional model for the Medway estuary [14]. This step was taken because, statistical models failed to give the desired results. Three models were developed; a model to predict water levels, a steady state water quality model which ignored photosynthesis and a time dependent model incorporating photosynthesis. The models were one dimensional, and longitudinally varying. The predictions from these models were good.

Micro-organisms and macro-organisms in water foul the cooling systems in Power Plants. Chlorine treatment is necessary to prevent this. However, byproducts due to this treatment will affect aquatic life. The knowledge of the transport and fate of these byproducts, will help one to evaluate the effects of discharging the cooling water. The paper [15] discusses the different kinds of biocides, their byproducts and the environmental effects due to the discharge of these byproducts. Sixteen models that can be used for cooling system discharges are listed. A model is presented which can predict the distribution of biocides in the upstream and downstream section of the outfall.

2.3.1.3 Two-Dimensional Models

A tidally averaged two-dimensional model was used to study the suspended solids in estuaries [16]. Suspended solids affect the transmission of light, growth of plants and phytoplankton, provide sites for growth of micro-organisms and absorb heavy metals and pesticides. The model was used in Sacramento - San Joaquin delta and James river estuary and Rappahnnock estuary of the Chesapeake Bay. A finite difference solution was used. It was found that the concentration of the solids was sensitive to the settling velocity of the solids. The conclusions arrived at by Fanger et al. were similar.

Lung and O'Connor [17], described a tidally averaged estuarine transport model. The method was suitable for laterally homogeneous estuaries; which were, partially stratified estuaries with respect to salinity. In model development, hydrodynamic and mass transport equations were averaged in the lateral direction. For the momentum equation, the vertical component of the convective acceleration was retained. These approximations were tested in the laboratory flumes and real data from estuaries. The results confirmed the hypothesis.

In hydrodynamic models for estuaries, the input requirements were enormous. The longitudinal momentum equation incorporated an advective acceleration term. Omitting this acceleration term had no effect on either the circulation or mass transport calculation. This hypothesis was confirmed with data from Sacramento - San Joaquin Delta [18].

The two-dimensional analysis of dissolved oxygen in the New York harbour was presented by O'Connor and Mueller [19]. A steady state analysis was used. Depending on site conditions, one dimensional, two dimensional (longitudinal-vertical) and two dimensional

(longitudinal-lateral) were used. The equations were based on the principle of conservation of mass. A finite difference approach was used to solve the equations. The application of this model to areawide planning was discussed. Recommendations were made as to the level of treatment necessary to achieve DO target levels in the New York harbour area.

2.3.1.4 Three-Dimensional Models

The model TEMPEST was a time dependent hydrothermal model [20]. A finite difference solution evaluated flow, turbulence, heat transfer and mass transport. The simulated results agreed well with field studies. The authors concluded that the model could assess the concentration and movement of toxic contaminants. The paper did not mention the decision taken at the end of the studies regarding the location of the outfall.

The effect of cooling water on the heat budget of a Bay in Japan was studied, using a three-dimensional model [21]. A high temperature zone exists when warm cooling water is discharged into a bay. Heat emanated into the atmosphere from this zone was expected to affect the meteorological conditions. The three-dimensional model was based on equations of fluid motion, continuity and diffusion with respect to temperature and salinity. Long wave radiation, sensible heat loss and latent heat were taken into account in the heat budget. The authors concluded that the change in heat balance was local and not sufficient to change the heat balance of the bay area.

2.3.2 Completely Stirred Tank Reactor (CSTR) Models

A CSTR model [22], was used to study oil pollution in the estuaries, in Australia. The author, defined oil pollution residue

(OPR) as a complex mixture with carbon numbers over 17 and a closed estuary as one in which fresh water input was negligible with the mean tidal flow over a half a cycle. He found that the settling rate was 0.22/day. The OPR varied from 1% to 3%. The mean value of 1.5% was ten times the values reported in the literature. According to his calculations, 8000 tons of OPR existed in the sediments and it would take several decades for it to decay.

2.3.3 Link Node Models

Dynamic estuary model is a link node model. The performance of the Dynamic estuary model for the Delaware and Potomac estuaries was presented by Ambrose and Roesch [23]. Although it was based on one dimensional assumptions, longitudinal and lateral values for the variables can be evaluated. Hydrodynamic, mass transport and water quality data were simulated for both estuaries. Statistical parameters were used to evaluate the performance. Standard error, relative error, average error, coefficient of variation and regression analyses were the statistical measures used to verify the predictions. The model predictions were good for the range it was calibrated. It cannot predict concentration gradients exceeding 5 km or 3 hours.

Water quality analysis simulation program is a link node model [24]. EUTRO1, EUTRO2, EUTRO3 and EUTRO4 are subroutines for this model. These represent eutrophication kinetics. The complexity of kinetic representation increases from EUTRO1 to EUTRO4. EUTRO1 uses four state variables, whereas, EUTRO4 employs twelve state variables. The study showed that, intermediate complex models like EUTRO3 could give satisfactory results without calibration.

2.3.4 Habitat Models

Habitat suitability index (HSI) model was used to study the impacts of estuarine fill operations. A value of 0.0 for HSI will indicate that the area does not have the ability to support the necessary species; whereas a value of 1.0 would indicate, ideal or optimal habitat. The study indicated that the construction activities did not have any long term effects, but some number of species would be destroyed. This number was expressed as average annual habitat units (AAHU). In order to rectify this, the suitability of two other marsh creation sites were studied and the results were presented [25].

2.3.5 Parameters Used in the Models

The numerical models used to study pollution events incorporate a number of parameters like dispersion coefficients, reaeration rate coefficients etc. The values assigned to these parameters affect the predictions of the model. The manual on Rates, Constants and Kinetics [26] contains an exhaustive review of the various formulations for these parameters. It is a good source of reference and the users of models could decide on which formula to use. It has been revised and a new manual [27] is available.

Fischer [28], disagreed with the presentation of the longitudinal dispersion coefficient by M. L. Thatcher and D. R. F. Harleman (JEE No. 1, ASCE, Vol. 107, 1981, pp. 11-27). He felt that their formulation was similar to that of Taylor's pipe flow analysis. He suggested that the formulation was not applicable for estuaries and recommended a square law relationship for the dispersion coefficient of the form

$$E \propto \left(\frac{ds}{dx} \right)^2 .$$

Dispersion is an important phenomenon in the reduction of concentration of pollutants in estuaries. The capability of models to predict pollutant concentrations in estuaries, depend on parameters like dispersion coefficients. According to Ozturk [29], the existing equations for the dispersion coefficient did not reproduce dispersion in estuaries. A new equation was developed. It represented dispersion in the Brisbane estuary, Australia, adequately. The new equation was a function of the flow depth and four thirds power of the tidal velocity.

$$E = K_i H U^{4/3},$$

where,

E = Dispersion coefficient

K_i = Consistency index

H = Depth of flow

U = Tidal velocity

Dispersion itself is a separate research topic. Review of papers related to dispersion is beyond the scope of the present work.

2.3.6 Verification of Water Quality Models

Thomann and Barnwell [30], reported the findings of a workshop on the verification of water quality models. The report contained 19 technical papers and reports from seven committees on the state of modeling. Each committee considered a different topic. Waste load generation, transport, salinity/TDS, DO/temperature, bacteria/virus, eutrophication and hazardous substances were the topics covered by these committees. Coordination between modeller and decisionmaker, statistical verification and post-audit data collection to verify previous model predictions were some of the recommendations.

The development of water quality models over the years was traced [31]. In the sixties, there were one-dimensional models for BOD and DO. Then there were one- and two-dimensional models, for six chemical variables. In the late seventies, 1, 2 and 3 dimensional models with nonlinear, interactive systems were developed. But then, there was no means of comparing the predictions of these models. The paper [31] presented some statistical methods for verifying the predictions. The use of regression analyses, relative error, comparison of means and root mean square error was encouraged. Case studies were presented, and the advantages and disadvantages of using this technique were also discussed.

2.4 Water Quality Monitoring

In the treatise monitoring is considered as collecting field measurements of physical, chemical and biological variables. Although biological monitoring is an important topic literature pertaining to it is not reviewed.

Water quality monitoring is a new field. Although, water quality measurements were taken for years, there was no scientific approach to how it should be done. During the last 15 years, a lot of emphasis has been placed on water quality monitoring. You do not find many scientific papers dealing with monitoring of estuaries. Therefore, the following notes contain only a few papers that deal with water quality monitoring of estuaries. A large number of them describe methods used for rivers and lakes. However, with slight modifications, the same principles can be used for estuaries too. Hence, their presentation here is appropriate.

Belle G. V. and J. P. Hughes [32], disagreed with the U.S. General Accounting Office (GAO) Report on "Better Monitoring Techniques are needed to assess the quality of rivers and streams". The major recommendation by the U. S. GAO was that the EPA and the USGS should discontinue the fixed station, fixed frequency sampling efforts and embark on small scale intensive surveys. The authors emphasized that short term intensive monitoring while helping to evaluate the changes in water quality during the period of study, would not help one to detect trends. However, if trend detection was the aim, biweekly or monthly sampling will be sufficient.

Couillard [33], summarized, the organizational and legal aspects of collecting water quality data in Canada, Finland and Sweden. In Canada the authority to collect data was derived from the Constitution. The Federal, Provincial and Municipal agencies were involved in data collection. National Board of Waters was responsible for water management in Finland. Permanent networks as well as temporary networks were used for data collection. The frequency of sampling varied depending on the type of water environment and legal requirements. Pollution control was administered by the Environmental Protection Agency in Sweden.

Flemer et al. [34], discussed in detail, the monitoring approach to Chesapeake Bay. Three levels of monitoring were advocated.

Level I : Descriptive - Describe statistically changes in variables measured over time and make trend assessments

Level II : Analytical - Derive correlation between variables with statistical significance, and

Level III : Interpretive - Determine cause and effect relationships among the variables and predict interactions among ecosystem components and effect changes.

The report recommended 122 stations for the bay, with sampling frequencies bimonthly or monthly depending on the variable to be measured.

The document, "Guidance for State water monitoring and waste load allocation Programs" [35], sets out guidelines to meet the requirements of the Clean Water Act. Section 1 covers the Water Quality Monitoring Program. Monitoring for water quality based controls, compliance and enforcement, water quality assessment, quality assurance and reporting are the major topics. Monitoring for total maximum daily loads and waste load allocations are given in Section 2. A Monitoring Checklist is also attached.

Gunnerson [36], contributed one of the first papers on water quality monitoring for estuaries. He felt that plenty of water quality data was collected, and that data collected may exceed the capacity of analysis. According to Gunnerson [36] time series analysis may help to determine an optimum interval for water quality monitoring in estuaries. Thirty one day record lengths of dissolved oxygen and specific conductance were analyzed. The analysis showed that for monthly record lengths, a 2-hr. sampling is sufficient and that it is not necessary to sample every 15 mins. or 30 mins.

The Canadian approach to water quality assessment was presented by Haffner [37]. They advocated an Index station network to acquire long term water quality data and a recurrent basin network to address

specific water quality concerns. The combination of these were serving the water quality objectives and environmental impact assessments of Canada.

The importance of statistics in environmental monitoring was emphasized by Hayne [38]. He recommended the employment of a statistician at the planning, execution and data analysis stages. Monitoring was defined as assembling data sets to detect a change in some variable or gathering information to determine trends in status. He felt that, what to monitor has to be decided at the policy level taking into account the cost, scientific losses if monitoring was at a low level and the damage to environment if contamination goes undetected. How often to monitor depended on the processes that took place, seasonality and spatial distribution. According to him, Cost of storage vs Loss of information due to not storing data should also be considered.

Karr [39], emphasized "Biological Monitoring". An important factor in water quality management was "the need to preserve life support systems that provide goods and services to human societies through the maintenance of healthy ecosystems". Biological monitoring should be integrated with physical and chemical monitoring. Fish was a better indicator than benthic organisms. An Index of biotic integrity was developed using the guild concept. Chemical monitoring misses impacts due to habitat alteration, reduced flow and changes in energy supplies. Hence, the necessity for the integration of physical, chemical and biological monitoring was recommended.

Kwiatkowski [40], analyses the importance of time in the design of large lake water quality networks. The theme was to discuss sampling

frequency and its importance in calculating seasonal or annual means. He calculated the number of samples needed to detect a 10% or 20% change in mean value for the WQ variable at different depths and seasons. Differences as great as 20% for the mean, occurred between samples taken at one metre versus the integrated value over 0-20 meter. Similarly, a 35% change was observed in the annual means as a result of a change in sampling frequencies.

The importance of defining water quality and reviewing the data collected in a monitoring program, was stressed [41]. The water quality monitoring program must suit the purpose for which the water was going to be used. It must be an active monitoring program and not a passive one. The time taken to review the collected data should not be more than 2 weeks in the case of discharges from waste water treatment plants. Although, the authors disagreed with some parts of the US GAO Report on Water Quality Monitoring (1981), they agreed that fixed station, fixed interval approach was not suitable for assessing the quality of a country's rivers.

Lerner [42], edited the Proceedings of a symposium held in Budapest, Hungary, by the International Association of Hydrological Sciences, in 1986. Two major factors were considered; designing monitoring systems to detect changes in quality of the water resources, and analyzing water quality data series to detect trends in time series. Nine papers discussed the design of monitoring systems for the detection of change in quality. Remote sensing and automatic monitoring were covered in five papers. Changes in quality due to non point source pollution are presented in ten papers. The rest of the papers, eight in number, presented ideas on the analysis of water

quality data. The book disseminates the latest findings in the design of water quality monitoring systems.

Moss [44], edited another set of proceedings "Integrated design of hydrological networks." Most of the papers presented recent approaches to the design of hydrological networks. Precipitation, runoff, water quality etc. were considered. There were a few papers which specifically dealt with water quality.

Made [43], presented a novel approach of conjunctive design of hydrological networks. It included surface water and ground water. According to him, simultaneous measurement of water quality and quantity was possible. Socio - economic factors were also important in the design of monitoring networks. The report gave several methods and approaches that could be used for the design of monitoring systems. Recent research on the design was also presented.

An optimization method was presented by Palmer and Mackenzie [45]. It was used to select an aquatic monitoring design that maximized cost-effectiveness. Defining the goals and purposes of a monitoring system was important. For their study, minimizing cost and maximizing statistical power were considered as the objectives. A modified ANOVA model was used. The gradient search procedure was able to select a design that maximized statistical power for a specified budget or minimized the cost for a specified statistical power.

The use of control charts and cumulative sum techniques to minimize monitoring requirements was discussed by Radford and West [46]. These techniques were used with a model to predict annual mean concentrations. Baseline data were used for subsequent sampling frequency determination. In the case of an estuary retention time was

one major factor that would determine frequency. The inner estuary may require a sampling frequency of 10-12 times/yr, while the river mouth zone may require only 2-4 times/yr.

The report, "Designing a river basin sampling system" [47], was based on the PhD thesis of Dr. T. G. Sanders. It presented methods to locate sampling stations and to determine the frequency of sampling for baseline concentrations and trend analysis. Sharp's method of locating the macrolocation of sampling stations, and the hydrodynamic mixing properties of a stream in the location of sampling stations were discussed. The techniques took into account the cost and economic implication of designing a system according to the methods envisaged. As a case study, the design was analyzed for the Massachusetts portion of the Connecticut river basin.

Sherwani and Moreau [48], assumed that there was a minimum flow requirement for a stream. They defined the design of a monitoring network as specifying the location of sites, frequency of sampling and the number of variables. Accidental spills were not considered and similarly toxic and hazardous substances. Coliforms, too, were omitted from the monitoring program. The water quality data fit the Log-Normal and Gamma distribution well. Information content was represented by the reciprocal of the variance. Time of travel was considered as an important variable. They recommended a network consisting of three components; extensive network, regulations network and an intensive network.

A method to optimize the sampling frequency was presented by Schilperroot et al. [49]. If the objective was to detect trends in water quality constituents, this approach was suitable. Optimization

of the location of the sampling stations, the number of analyses and the sampling method, were not considered. Direct techniques were considered, and indirect techniques which took into account the physical processes were not considered. The method was based on the Lettenmaier technique. The study showed that an increase in sampling frequency will not give the required improvement in detecting trends because of the high variance and interdependency of the observations.

The cost of monitoring and the effectiveness of monitoring are dependent on the frequency, the number of locations and the number of variables to be monitored, as per Schilperoot and Groot [50]. They said that, effectiveness of the information can be related to statistical concepts. The use of time series analysis was thought to aid in optimizing parts of the problem. Kriging and Kalman filtering methods were also, discussed.

Steele [51], presented the major factors to be considered in the design of water quality monitoring. Programme goals and objectives depended on government regulations, time and space. The design of network depended on the interrelationships of variables, frequency of sampling, site selection, sampling protocol, quality assurance/quality control, data processing and data analysis. The value of data and the transformation of data into information was also important. Costing of how information was to be used was difficult. Some future considerations were, the increase in the number of WQ variables to be monitored, regulations on hazardous wastes, technological breakthrough in measurement techniques and obtaining real time information from monitoring.

Sampling frequency was the basis for the cost-effectiveness analysis as discussed by Ward and Vanderholm [52]. Two different networks were considered; Primary network for spill detection and Secondary network for trend data. A model was used to predict the performance of water quality networks and the method was tested in Colorado. From their analysis, design curves were developed. For a given effectiveness level, the cost of the system can be determined or vice versa, from these curves.

The implications of using statistics and water quality hydrology in the management arena was the theme of the paper, by Ward and Loftis [53]. Although, Log-Pearson Type III statistical models were available for flood analysis, such methods were not available for water quality management. The authors note that results from a statistically designed monitoring system would be incompatible with legal standards. The advantages and disadvantages in using statistics were analyzed. The water quality managers felt that using statistics may lead to increased pollution. Use of standards for legal enforcement was recommended. The use of standards for technical and other matters was discouraged.

"Proceedings of a Workshop on water quality monitoring in Colorado" [54], is a report of a 1-day workshop held at Colorado State University. The existing practices in the field and research efforts were discussed. The government agencies presented their activities in monitoring. Ward discussed the systems approach to monitoring. Sanders emphasized the importance of statistics in analyzing water quality data. Foster insisted that scientists must present ways by which flexibility can be included in the decisionmaking process of

water quality management. "Water quality monitoring must be given the same importance as a research project" was emphasized by Averett.

"The 'Data-rich but Information poor' syndrome in water quality monitoring" [55], asserted that while there was plenty of data, information was lacking. The authors defined water quality monitoring as the effort by an enterprise to obtain an understanding of the various characteristics of water via STATISTICAL SAMPLING. The major emphasis was on information. Further, a five step procedure was recommended for the design of a water quality monitoring system.

Step 1 : Evaluate information expectations

Step 2 : Establish statistical design criteria

Step 3 : Design monitoring network

Step 4 : Develop operating plans and procedures

Step 5 : Develop information reporting procedures

Not only physical, chemical and biological monitoring, but the monitoring of hazardous organic compounds was also recommended.

The 'Systems Approach' to monitoring design was reviewed [56], and the authors suggested that statistics played a major role in the following:

(a) Determining the characteristics of background water quality.

(b) Detecting changes in water quality, that is, departure from background conditions, including trends and violations.

Statistical methods that can be used to accomplish the above two factors were discussed. Design criteria for monitoring programs had to be expressed in statistical terms in order to achieve maximum results. The authors still felt that a designer had to make further assumptions

and formulate his/her own criteria in addition to the steps mentioned in the systems approach.

Wetering and Groot [57], reviewed water quality monitoring in the Netherlands for the past three decades. In the Netherlands, sampling stations increased from 4 to 400 during the period 1950 to 1981. There was a shift from macro quality variables to micro quality variables. The objectives of monitoring were defined by law. Choice of sampling stations, water quality variables and sampling frequency were important factors. Laboratory capacity was another factor to be considered. In optimizing the monitoring network two techniques could be used; direct, which does not take into account the physical processes, and indirect, which makes use of the knowledge of water quality processes. In the Netherlands direct technique, the Lettenmaier technique was used because they did not have any experience in using the indirect technique, the Kalman filter algorithm.

2.5 Kalman Filter in Water Quality Management

2.5.1 Optimal Estimation

The objective of designing a monitoring system for an estuary using the physical understanding as reflected by water quality models is possible when OPTIMAL ESTIMATION is used. Gelb (69) defines optimal estimation as "A computational algorithm that processes measurements to deduce a minimum error (in accordance with some stated criterion of optimality) estimate of the state of a system by utilizing: knowledge of system and measurement dynamics, assumed statistics of system noises and measurement errors, and initial condition information." Such an estimation technique was developed by Kalman for estimating the state of a linear system. Although it is popularly known as Kalman filter,

the algorithm can be used for smoothing, filtering and prediction [70]. However, the algorithm per se will not give the best monitoring schedule. We have to assign additional design specifications to obtain the best schedule. The applications of linear Kalman filter, and the use of its off shoots the extended Kalman filter and adaptive Kalman filter are further reviewed in the following section.

2.5.2 Linear Kalman Filter (LKF)

The use of LKF, for state and parameter estimation is discussed in Rinaldi et al. [58] for the Yomo river, Japan. In order to increase efficiency and computer time, suboptimal recursive filters (SMART) and recursive filter in time and space (RFTS), were also used for the analysis of data of the same river. All three gave satisfactory results. When the algorithm was used for groundwater level predictions in the San Jacinto groundwater basin [59], the filter performed as desired. However, the filtered predictions were not better than the model predictions. The technique was used for the analysis of groundwater monitoring networks in the Netherlands. The authors were able to reduce the number of wells from 18 to 10 for a specified threshold value of the standard deviation surface [60,61]. It was also used for air pollution monitoring [62].

2.5.3 Extended Kalman Filter (EKF)

As environmental systems are non linear, LKF was modified, and was known as Extended Kalman Filter. It enables the recursive estimation of the state variables and the parameters, whereas in LKF, parameters were assumed to be known in state estimation. It was used for state and parameter estimation for Cam river (England) [58]. In monitoring pollution by chlorinated solvents, Jinno et al. [63] used EKF to

recursively estimate dispersion coefficients, of a two-dimensional convective dispersion equation which described pollutant transport in groundwater. The coefficients converged to constant values after 100 time steps. Moore [68] used the EKF to analyze water quality monitoring design. However, it was used for a simulated river system and the "objectives of this research were primarily methodological, data from a real system were not utilized" [68].

2.5.4 Adaptive Kalman Filter (AKF)

In order to use the Kalman filter techniques one should be able to estimate the model error and the measurement error. If it cannot be estimated they have to be assumed. (Details of the measurement error, and model error in the filter algorithm are explained in Chapters 3 and 5, and in Appendix A-4.) Mehra [64] describes a method of estimating these errors and using them in the filter. Incorporating this in the filter algorithm is known as adaptive filtering.

Kaweamura et al. [65] used such a technique to analyze water quality time series. They found that, adaptive filtering predicted sudden pollution events better than the linear Kalman filter.

2.6 Summary

The review of literature indicates a limited application of Kalman filter, either in water quality monitoring network design or model use. Optimization of groundwater level monitoring was the sole concern of Van Geer [60,61] and water quality variables were not considered. Although, applying Kalman filtering techniques to monitoring was discussed [49,50,57,65] specific applications were not given. Up to now there has been no systematic design of water quality monitoring networks for the estuarine environment. Although, Chesapeake Bay has a

coordinated monitoring network, it is not scientifically designed [34]. The existing program was unable to achieve the monitoring goals as envisaged in, "Chesapeake Bay: A Framework for Action." Management was having difficulties in achieving Levels II and III of the monitoring goal [67]. They are namely,

Level II : Deriving meaningful correlations among variables measured over time, with statistical significance.

Level III : Determining cause and effect relationships, and predict interactions among ecosystem components and probable effects of changes, statistically.

In conclusion, models have not been used to design water quality monitoring systems for an estuary.

CHAPTER 3

APPROACH

3.1 Introduction

Information necessary for any water quality management plan is usually acquired either through the use of statistical analysis of water quality data, or by physical modeling of the particular environment. It is proposed that instead of using them individually a combination of both will permit the acquisition of knowledge about water quality behavior in an estuary at a reasonable cost. The flow chart in Figure 3.1 illustrates the intended approach to obtaining the information necessary for water quality management of estuaries. The approach consists of two major components;

- (i) Determining the number of sampling locations with the combined use of a physical model and field measurements, and
- (ii) Statistical analysis of trends.

However, the main aim is to determine the sampling locations using a model. Hence, the second component of statistical analysis of trends will not form part of the main dissertation. The details of statistical analysis are provided in Appendix A-9.

Our approach involves several phases to achieve the objective of determining the "optimum" number of sampling locations using the behavior of the estuary. The steps in the approach are:

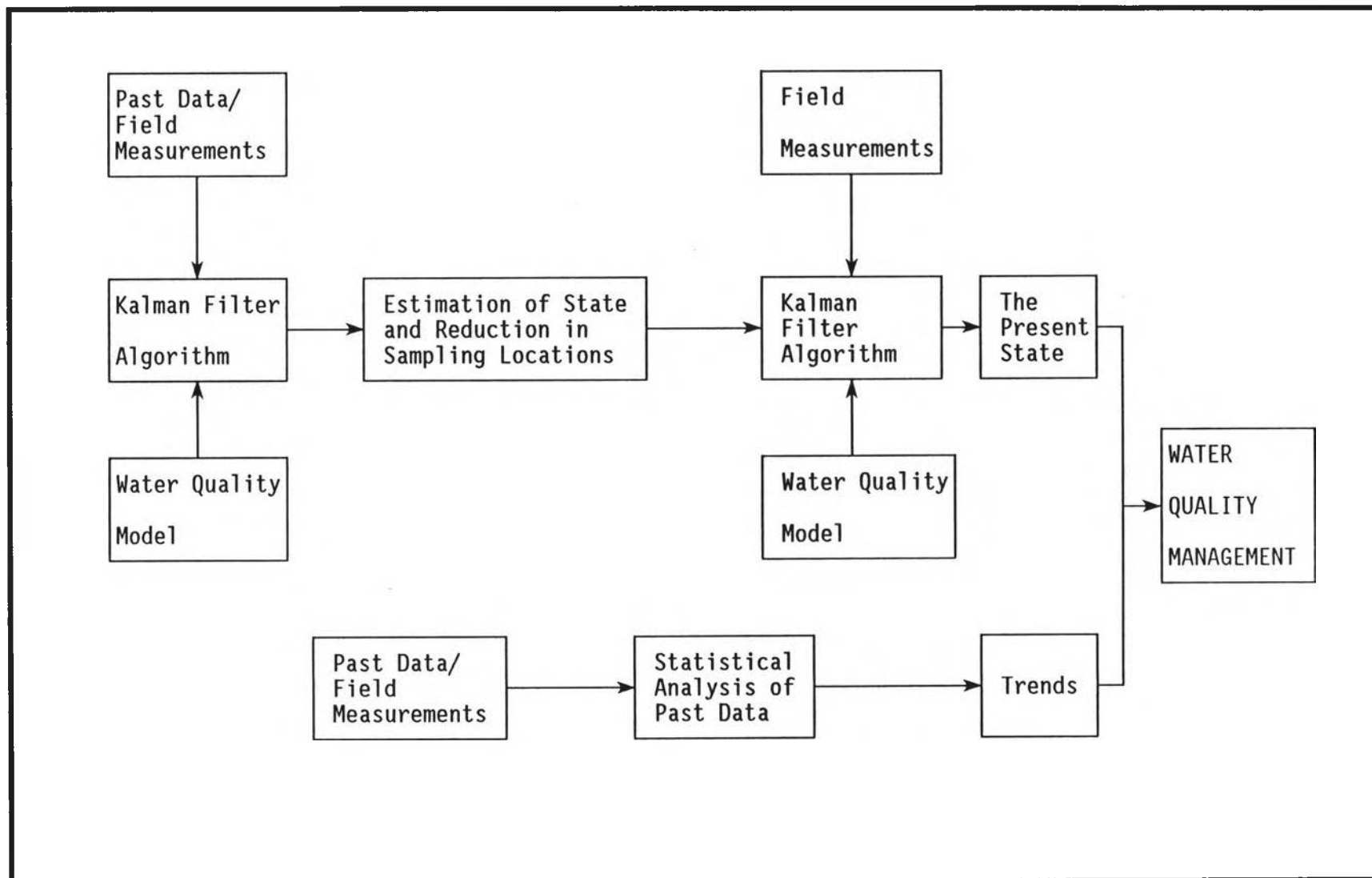


Figure 3.1. Flow Chart for Water Quality Management.

- (i) Choosing an indicator for water quality
- (ii) Developing a theory for the physical model
- (iii) Collecting data
- (iv) Testing the model with the collected data, and
- (v) Obtaining results

The following sections in this chapter provide the basic information on these phases (steps in the process).

3.2 Choice of Dissolved Oxygen (DO)

Water quality problems encountered by estuaries are similar. The important ones encountered in the Potomac are, nutrient enrichment, algal blooms, dissolved oxygen, sedimentation and living resources [1].

The technical support manual on Use Attainability Analyses for Estuarine Systems [2] recommends the use of submerged aquatic vegetation (SAV) as the water quality indicator for an estuary. However, there is controversy over its use. "Scientists do not fully understand the complex interactions of a variety of factors that appear to influence SAV distribution and abundance.... it is not known why the plants declined, and why some have returned" [3]. Further, there are some kinds which are detrimental to the quality.

DO is necessary for the survival of organisms. The DO concentration at the bottom of the estuary dictates the presence and heterogeneity of shellfish. Its concentration at the surface and mid-depth is also important for finfish. DO is included in most general water quality index formulations. It is one of the water quality variables whose kinetics has been studied for more than five decades. Even if questions still remain to be answered about its replenishment rates, the choice is good; it is valid; it indicates water quality.

The general framework developed herein to tie modeling to monitoring could be followed with other water quality variables. Dissolved oxygen was chosen primarily for the exhaustive modeling already done on this variable.

3.3 Theoretical Development

The development of the theory itself can be divided into four parts:

- (i) Water quality modeling
- (ii) Water quality monitoring
- (iii) Kalman filter algorithm, and
- (iv) Criteria for monitoring

The physical behavior of the estuary (i.e. the water quality model) is expressed as a one-dimensional differential equation. A finite difference technique, using Euler's Scheme was employed to solve the differential equation. This resulted in a recursive numerical solution for the model. A recursive numerical solution is essential for the use of Kalman filter algorithm, which is discussed later on. The field measurements, that is, water quality monitoring is then expressed as an equation incorporating an error term. The recursive solution from the model and the field measurements are combined using the Kalman filter algorithm to obtain the best value of dissolved oxygen in a segment. The algorithm also puts bounds on this estimated value of DO.

Although the filter algorithm combines the model prediction and the field measurement it does not tell us how to determine the sampling locations. Therefore, we have to define or develop a measure by which the number of locations can be obtained. The measure used in this study is the term TRACE OF ESTUARY (TOE). Using this measure,

hypotheses have to be formed indicating how TOE would vary depending on the sampling locations, and how sampling locations would vary depending on the accuracy of the model.

3.4 Data Collection

Once a theory is developed it has to be tested in a real life situation. The Potomac estuary on the eastern coast of the U. S. was selected, and data from the months of May 1982 to December 1983 was used. The estuary is described in Chapter 5.

The Metropolitan Washington Council of Governments organized a regional monitoring program in 1982 for the Potomac River. About eleven agencies were involved in the data collection program. A total of 59 stations were established within 43 miles upstream and 107 miles downstream of Chain Bridge [4]. The frequency of sampling varied; weekly, fortnightly and monthly. While on some occasions the sampling was done at various depths, on several occasions it was done just below the water surface.

3.5 Test of the Theory

In order to use the theory, the estuary had to be idealized to suit the research needs. The inflows from the various tributaries into the study area were omitted, and an idealized version of the estuary was obtained. The idealized estuary was then divided into suitable segments. The segments were further idealized as rectangular boxes. These were then combined in a specific manner to evaluate the TOE of the various combinations of the segments.

3.6 Results

The prediction of dissolved oxygen along the estuary as the number of segments are reduced is presented first, in Chapter 5. Then the variation of TOE with the number of segments, (when dissimilar sized segments are used) is then given for 18 months in the same chapter. The results are critically evaluated in the chapter on Discussion.

CHAPTER 4

INTEGRATING MODELS AND MONITORING

4.1 Introduction and Hypothesis

The literature review revealed that modeling and monitoring have been evolving independently; especially in the management of estuaries. Our hypothesis is that the combined use of both models and monitoring in the water quality management of estuaries will be advantageous. In order to combine these two, it is necessary to identify the models that solved the convective-diffusion equation for a particular variable of interest. The solution to the convective-diffusion equation is expressed in a form where it recursively estimates the concentration of a variable. The measurements are written as equations incorporating possible errors. It is possible to combine the recursive solution and the field measurements using the Kalman filter algorithm. The following sections exemplify the above statements and describe how the monitoring system is chosen.

4.2 Description of the Theory

4.2.1 Mass Balance Equation

The basic theory behind the development of the models is a three dimensional convective-diffusion equation. Figure 4.1 shows a cube of size $[dx \ dy \ dz]$. When you consider a non-conservative substance flowing from one side of the cube to the other side of the cube, we obtain the following 3-dimensional convective diffusion equation

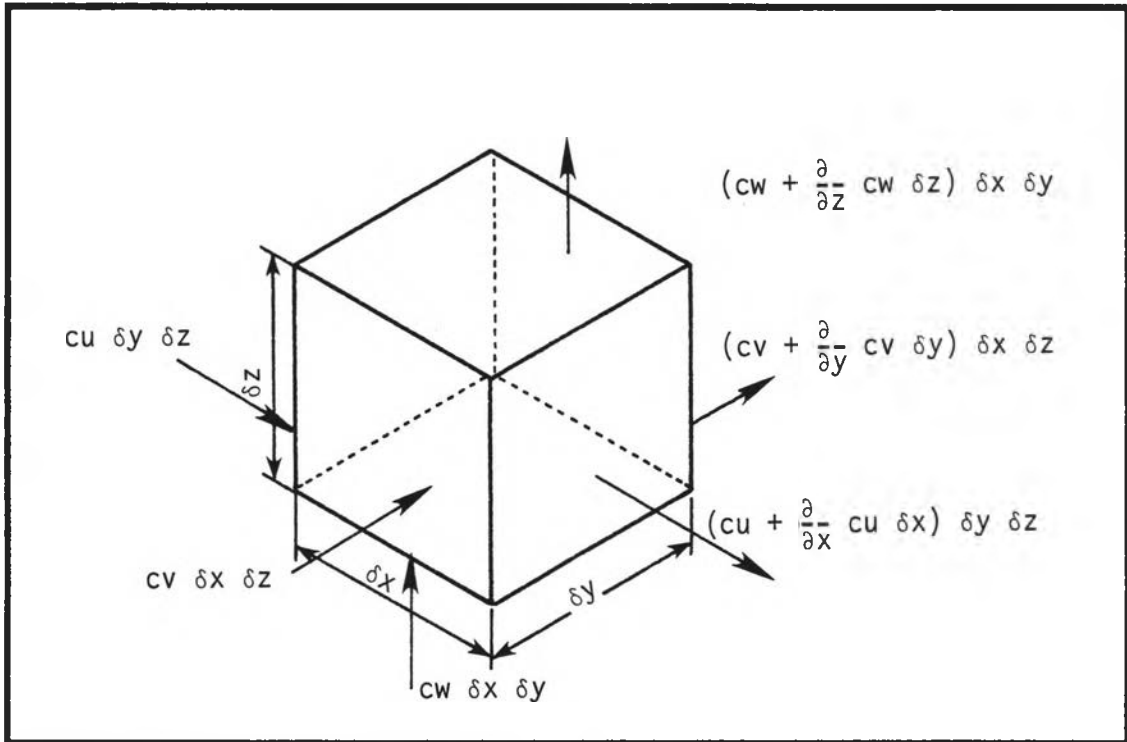


Figure 4.1. Conservation of Mass - Cube.

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} - \frac{\partial}{\partial x} \left(D_x \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial y} \left(D_y \frac{\partial c}{\partial y} \right) - \frac{\partial}{\partial z} \left(D_z \frac{\partial c}{\partial z} \right) \pm S = 0$$

Eqn. (4.1)

where,

c : concentration of the substance

u, v, w : velocity in the x, y, z directions

t : time

D_x, D_y, D_z : dispersion coefficient in the x, y, z directions

S : source/sink term

Equation (4.1) is obtained at an instantaneous point. However when averaged over the cross-section we obtain the Equation (4.2).

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - \frac{\partial}{\partial x} \left(E \frac{\partial c}{\partial x} \right) \pm S = 0$$

Eqn. (4.2)

When the above equation is multiplied by the cross-sectional area A , we arrive at Equation (4.3).

$$\frac{\partial(AC)}{\partial t} + \frac{\partial}{\partial x} (AUC) - \frac{\partial}{\partial x} \left(EA \frac{\partial C}{\partial x} \right) \pm AS = 0 \quad \text{Eqn. (4.3)}$$

The term 'E' is known as the effective dispersion coefficient. The term incorporates effects due to averaging over cross-section and also factors which we do not know. The use of the term effective dispersion E is well explained in references [1] and [2].

4.2.2 Finite Difference Solution

Portions of this material are adapted from reference [3] with corrections, additional figures and descriptions.

The variation of concentration 'C' of a substance along distance 'x' and the corresponding physical representation of the channel are given in Figures 4.2(a), 4.2(b) and 4.2(c).

Using Taylor series expansion, for the concentration at points $x_0 + \Delta x$ and $x_0 - \Delta x$

$$C_{x_0 + \Delta x} = C_{x_0} + \frac{\Delta x}{1!} \left(\frac{\partial C}{\partial x} \right)_{x_0} + \frac{\Delta x}{2!} \left(\frac{\partial^2 C}{\partial x^2} \right)_{x_0} + \frac{\Delta x}{3!} \left(\frac{\partial^3 C}{\partial x^3} \right)_{x_0} + \dots \quad \text{Eqn. (4.4)}$$

$$C_{x_0 - \Delta x} = C_{x_0} - \frac{\Delta x}{1!} \left(\frac{\partial C}{\partial x} \right)_{x_0} + \frac{\Delta x}{2!} \left(\frac{\partial^2 C}{\partial x^2} \right)_{x_0} - \frac{\Delta x}{3!} \left(\frac{\partial^3 C}{\partial x^3} \right)_{x_0} + \dots \quad \text{Eqn. (4.5)}$$

Assuming that the 3rd order and higher order terms are negligible, and subtracting Equation (4.5) from Equation (4.4)

$$C_{x_0 + \Delta x} - C_{x_0 - \Delta x} = 2 \Delta x \left(\frac{\partial C}{\partial x} \right)_{x_0}$$

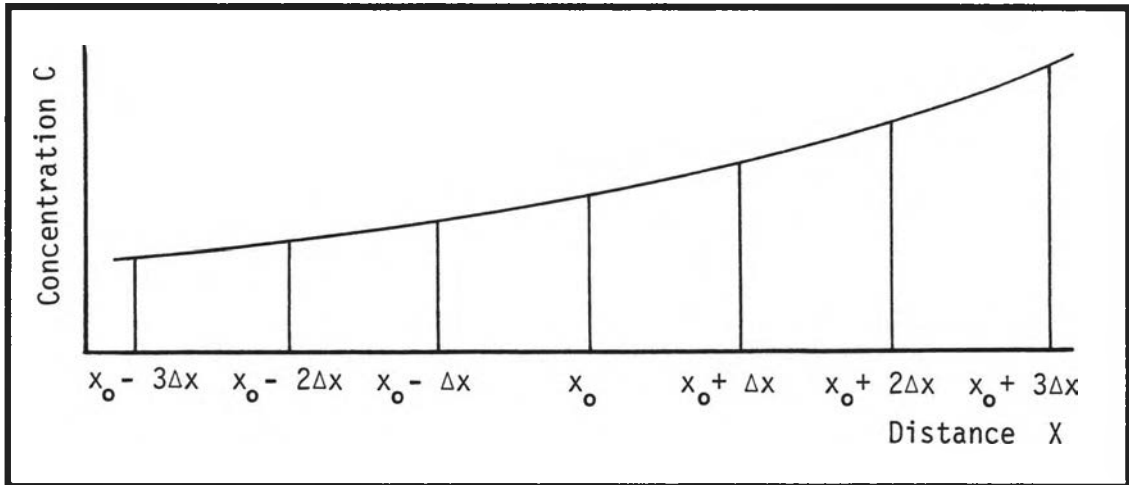


Figure 4.2(a). Variation of Concentration with Distance.

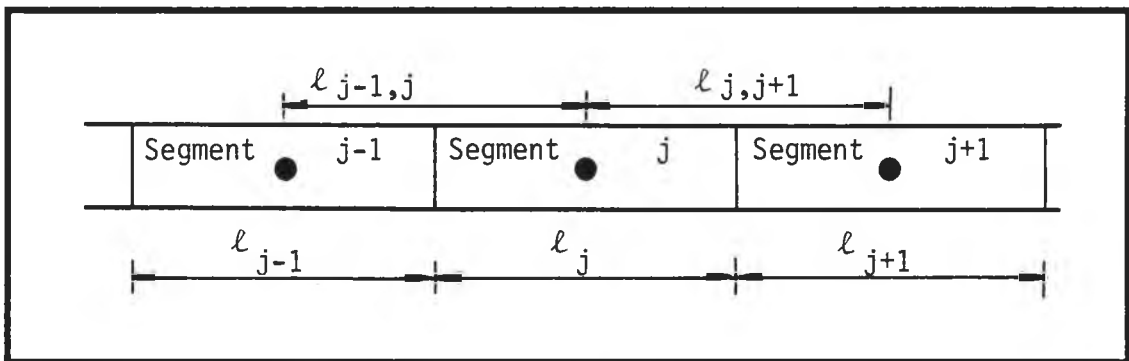


Figure 4.2(b). Layout of Segments.

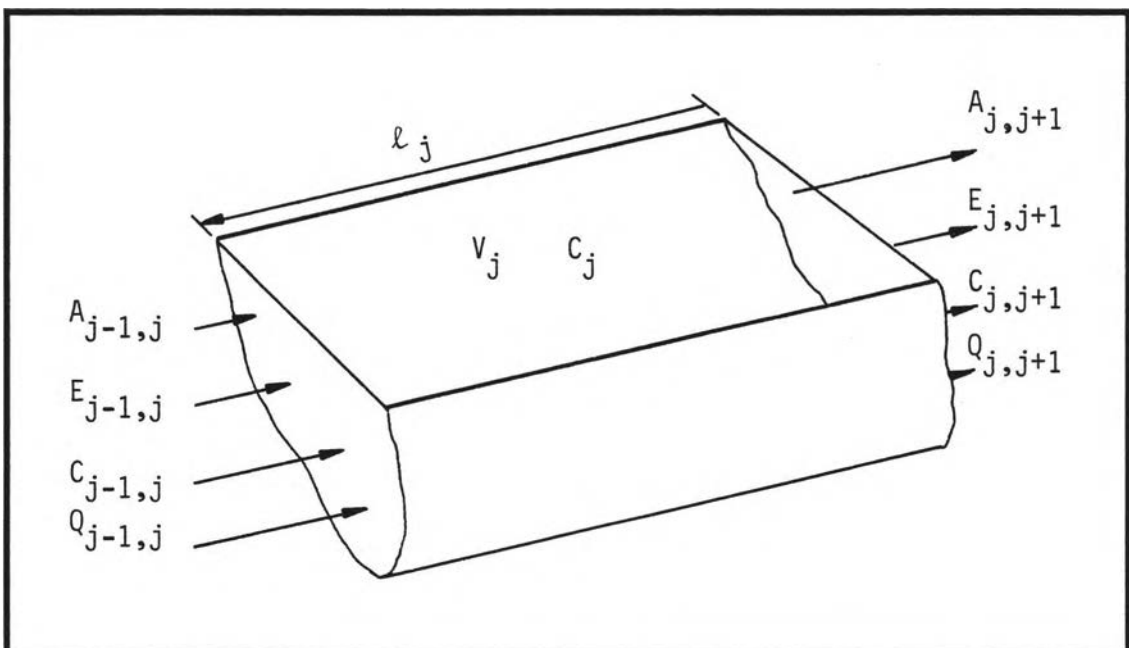


Figure 4.2(c). Three-dimensional View of a Segment.

$$\text{Therefore, } \left(\frac{\partial C}{\partial x} \right)_{x_0} = \frac{C_{x_0 + \Delta x} - C_{x_0 - \Delta x}}{2 \Delta x} \quad \text{Eqn. (4.6)}$$

Now considering Equation (4.3),

$$\frac{\partial (AC)}{\partial t} + \frac{\partial}{\partial x} (AUC) - \frac{\partial}{\partial x} \left(EA \frac{\partial C}{\partial x} \right) \pm AS = 0$$

if we represent $Q = AU$, where Q is the volumetric inflow,

$$\frac{\partial (AC)}{\partial t} + \frac{\partial}{\partial x} (QC) - \frac{\partial}{\partial x} \left(EA \frac{\partial C}{\partial x} \right) \pm AS = 0 \quad \text{Eqn. (4.7)}$$

In finite difference form, the second and third expressions in Equation (4.7), can be represented as

$$\frac{\partial}{\partial x} (QC) = \frac{Q_{x_0 + \Delta x} C_{x_0 + \Delta x} - Q_{x_0 - \Delta x} C_{x_0 - \Delta x}}{2 \Delta x}$$

$$\frac{\partial}{\partial x} \left(EA \frac{\partial C}{\partial x} \right) = \frac{(EA)_{x_0 + \Delta x} \left(\frac{\partial C}{\partial x} \right)_{x_0 + \Delta x} - (EA)_{x_0 - \Delta x} \left(\frac{\partial C}{\partial x} \right)_{x_0 - \Delta x}}{2 \Delta x}$$

$$\frac{\partial}{\partial x} \left(EA \frac{\partial C}{\partial x} \right) = \frac{(EA)_{x_0 + \Delta x} \left[\frac{C_{x_0 + 2\Delta x} - C_{x_0}}{2 \Delta x} \right] - (EA)_{x_0 - \Delta x} \left[\frac{C_{x_0} - C_{x_0 - 2\Delta x}}{2 \Delta x} \right]}{2 \Delta x}$$

When the difference approximations are superimposed with the segments of the channel,

$$Q_{x_0 + \Delta x} = Q_{j,j+1} \quad : \quad \text{flow passing through boundary of segment } j \text{ and segment } j+1$$

$$C_{x_0 + \Delta x} = C_{j,j+1} \quad : \quad \text{concentration at the boundary of segments } j \text{ and } j+1$$

$$\left. \begin{aligned}
 C_{x_0 - 2\Delta x} &= C_{j-1} \\
 C_{x_0} &= C_j \\
 C_{x_0 + 2\Delta x} &= C_{j+1}
 \end{aligned} \right\} \begin{array}{l} \text{Concentrations of segments } j-1, j \text{ and } j+1 \\ \text{measured at the center of segment} \end{array}$$

$(EA)_{x_0 + \Delta x} = (EA)_{j,j+1}$: dispersion through the boundary of segments j and $j+1$

$(EA)_{x_0 + \Delta x} = (EA)_{j-1,j}$: dispersion through the boundary of segments $j-1$ and j

Substituting the above expressions in Equation (4.7)

$$\begin{aligned}
 \frac{\partial}{\partial t} (A_j C_j) &= - \frac{Q_{j,j+1} C_{j,j+1} - Q_{j-1,j} C_{j-1,j}}{\ell_j} \\
 &+ \frac{(EA)_{j,j+1} \left(\frac{C_{j+1} - C_j}{\ell_{j,j+1}} \right) - (EA)_{j-1,j} \left(\frac{C_j - C_{j-1}}{\ell_{j-1,j}} \right)}{\ell_j} \\
 &\pm A_j S_j
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial}{\partial t} (A_j C_j) &= - \frac{Q_{j,j+1} C_{j,j+1} - Q_{j-1,j} C_{j-1,j}}{\ell_j} \\
 &+ (EA)_{j,j+1} \frac{(C_{j+1} - C_j)}{\ell_j \ell_{j,j+1}} - (EA)_{j-1,j} \frac{(C_j - C_{j-1})}{\ell_j \ell_{j-1,j}} \\
 &\pm A_j S_j
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial}{\partial t} (\ell_j A_j C_j) &= - Q_{j,j+1} C_{j,j+1} + Q_{j-1,j} C_{j-1,j} \\
 &+ \left(\frac{EA}{\ell} \right)_{j,j+1} (C_{j+1} - C_j) - \left(\frac{EA}{\ell} \right)_{j-1,j} (C_j - C_{j-1}) \\
 &\pm \ell_j A_j S_j
 \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial t} (V_j C_j) = & - Q_{j,j+1} C_{j,j+1} + Q_{j-1,j} C_{j-1,j} \\ & + R_{j,j+1} (C_{j+1} - C_j) - R_{j-1,j} (C_j - C_{j-1}) \\ & \pm V_j S_j \end{aligned} \quad \text{Eqn. (4.8)}$$

where,

V_j : volume of the segment m^3

$R_{j,j+1}$: dispersive flow at the boundary of the segment m^3/sec and

$$\text{and } R_{j,j+1} = \left(\frac{EA}{\ell} \right)_{j,j+1}$$

$\ell_{j,j+1}$: characteristic length m

Euler scheme is used to obtain the solution to Equation (4.8)

$$\left(V_j C_j \right)_{t + \Delta t} = \left(V_j C_j \right)_t + \frac{\partial}{\partial t} \left(V_j C_j \right) \cdot \Delta t \quad \text{Eqn. (4.9)}$$

$$\left(M_j \right)_{t + \Delta t} = \left(M_j \right)_t + \left(r_j \right)_t \quad \text{Eqn. (4.10)}$$

where,

$$M_j = V_j C_j$$

$$r_j = \frac{\partial}{\partial t} \left(V_j C_j \right) \Delta t$$

Equation (4.10) is a predictive equation. Knowing ' r_j ' and the mass of the non-conservative substance in segment 'j' at time 't', it predicts the mass in segment 'j' at time 't + Δt '. The water quality model makes use of Equation (4.10) to predict the concentration of the different variables in the water body.

However, the predicted concentrations are not the correct/accurate values. The reasons are many. For example, the irregular shape of the water body will be approximated as either rectangular or trapezoidal channels to determine the volume of segments. Dispersion coefficients will be estimated. Rate constants to be used in determining the decay of non-conservative substances will be assumed. Hence, Equation (4.10) can be written as

$$\left[M_j \right]_{t + \Delta t} = \left[M_j \right]_t + \left[r_j \right]_t + \left[\xi_j \right]_t \quad \text{Eqn. (4.11)}$$

incorporating an error term $(\xi_j)_t$ to reflect the various approximations made.

In developing the model, the determination of the term r_j , which is equal to $\frac{\partial}{\partial t} (V_j C_j) \cdot \Delta t$ is important. The term $\frac{\partial}{\partial t} (V_j C_j)$ incorporates the following three quantities;

- Change in mass due to volumetric inflows and outflows from the segment

$$- Q_{j,j+1} C_{j,j+1} + Q_{j-1,j} C_{j-1,j}$$

- Change in mass due to dispersive flow in the segment

$$R_{j,j+1} (C_{j+1} - C_j) - R_{j-1,j} (C_j - C_{j-1})$$

- Change in mass due to kinetics of the non-conservative substance

$$V_j S_j$$

However, for the case study, the Potomac estuary is idealized as having twelve segments. Each of these segments are assumed to behave like completely stirred tank reactors, (CSTR). The assumption is valid owing to the residence time in the estuary, 85 days [4]. As the segments duplicate CSTR's, the changes due to volumetric

inflows/outflows, and dispersive flows are negligible. Hence, in the model, only the kinetics of the non-conservative substance is taken into account, that is the $V_j S_j$ term.

Further, in the particular case of dissolved oxygen, algal respiration, sediment oxygen demand, photosynthesis etc., are neglected. This will lead to the following expression for the source/sink term, S in the j th segment.

$$S_j = K_2 [C_s - C_{6,j}] - K_d C_{5,j} \quad \text{Eqn. (4.12)}$$

where,

- K_2 : reaeration rate coefficient
- C_s : saturation value of the dissolved oxygen
- $C_{6,j}$: dissolved oxygen in the j th segment
- K_d : deoxygenation rate coefficient
- $C_{5,j}$: biochemical oxygen demand in the segment

4.2.3 Field Measurements/Observations

When a monitoring scheme is employed, measurements are taken at specified locations at certain times. These measurements are affected by errors in the measuring equipment, errors while entering the data, errors while reading and so on. We can write an equation incorporating the errors, and this is known as the measurement equation. For a particular segment ' j '

$$(y_j)_{t + \Delta t} = (M_j)_{t + \Delta t} + (\eta_j)_{t + \Delta t} \quad \text{Eqn. (4.13)}$$

where,

$y_{t + \Delta t}$: field measurement at time $t + \Delta t$

$x_{t + \Delta t}$: real value of the measured variable

$\eta_{t + \Delta t}$: error in the measurement/observation

In the case of dissolved oxygen, we express the measurements as concentrations in mg/liter. However, for the development of the theory, the variables in Equation (4.13) are in weight units expressed in kilograms.

A major assumption is being made in writing down Equation (4.13), and is explained below. Figure 4.3 illustrates a segment of an estuary. At any one time field measurements can be made at an infinite number of points within the segment, say at locations A, B, C and so on. The assumption is that the field measurements are identical irrespective of wherever they are made, A, B, or C.

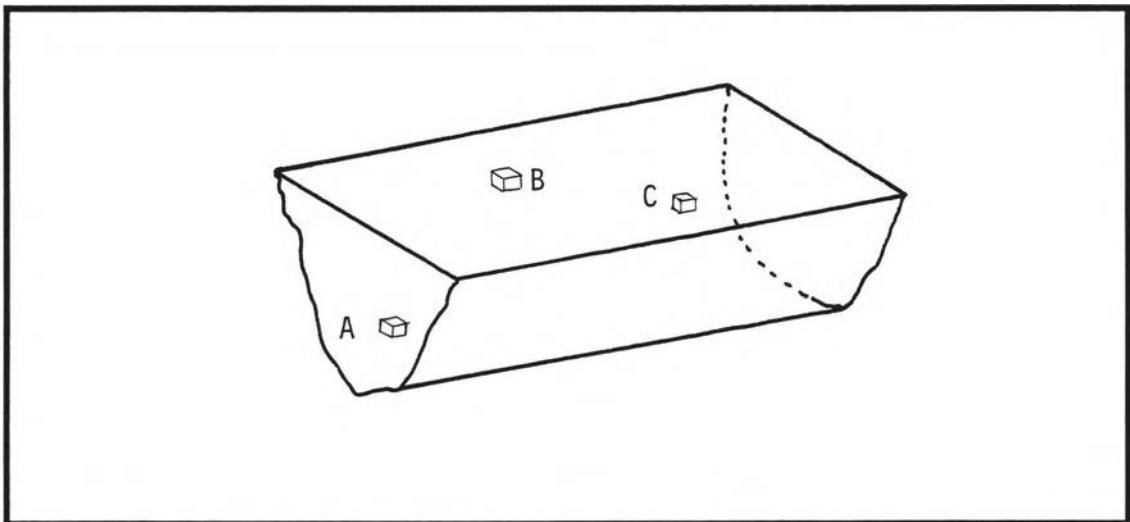


Figure 4.3. Field Measurements Within a Segment.

4.2.4 Kalman Filter Algorithm

It is not intended either to derive or explain in detail the Kalman filter algorithm. Excellent sources exist [5,6,7] elsewhere,

and these describe in detail the algorithm and its applications in water resource systems. However, the algorithm, as briefly explained in Appendix A-4, is summarized in five steps and a flow chart, Figure 4.4, illustrates the various steps. Consider a segment 'j'.

The basic philosophy behind the filter algorithm is obtaining the best estimate $[(M'_j)_{t+\Delta t}]$ of the state of the system as represented by a specific variable, making use of the model prediction of the variable $[(M_j)_{t+\Delta t}]$, and field measurements of that variable $[(y_j)_{t+\Delta t}]$. This is achieved by weighting $[(k_j)_{t+\Delta t}]$ the difference between the model prediction and the field measurement $[(y_j)_{t+\Delta t} - (M_j)_{t+\Delta t}]$, and adding the weighted difference $\{[(k_j)_{t+\Delta t}][(y_j)_{t+\Delta t} - (M_j)_{t+\Delta t}]\}$ to the model prediction $[(M_j)_{t+\Delta t}]$. This is illustrated in step 4, as posterior forecast.

The algorithm not only evaluates the best estimate but also puts bounds on this best estimate. This is given in step 5 as forecast variance update. In the process, the weighting factor is also recursively estimated as shown in step 3. However, in order to begin the execution of the algorithm we should know the initial state, and the error associated with it. These are obtained from steps 1 and 2 respectively.

1. Prior forecast

$$\begin{bmatrix} M_j \end{bmatrix}_{t + \Delta t} = \begin{bmatrix} M_j \end{bmatrix}_t + \begin{bmatrix} r_j \end{bmatrix}_t$$

2. Forecast error/forecast variance

$$\begin{bmatrix} \sigma_j^2 (-) \end{bmatrix}_{t + \Delta t} = \begin{bmatrix} \sigma_j^2 (+) \end{bmatrix}_t + \sigma_{\text{model}}^2$$

3. Kalman gain/filter gain

$$\left[K_j \right]_{t + \Delta t} = \frac{\left[\sigma_j^2 (-) \right]_{t + \Delta t}}{\sigma_{\text{measurement}}^2 + \left[\sigma_j^2 (-) \right]_{t + \Delta t}}$$

4. Posterior forecast

$$\left[M'_j \right]_{t + \Delta t} = \left[M_j \right]_{t + \Delta t} + \left[K_j \right]_{t + \Delta t} \left[\left[y_j \right]_{t + \Delta t} - \left[M_j \right]_{t + \Delta t} \right]$$

5. Forecast variance update

$$\left[\sigma_j^2 (+) \right]_{t + \Delta t} = \left[1 - \left[K_j \right]_{t + \Delta t} \right] \left[\sigma_j^2 (-) \right]_{t + \Delta t}$$

- M_j : Mass in segment.
- r_j : Changes in mass due to physical processes that take place in segment.
- $\sigma_j^2 (-)$: Variance of the indicator variable before the field measurements are made.
- $\sigma_j^2 (+)$: Variance of the indicator variable after the field measurements are made.
- σ_{model}^2 : Variance of the model prediction of the indicator variable.
- $\sigma_{\text{measurement}}^2$: Variance of the measurement of the indicator variable.
- k_j : Weighting factor/Kalman gain/Filter gain.
- M'_j : Mass after field measurements are made in segment.

At the next time step, the results from 4 and 5 are used as inputs for steps 1 and 2. The signs (-) and (+) indicate the values of the variance σ^2 before and after the measurements, respectively. The

ASSUMPTIONS

The following are known: $M(t,j)$, $P(t,j)$ for $t = 1$ and $j = 1, 2, \dots, N$

$$\begin{array}{l} P_{\text{model}} \\ P_{\text{measurement}} \end{array}$$

The signs (-) and (+) indicate the value of the variance P , before and after the field measurements are made.

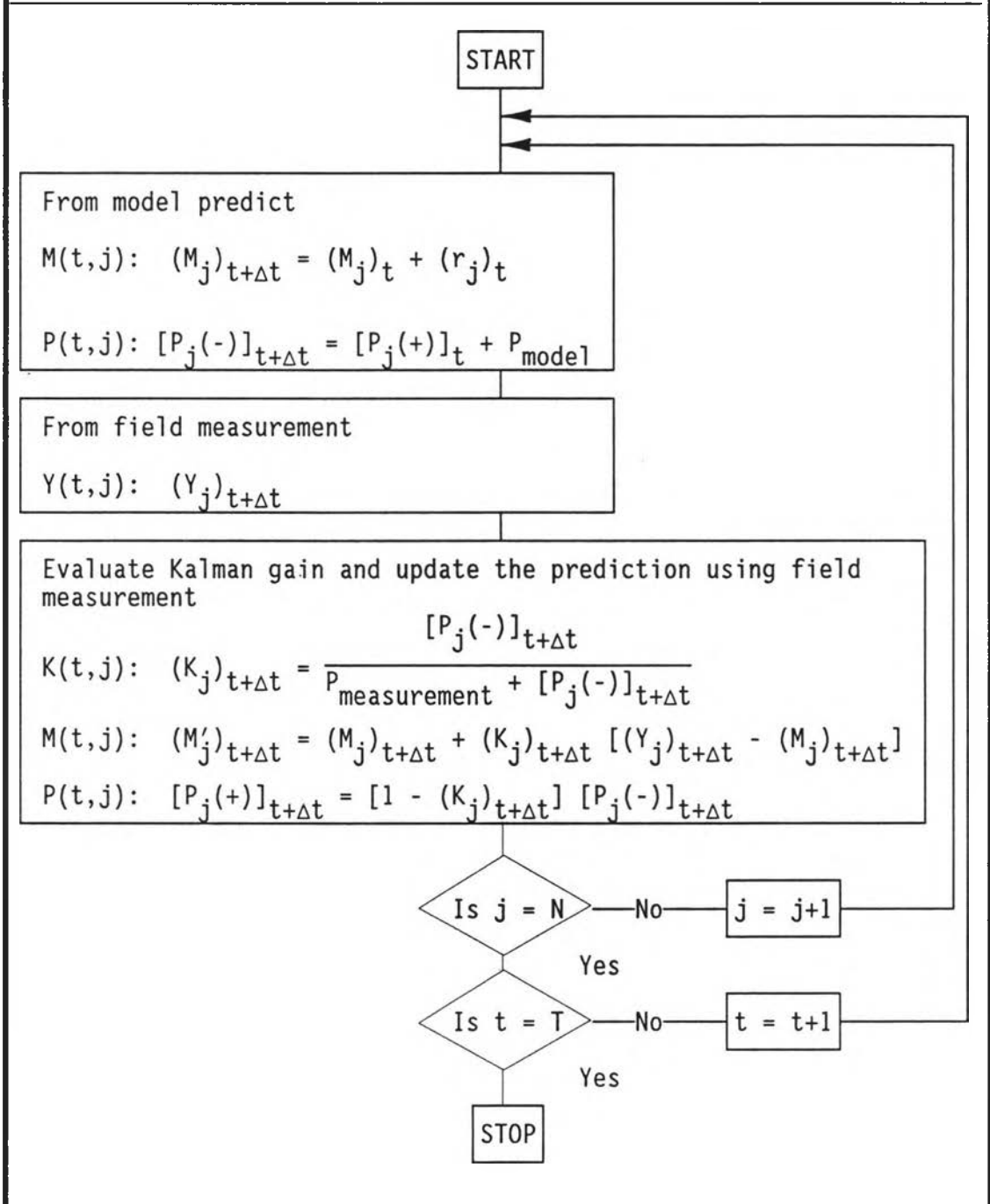


Figure 4.4. Flow Chart for Kalman Filter Algorithm.

updated variance shown in Step 5 is the key to the selection of monitoring locations and is explained in the next section.

4.3 Selection of Models and Monitoring

4.3.1 Criteria for Monitoring

In order to analyze the ongoing monitoring system in an estuary, a new term "TRACE OF ESTUARY" (TOE) is defined. The term TRACE is obtained from matrix terminology. It is the sum of the diagonal terms of the matrix, and is used in a similar context.

The estuary is divided into 'j' segments. The forecast variance update illustrated in section 4.2.4 is evaluated for each and every segment at each time step. If we assume that the forecast variance update is not correlated in space, the forecast variance update for the segments at a specific time step can be represented in matrix form as follows:

$$[A_j] = \begin{bmatrix} a_{11} & 0 & \cdot & \cdot & \cdot \\ 0 & a_{22} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & a_{jj} \end{bmatrix}$$

The trace of the matrix A_j is given by

$$\text{trace } [A_j] = \sum_{i=1}^j a_{ii}$$

For easy notation let us denote

$$\text{trace } [A_j] = T_j$$

Further, if one can define a total acceptable error, we assume that it is related to the trace of estuary (TOE), T_j . The units of T_j will be kilogram² in our case. Further the value of T_j is dependent on the

number of segments 'j'. In other words it is dependent on the number of sampling locations; because a monitoring station exists in every segment. There is an optimum value of T corresponding to a particular 'j' that will determine the number of sampling locations. This value of T is defined as the 'OPTIMUM TRACE OF ESTUARY'. The number of sampling locations corresponding to the optimum trace of estuary is the minimum number necessary for effective water quality management.

The total cost to the management is the combined cost of modeling and monitoring. The reduction in the number of locations due to the use of a sophisticated model does not necessarily mean reduction in cost. This is because the reduction in cost due to fewer number of monitoring stations may be offset by the increase in cost due to the development or use of a sophisticated model.

4.3.2 Hypothesis

- (i) It is postulated that the trace of estuary (TOE) varies inversely with the number of sampling locations. That is, it decreases with the increase in the number of sampling locations as shown in Figure 4.5(a).
- (ii) Secondly, the curve of TOE vs Number of Sampling locations is dependent on the accuracy of the model. For a given number of sampling locations, the curve of TOE vs Locations will shift down for an accurate model as indicated in Figure 4.5 (b).
- (iii) Thirdly, for a predetermined value of TOE, the accuracy of the model dictates the number of sampling locations. Figure 4.5 (c) portrays the fact that an accurate model

will give a lesser number of locations than a less accurate model.

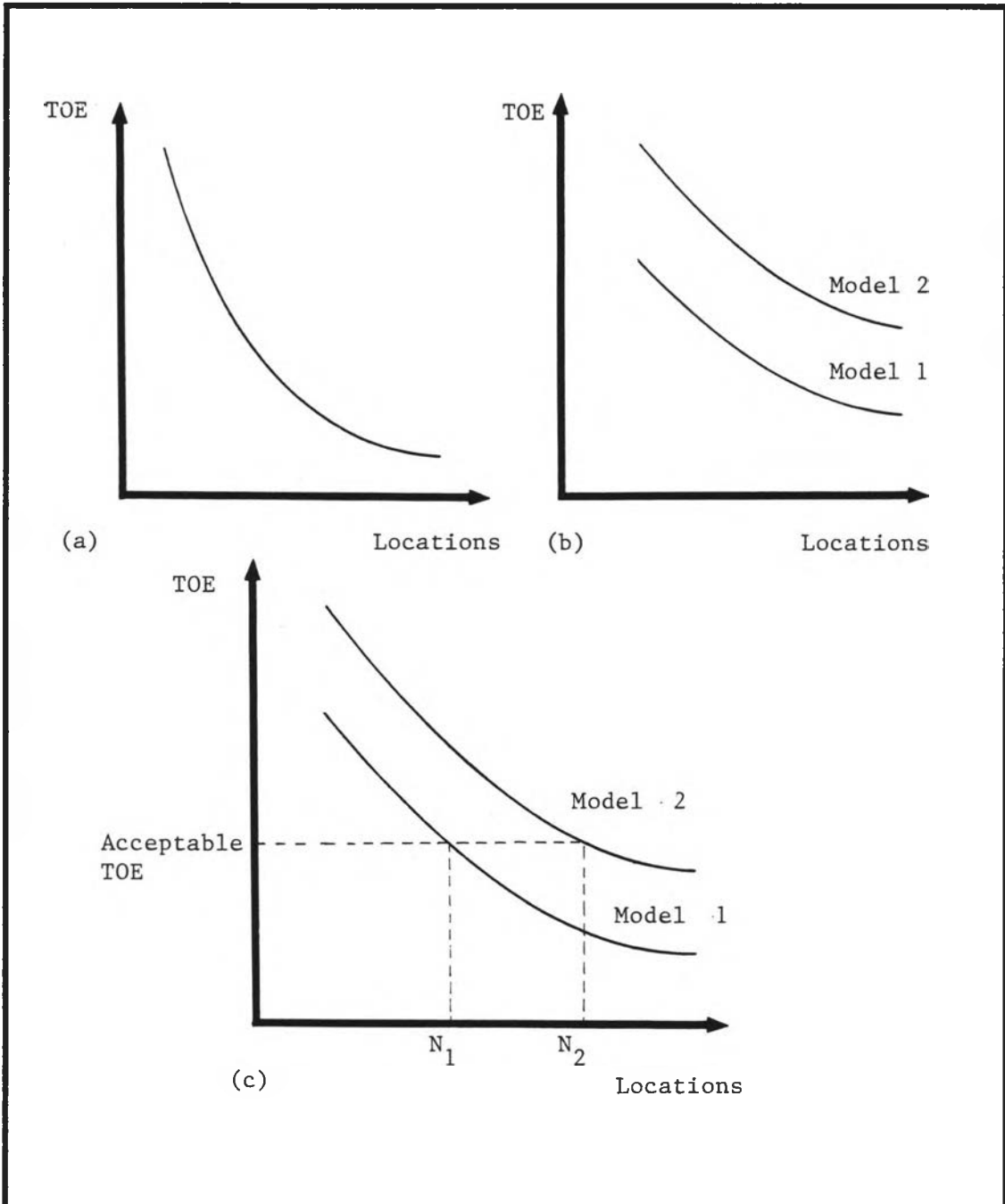


Figure 4.5. Trace of Estuary vs No. of Locations.

CHAPTER 5

CASE STUDY - POTOMAC ESTUARY

5.1 Study Area

The Potomac River which flows in the eastern part of the United States was discovered in 1608 by John Smith. It flows 383 miles, and joins the Chesapeake Bay. The water in the Potomac is critical, and "It is water, not politics that unifies portions of Pennsylvania, West Virginia, Virginia, Maryland, and all of the District of Columbia" [1].

Since 1608, the English, French, Germans and Scotch-Irish, all from Europe, settled in the region. The initial settlers grew tobacco. Subsequently, tobacco gave way to wheat. Wheat was ousted by dairy farming, when electric trains were introduced. Over-use of the natural resources and population growth led to pollution and silt in the river, and hindered economic stability in the region. "The river no longer yields up the abundant harvests of oysters and fish as it did in the 1880s and 1890s" [2].

As the quality of water in the estuary is important, several institutions are engaged in research, trying to understand the water quality characteristics of the estuary. The literature on the Potomac estuary is enormous. The annotated bibliography [2] by the Library of Congress, lists publications since 1965 for a period of 15 years. The region selected for the present research is shown in Figure 5.1 [3].

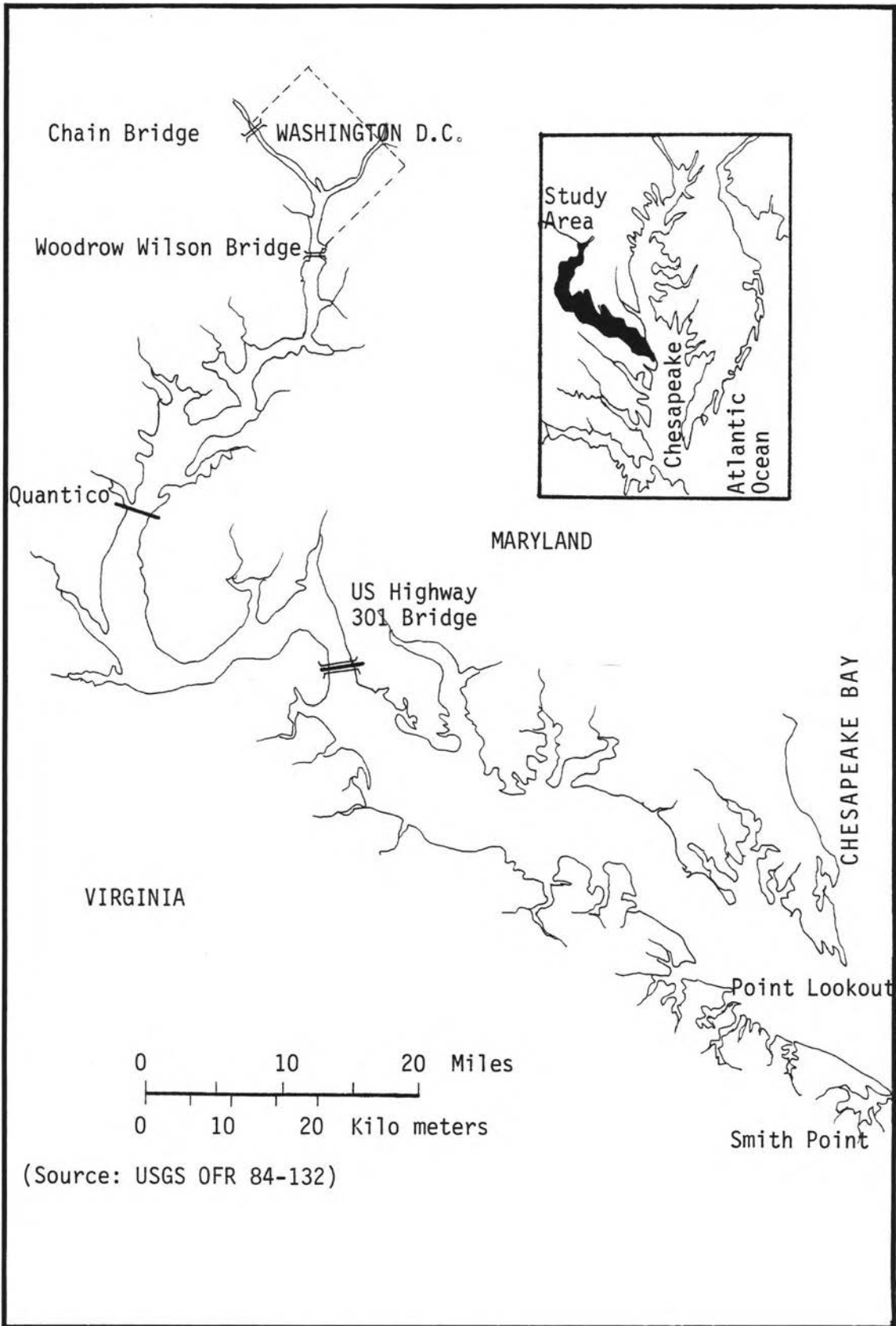


Figure 5.1. Study Area - Potomac Estuary.

The study area was briefly described in the preceding paragraphs. The next few sections illustrate the results of the completely stirred tank reactor (CSTR) model predictions, Kalman filter predictions, and the variation of Trace of Estuary (TOE) with the number of sampling locations.

5.2 Completely Stirred Tank Reactor (CSTR) Model

5.2.1 Segmenting the Estuary

The theory for developing the CSTR model was described in Chapter 4. In order to use the model, the Potomac estuary was divided into twelve segments. Each segment was idealized as being rectangles in Plan and Cross-sectional views. This is graphically illustrated in Figure 5.2.

Nautical chart 12285 [4] was used to divide the estuary into segments. Segments were selected such that water quality monitoring stations were located at the center of each segment. The area in Plan view was obtained using a Planimeter. The area divided by the length gave the mean width of segment. Cross-sections at the centers of segments were also obtained from nautical chart 12285. The mean depth of the segment was obtained by dividing the cross-sectional area by the mean width obtained previously. The depths in the chart used for obtaining the cross-section were with reference to mean lower low water (MLLW). MLLW is defined as the average of the lowest low water height of each tidal day observed over the national tidal datum epoch [5]. This average is normally taken over a period of 19 years.

The locations, lengths, widths and depths of the idealized estuary are given in Appendix A-2.

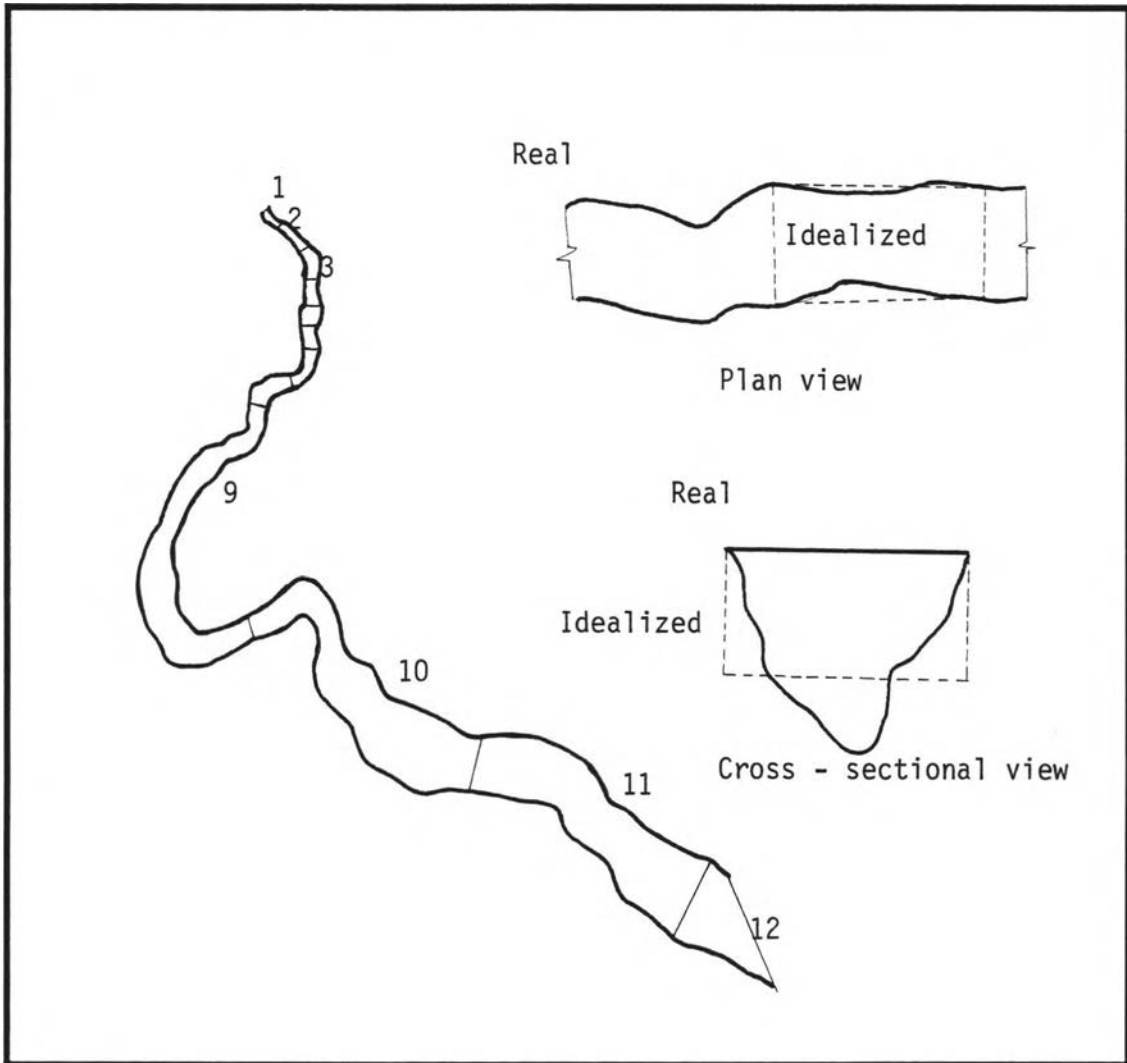


Figure 5.2. Segmentation and Idealization.

5.2.2 Segment Volumes

Owing to the tides, the heights of the water level vary from the MLLW. The water heights (high water predictions) at the monitoring locations were predicted with the aid of tide tables [5,6] for a period of 24 months (1982-83). These heights were added to the mean depth, and volumes of each of the segment during the 24 month period were calculated. The calculated volumes are shown in Appendix A-6 as output of program EULER.

5.2.3 Dissolved Oxygen (DO) and Biochemical Oxygen Demand (BOD)

The dissolved oxygen concentration values for this period were obtained from the report published by the Council of Governments [7]. In case of missing values at intermediate stations, the mean values of the neighboring stations were used. The point source ultimate BOD loading along the estuary was obtained from reference [3] for the 12 months, January-December, in 1980. This was assumed as being representative loads for 1982 and 1983. A non point source load of 5000 kg/day was also assumed for each of the segments. These values are also given in Appendix A-6 as output of program EULER.

5.2.4 Model Predictions

The CSTR model predictions for one particular time period, with field observations are illustrated in Figure 5.3.

5.3 Kalman Filter Predictions

5.3.1 Combining Segments

The approach of the research was to reduce the number of sampling locations and evaluate the predicted variance of DO for the entire estuary defined as Trace of Estuary (TOE), using Kalman filter algorithm. It was mentioned in the previous section that each segment had a monitoring station at its center. In order to reduce the sampling locations, segments were combined one at a time. When segments were combined, the monitoring station at the far left segment was retained. Measurements from this sampling location were considered as being representative of the combined segment. These values were then used in the filter algorithm. The manner in which segments are combined is graphically illustrated in Figure 5.4.

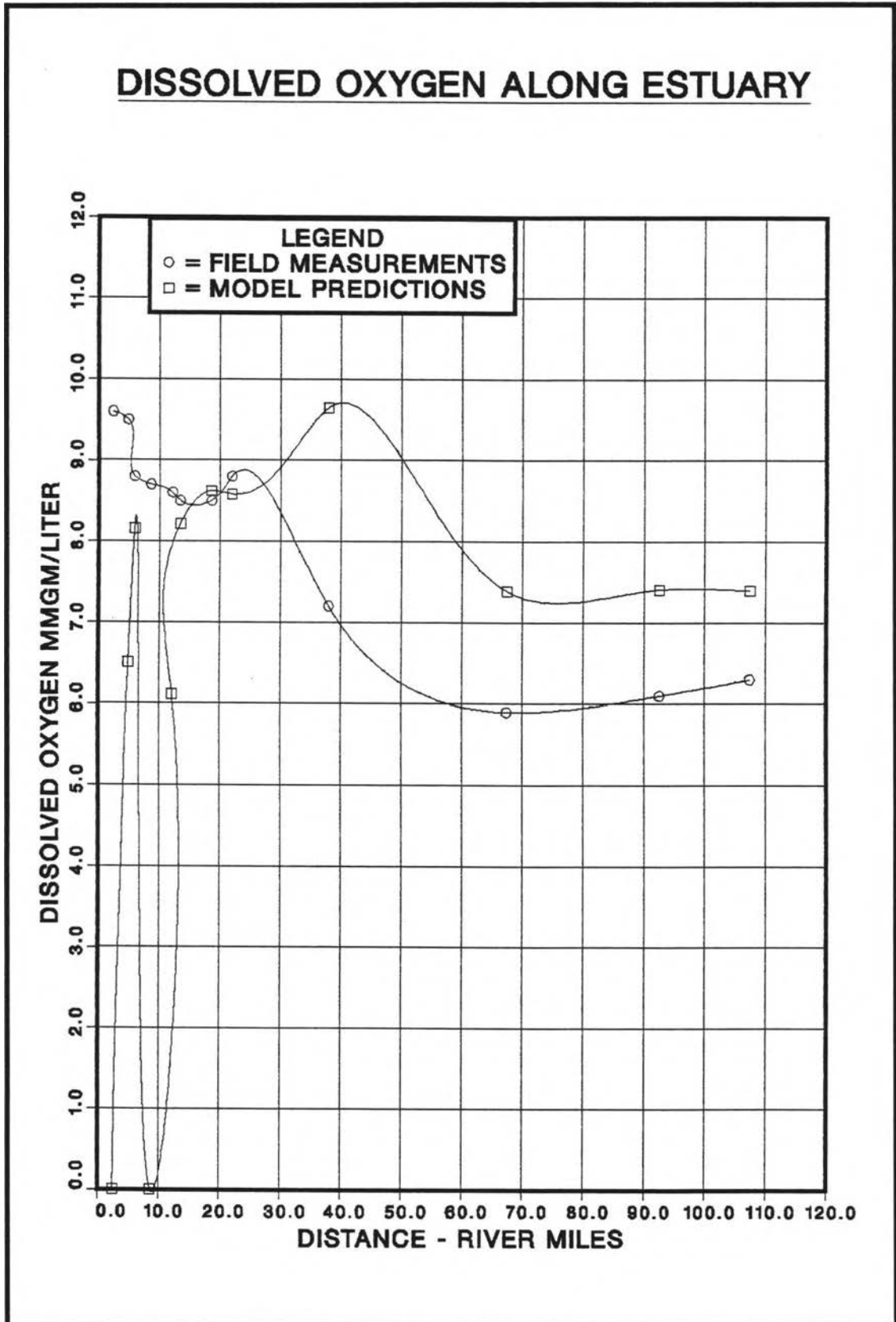


Figure 5.3. CSTR Model Prediction and Field Measurements.

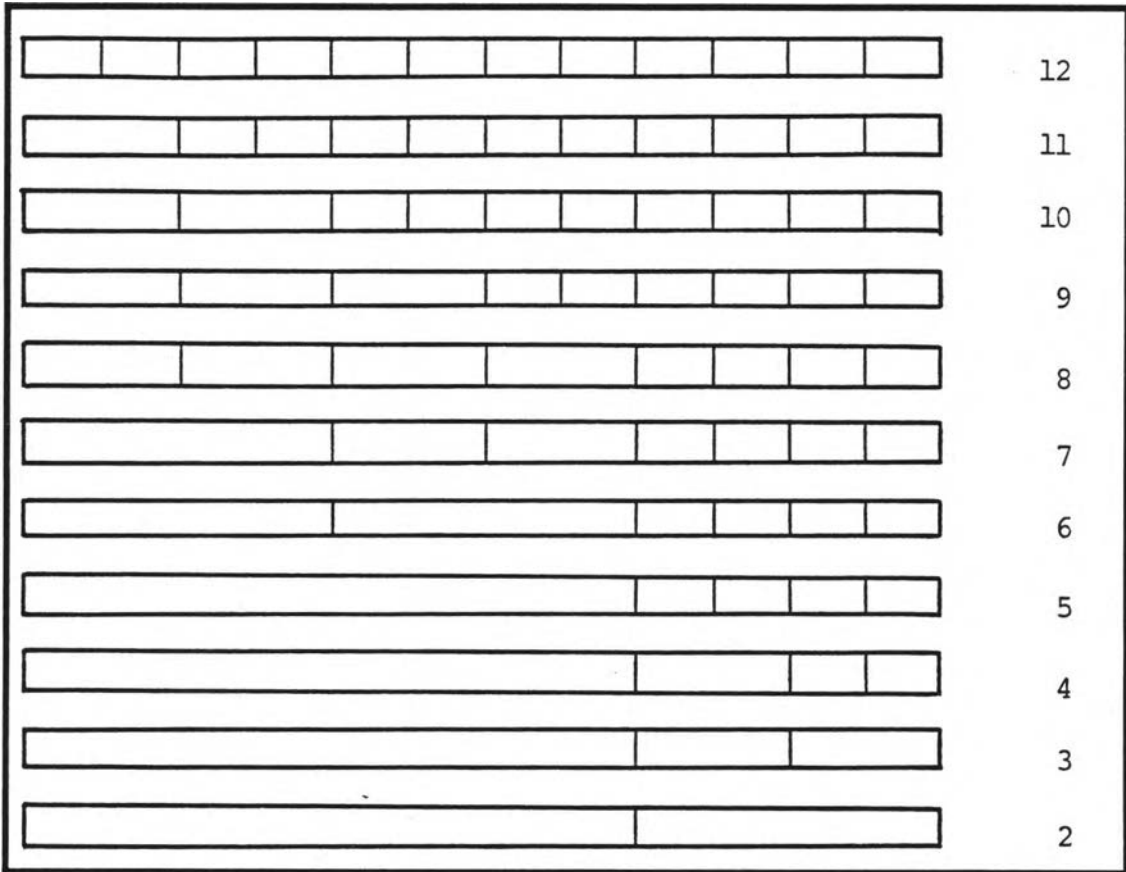


Figure 5.4. Combining Segments.

5.3.2 Measurements, CSTR Model Prediction, and Filter Prediction

The field observations, CSTR model predictions, and filter predictions are shown in Figure 5.5 for one time period. The field observations from 12 sampling locations, considered as the ideal situation, together with filter predictions as sampling locations are reduced, are illustrated in Figures 5.6 - 5.11, for one period. The values are given in Tables 5.1 and 5.2.

5.3.3 Variation of the Trace of Estuary with Sampling Locations

The predicted variance of DO for the entire estuary, expressed as the trace of estuary versus the number of sampling locations is graphically illustrated in Figure 5.12 - 5.20 for the entire period of analysis. The numerical values are tabulated in Appendix A-3.

DISSOLVED OXYGEN ALONG ESTUARY

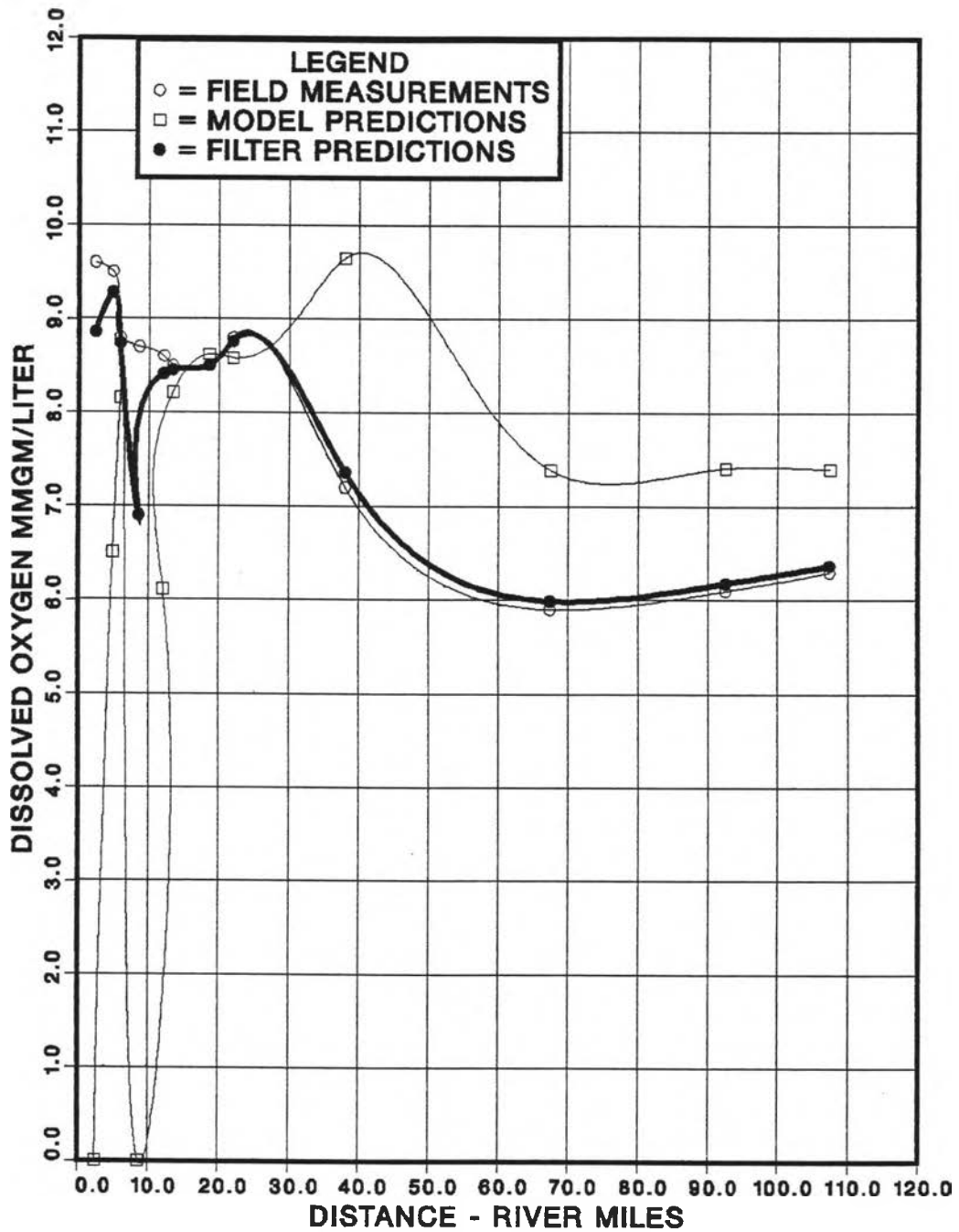
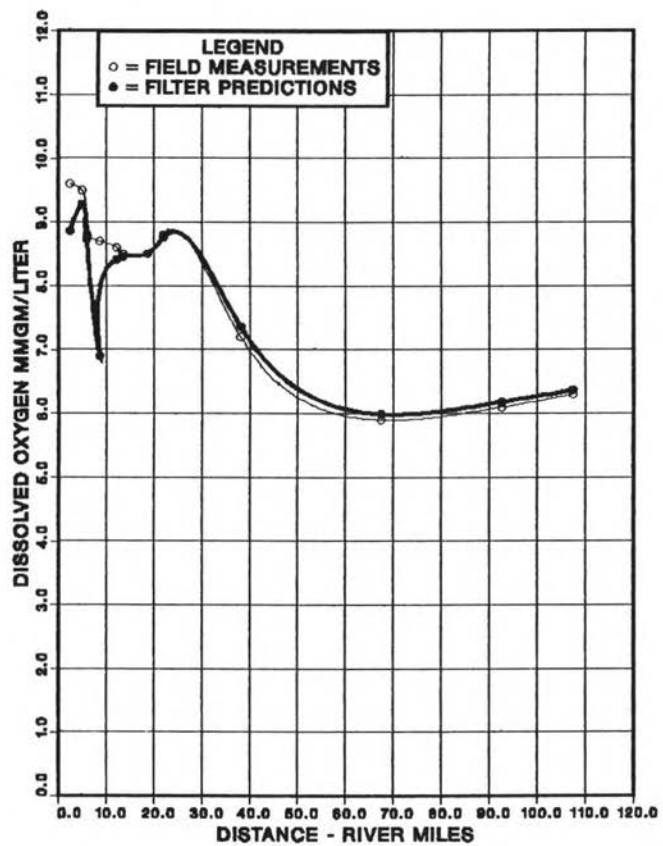


Figure 5.5. Comparison of Field Measurements, CSTR Model Prediction and Filter Prediction.

DISSOLVED OXYGEN ALONG ESTUARY



DISSOLVED OXYGEN ALONG ESTUARY

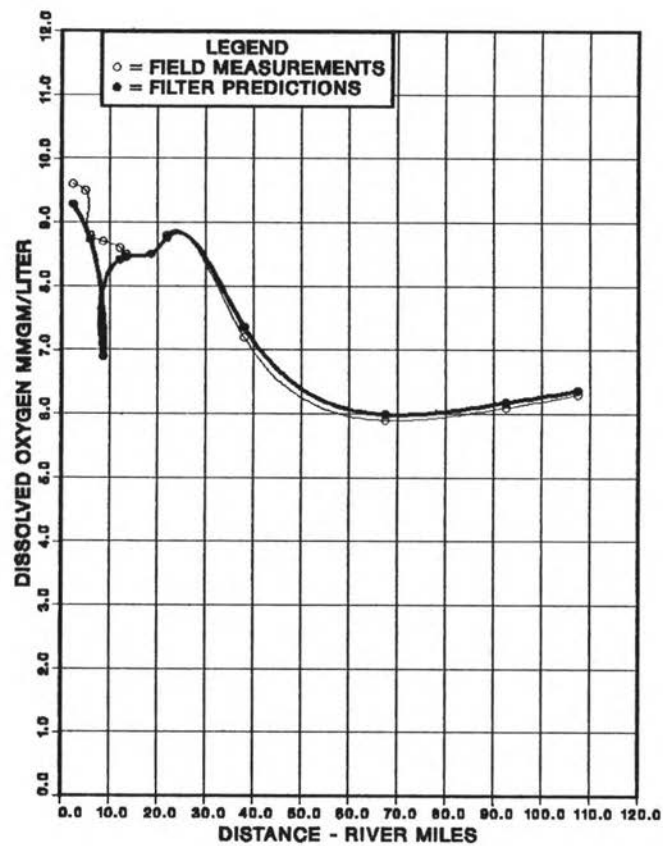
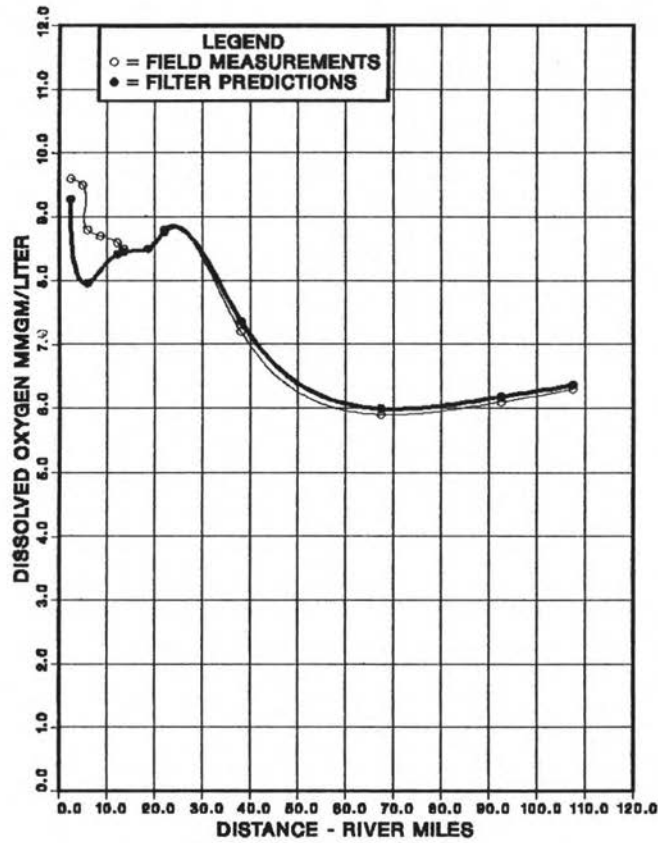


Figure 5.6. Field Measurements and Filter Predictions; 12 Segments and 11 Segments.

DISSOLVED OXYGEN ALONG ESTUARY



DISSOLVED OXYGEN ALONG ESTUARY

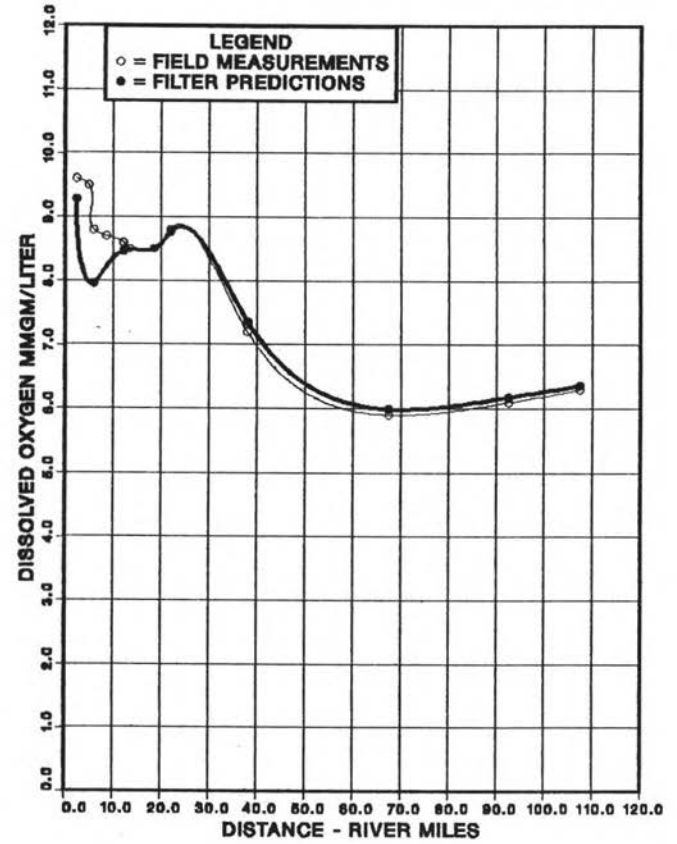
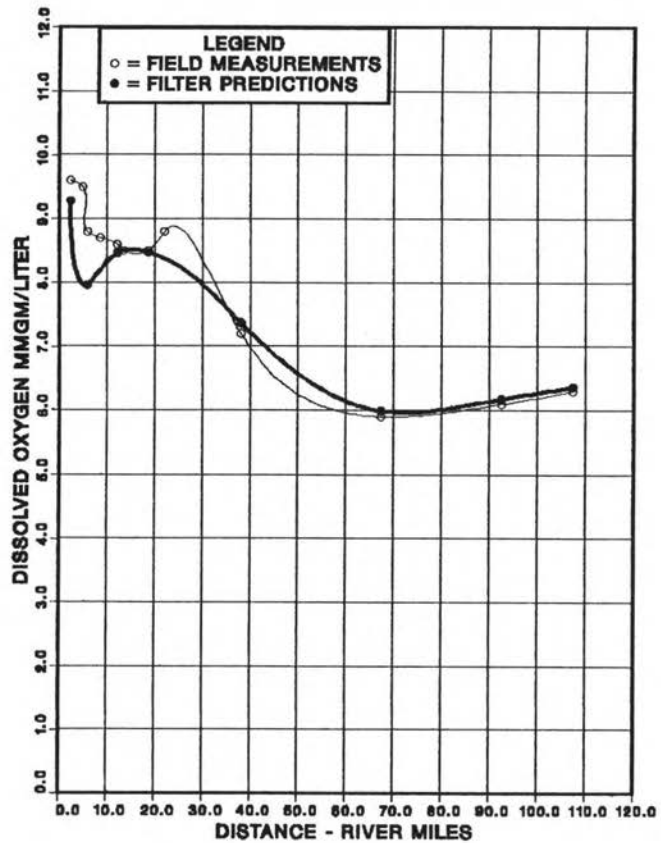


Figure 5.7. Field Measurements and Filter Predictions; 10 Segments and 9 Segments.

DISSOLVED OXYGEN ALONG ESTUARY



DISSOLVED OXYGEN ALONG ESTUARY

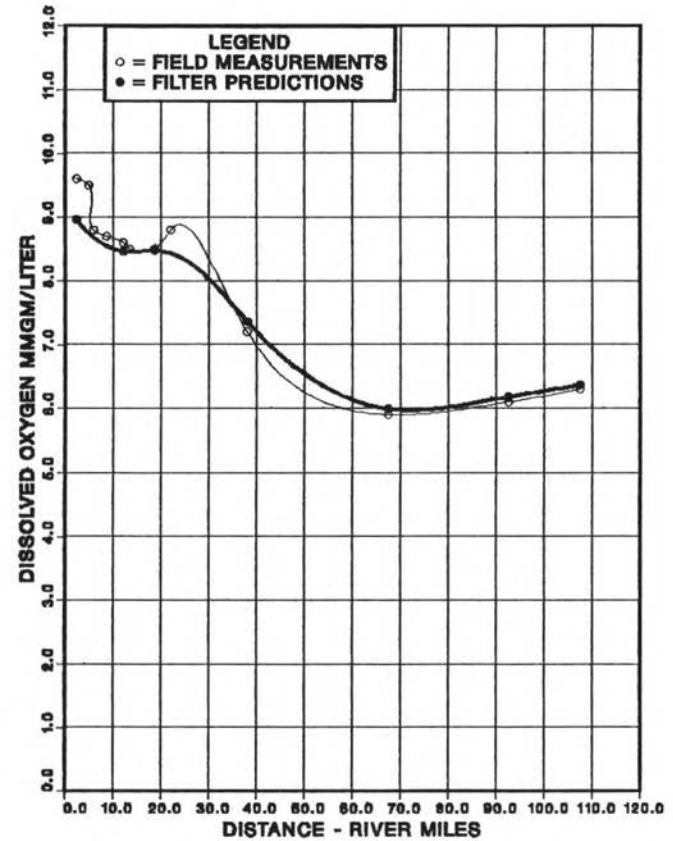
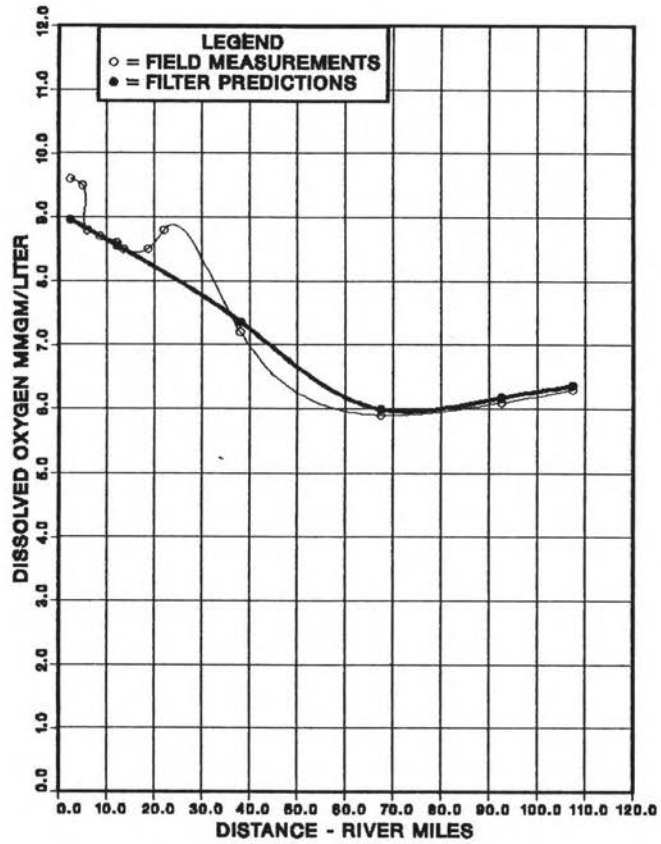


Figure 5-8. Field Measurements and Filter Prediction; 8 Segments and 7 Segments.

DISSOLVED OXYGEN ALONG ESTUARY



DISSOLVED OXYGEN ALONG ESTUARY

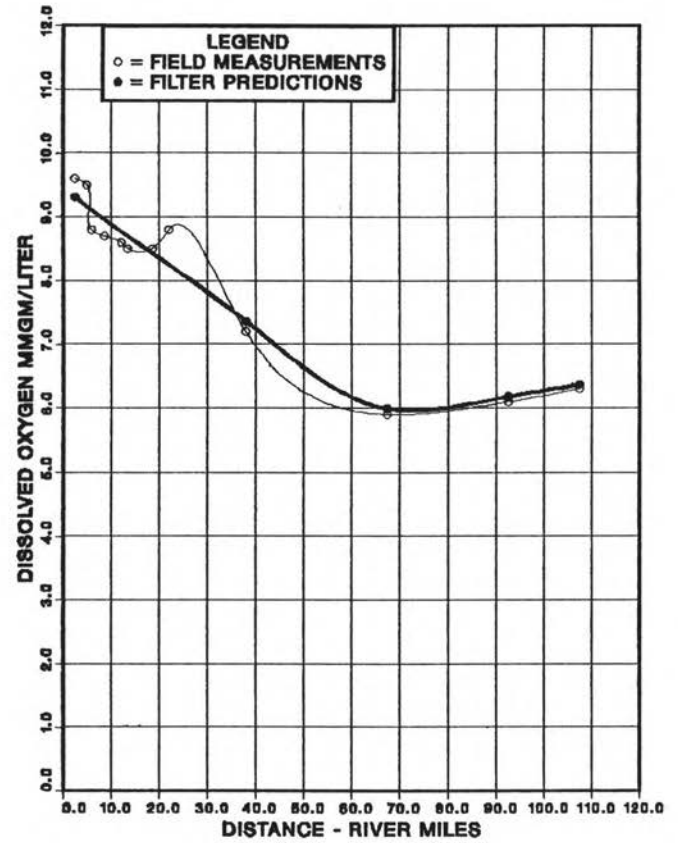
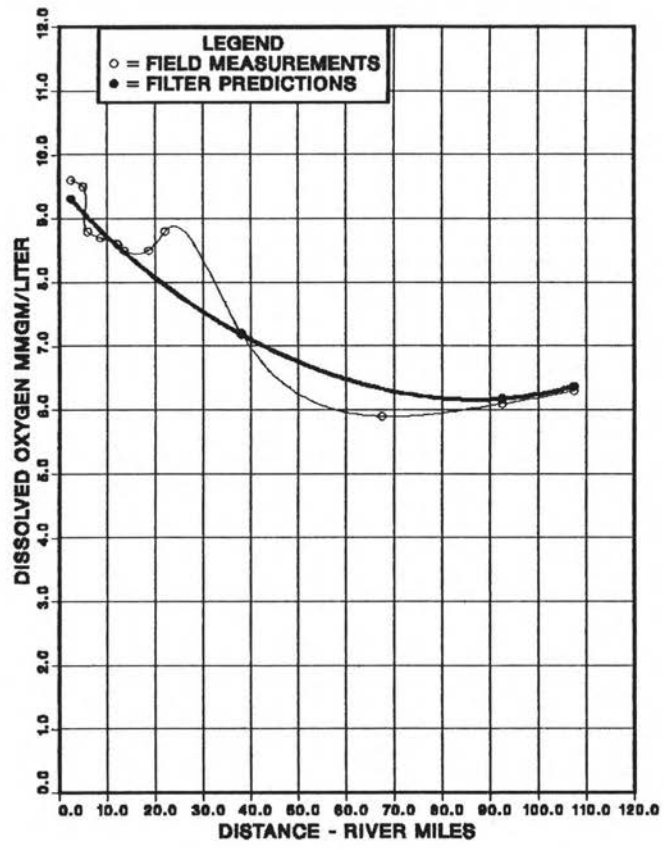


Figure 5.9. Field Measurements and Filter Prediction; 6 Segments and 5 Segments.

DISSOLVED OXYGEN ALONG ESTUARY



DISSOLVED OXYGEN ALONG ESTUARY

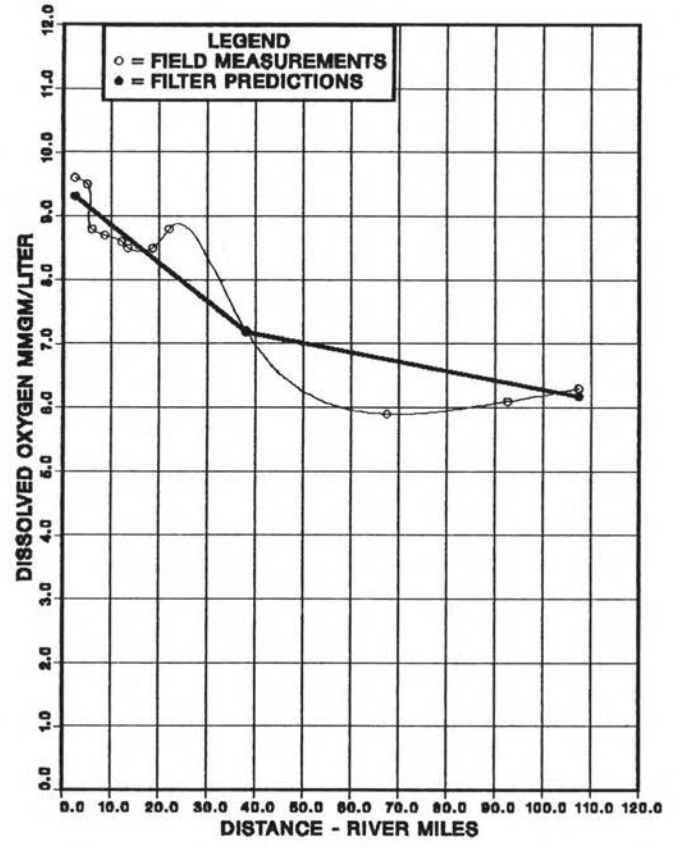


Figure 5.10. Field Measurements and Filter Prediction; 4 Segments and 3 Segments.

DISSOLVED OXYGEN ALONG ESTUARY

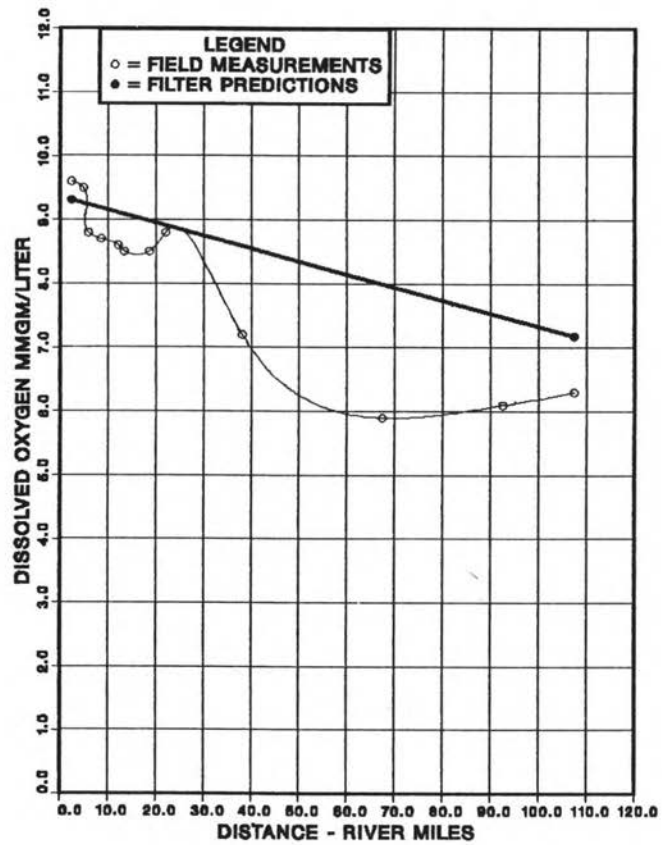
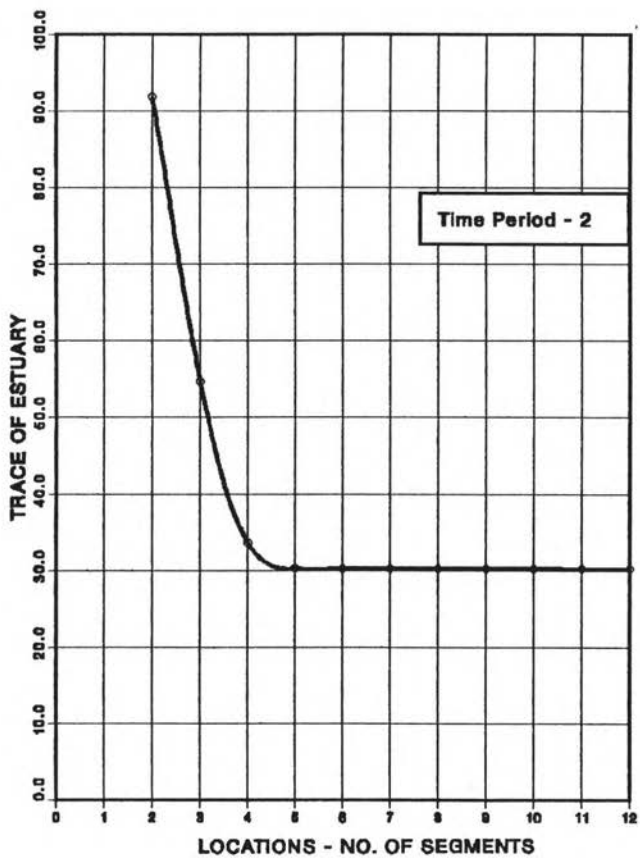


Figure 5.11. Field Measurements and Filter Prediction; 2 Segments.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

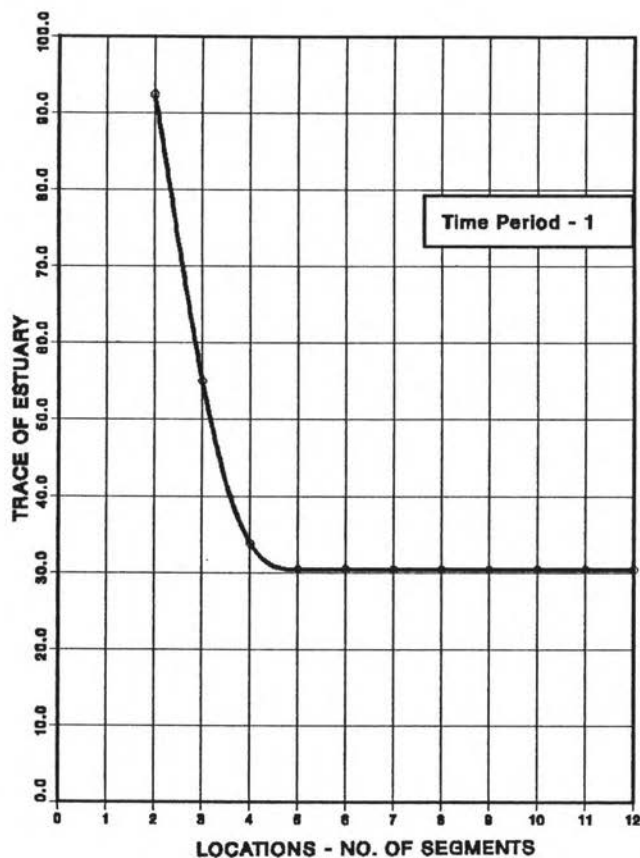
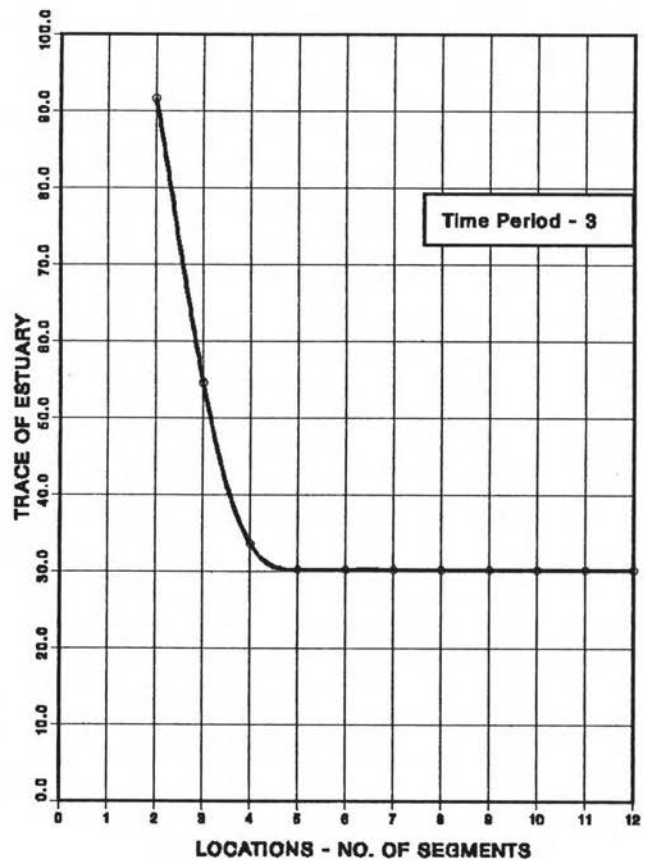


Figure 5.12. Trace of Estuary vs. Locations, Time Periods 1 and 2.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

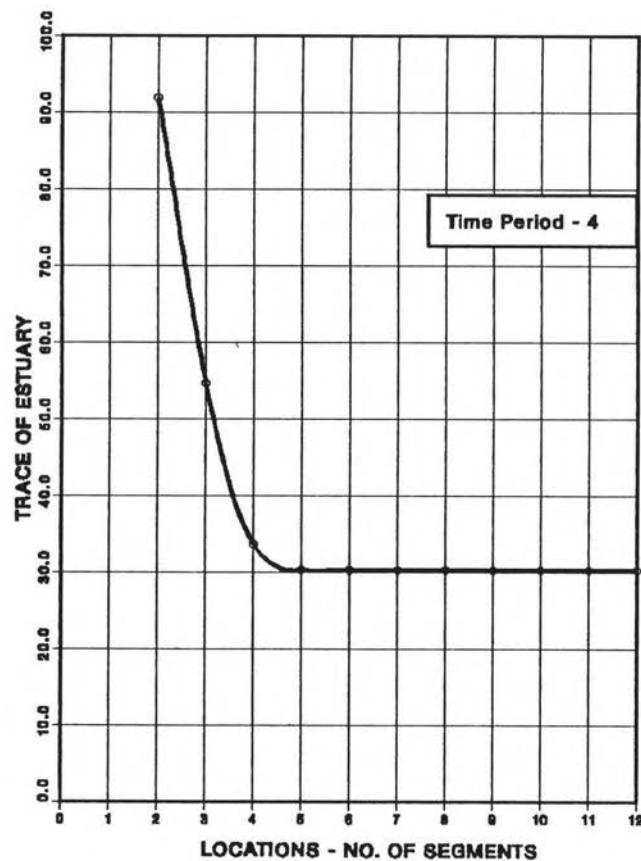
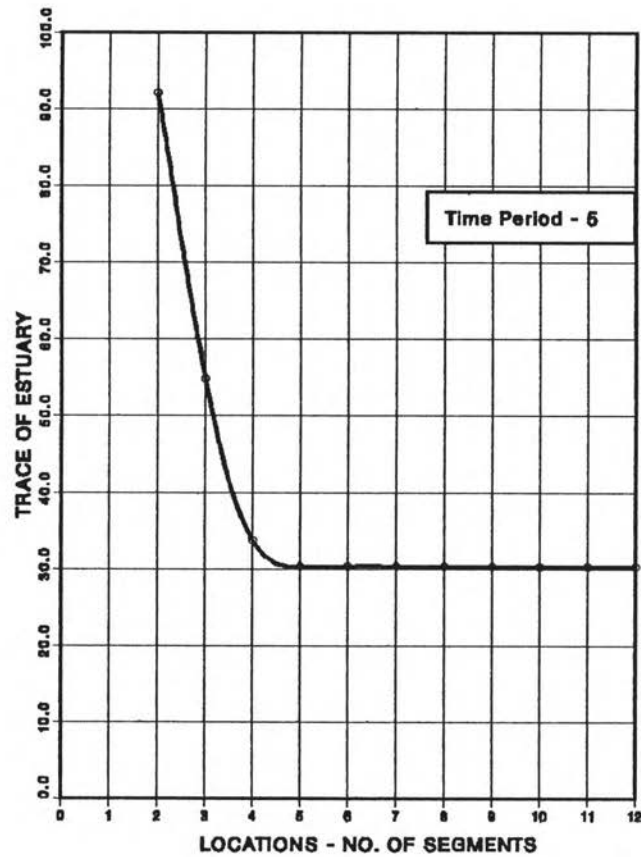


Figure 5.13. Trace of Estuary vs. Locations, Time Periods 3 and 4.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

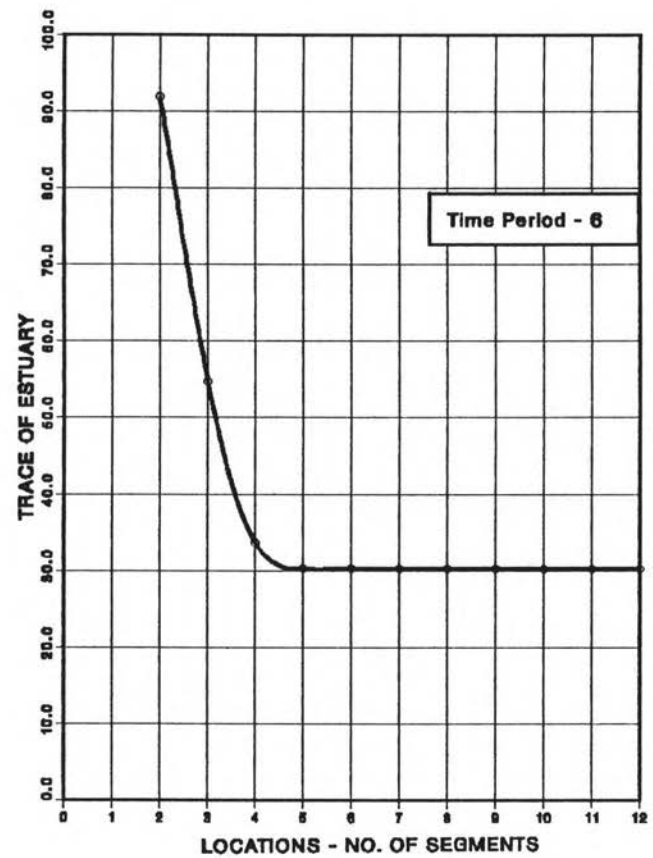
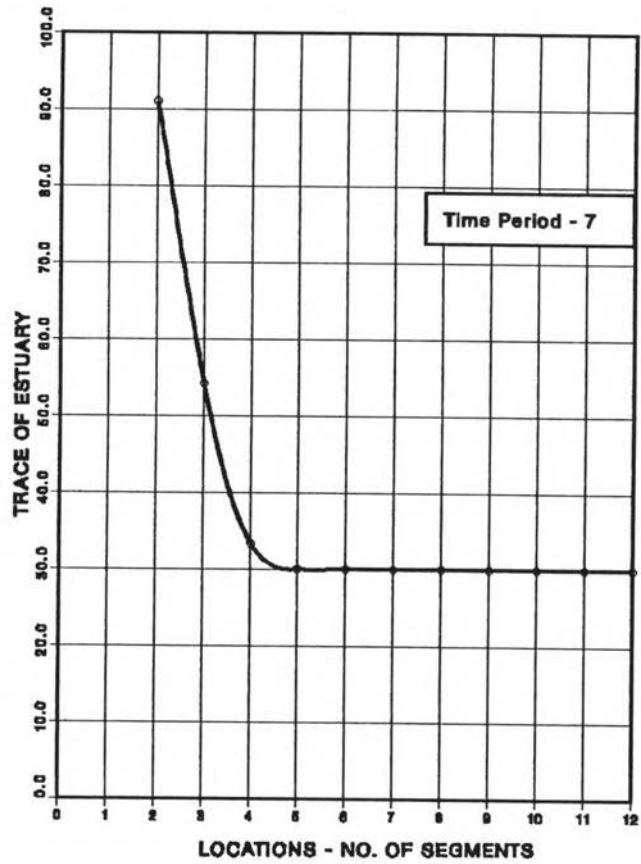


Figure 5.14. Trace of Estuary vs. Locations, Time Periods 5 and 6.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

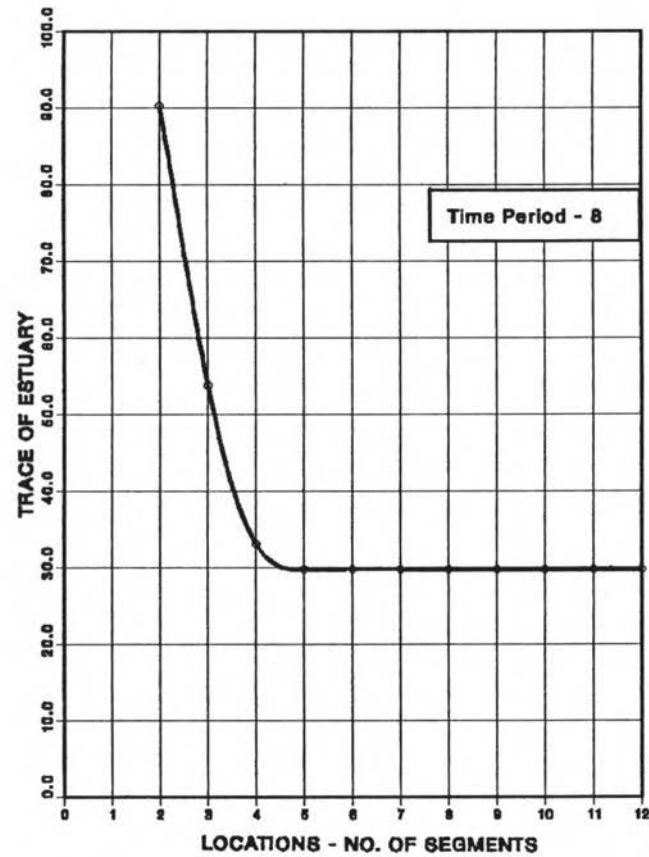
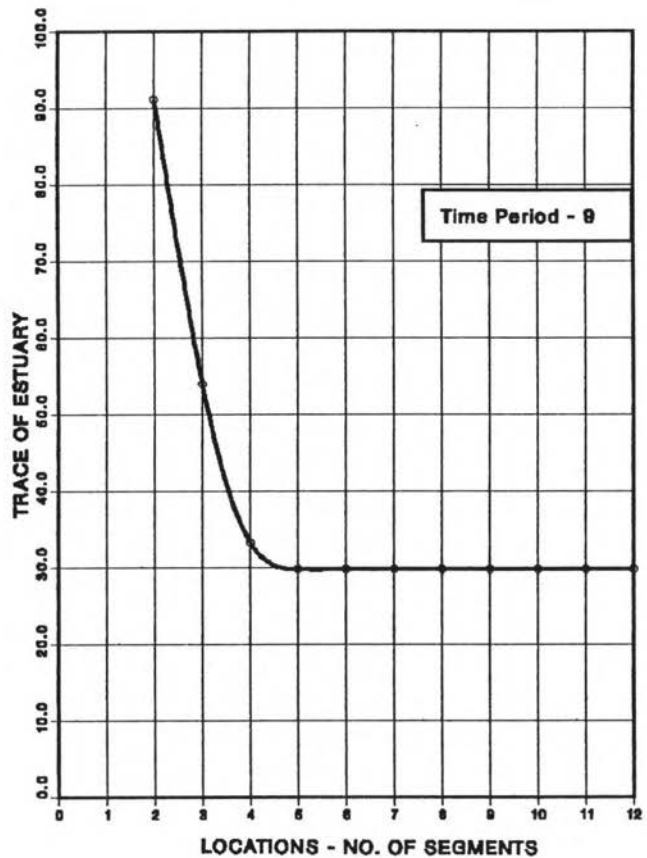


Figure 5.15. Trace of Estuary vs. Locations, Time Periods 7 and 8.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

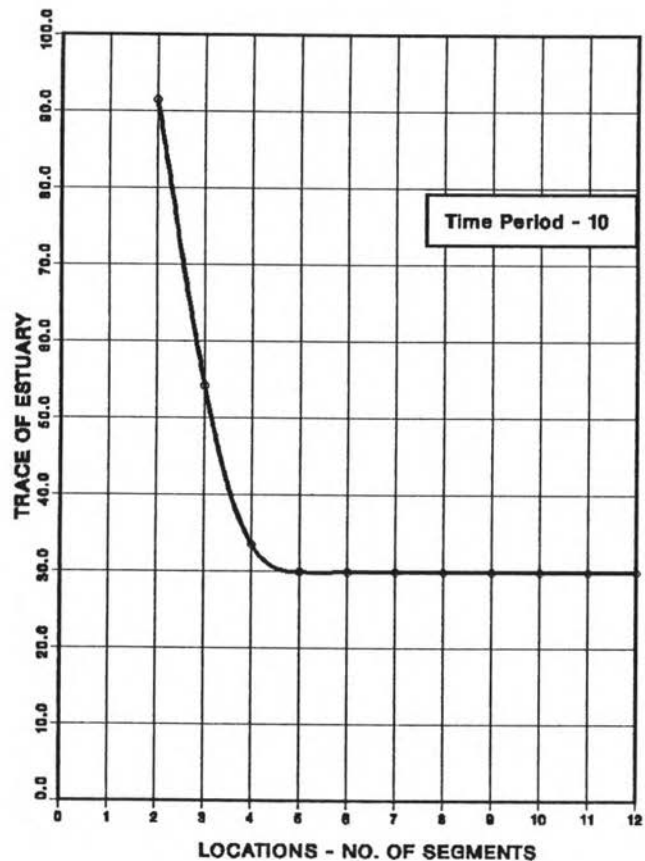
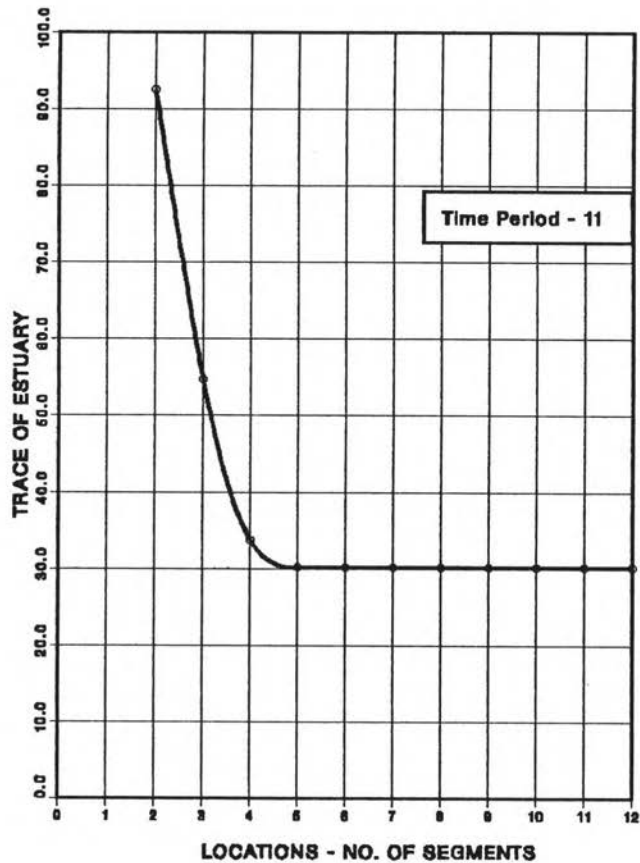


Figure 5.16. Trace of Estuary vs. Locations, Time Periods 9 and 10.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

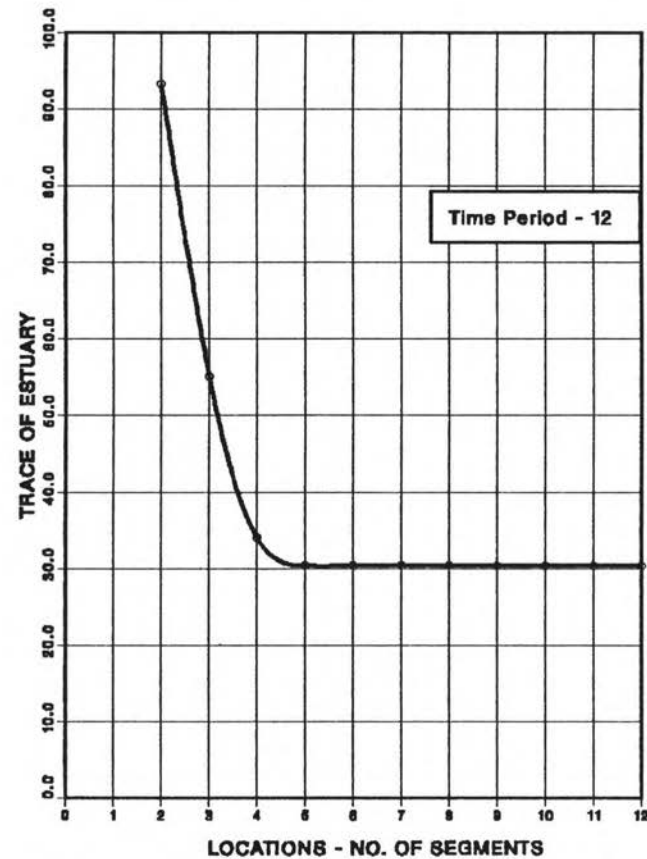
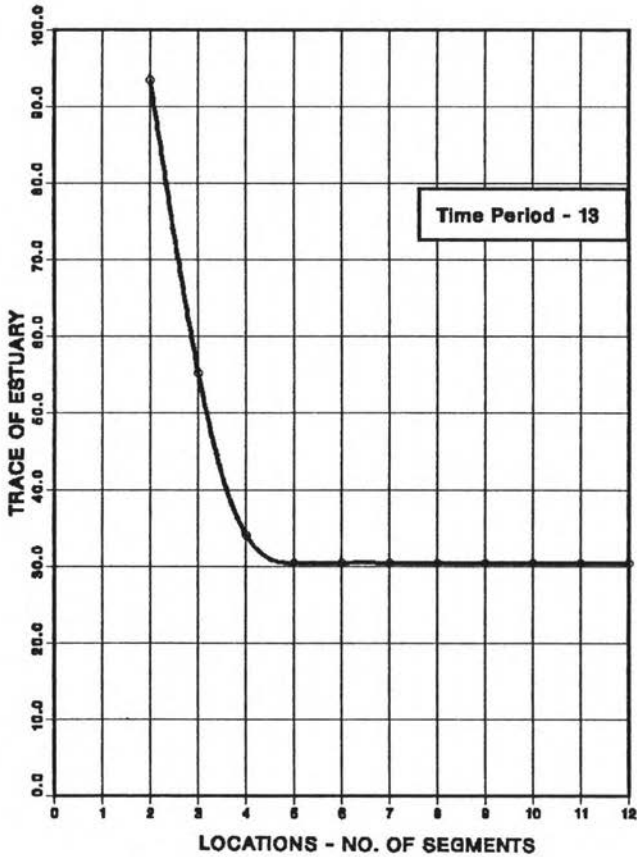


Figure 5.17. Trace of Estuary vs. Locations, Time Periods 11 and 12.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

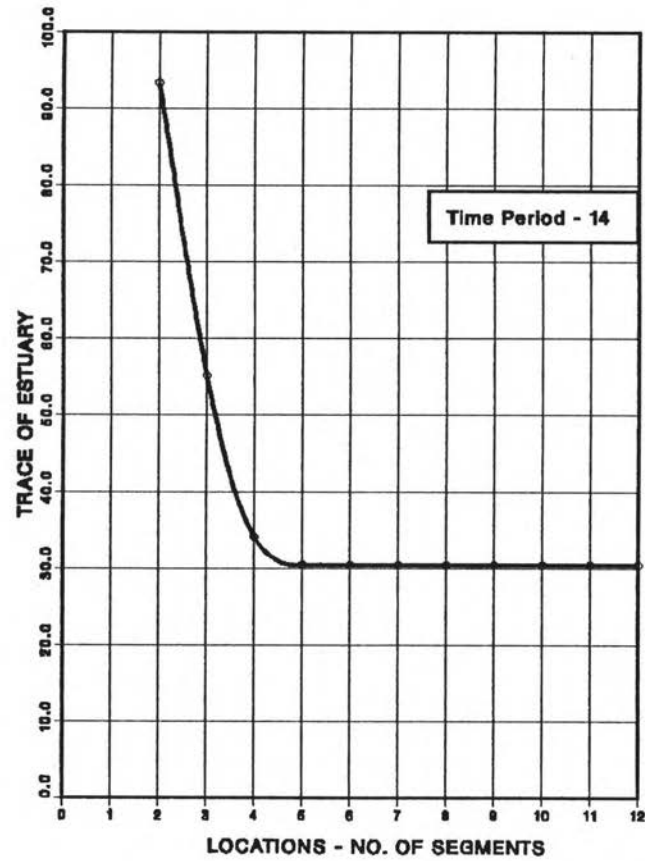
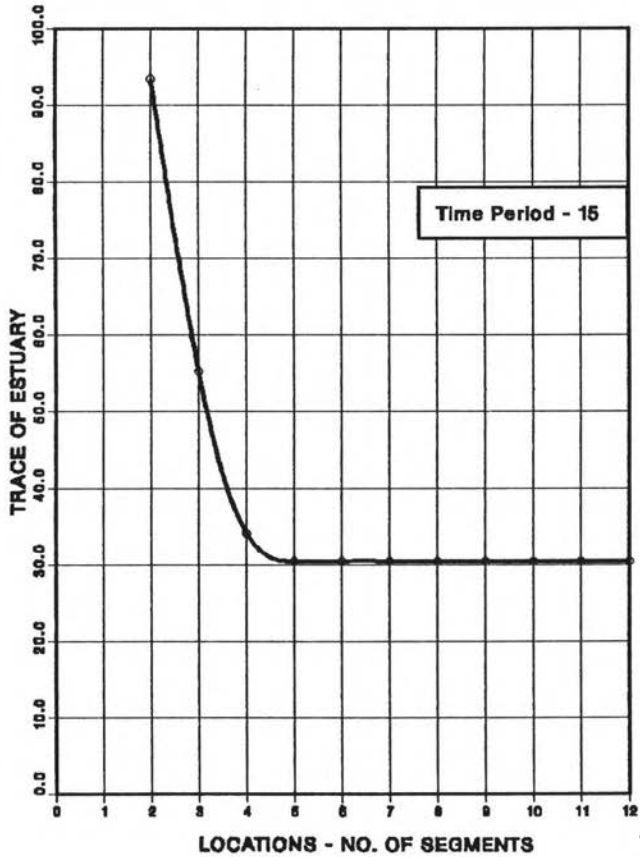


Figure 5.18. Trace of Estuary vs. Locations, Time Periods 13 and 14.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

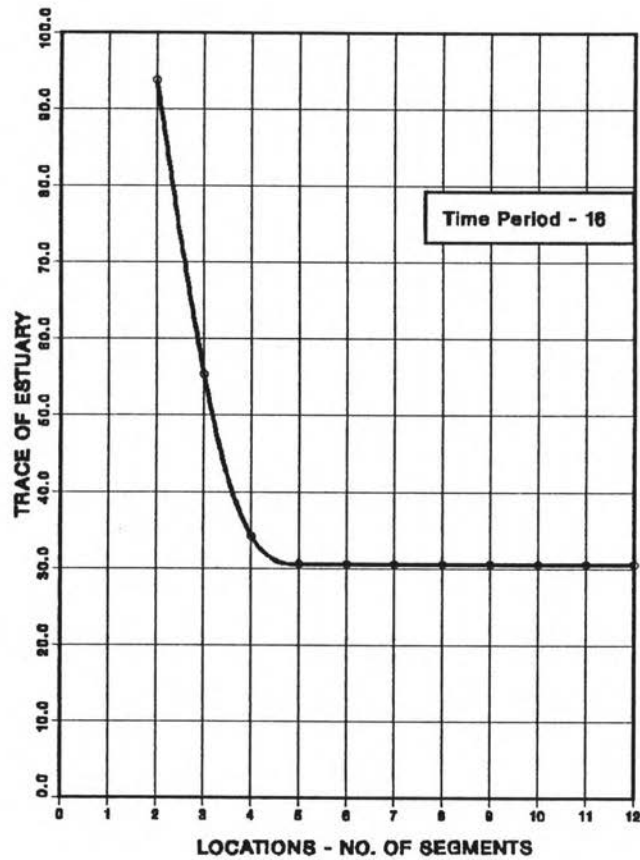
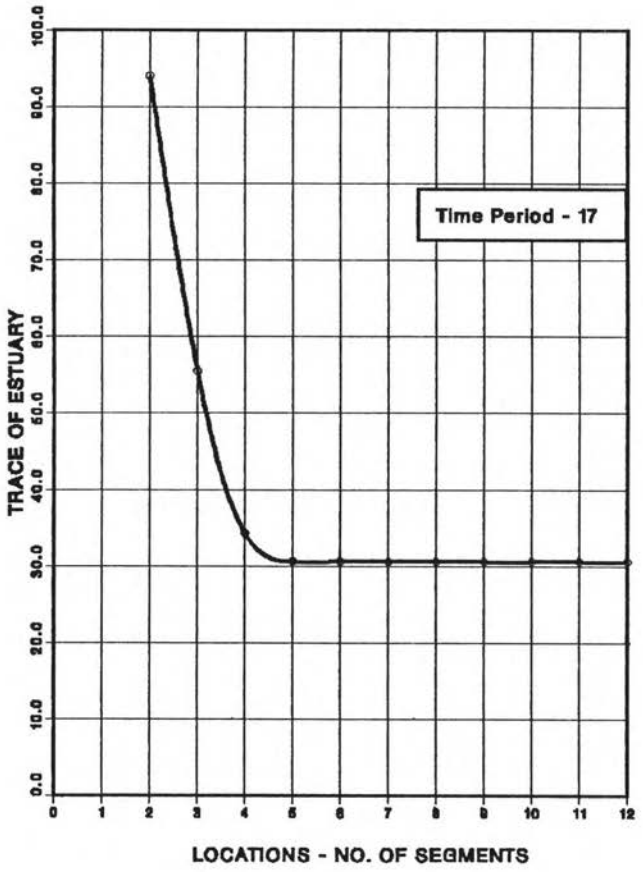


Figure 5.19. Trace of Estuary vs. Locations, Time Periods 15 and 16.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

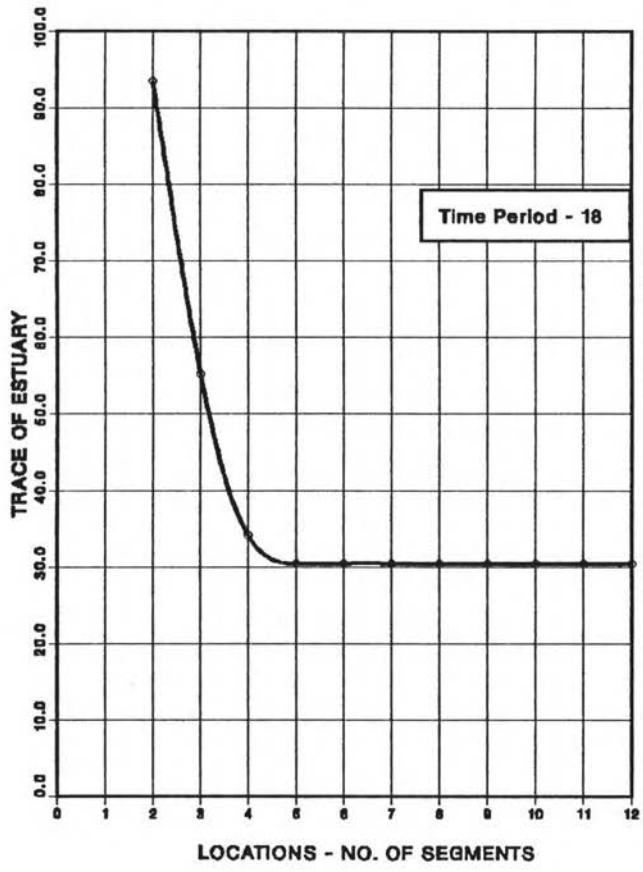


Figure 5.20. Trace of Estuary vs. Locations, Time Periods 17 and 18.

However, Table 5.3 contains one set of values for the period (time period - 1) June 1982. The graph is almost flat until a certain reduction in the sampling locations and rises steeply with further reduction.

Table 5.3. Trace of Estuary and No. of Locations.

Number of Locations	Trace of Estuary (TOE) kg ² x10 ¹²
12	30.476714
11	30.476977
10	30.477838
9	30.478725
8	30.484498
7	30.486882
6	30.496803
5	30.518948
4	33.939778
3	55.029178
2	92.497978

5.4 Summary

This chapter illustrated the study area, the Potomac estuary. The results from the Completely Stirred Tank Reactor (CSTR) model and the Kalman filter predictions were presented. In Chapter 6, the assumptions in the research and the interpretation of the results are explained.

CHAPTER 6

DISCUSSION

6.1 Introduction

Assumptions and justifications were made; various approaches were selected; theories were developed; and results were presented in the earlier chapters. The focus of this chapter is to discuss the choices, the assumptions and approximations made, the results, and why such choices, assumptions and approximations were made. This is achieved by dividing the chapter into three sections: answering criticism from the scientific community, the water quality model predictions and the outcome of using the Kalman filter algorithm.

6.2. Criticism by the Scientific Community

This type of management research is often criticized in the scientific community [1] because:

- (i) Paucity of data base that cannot reveal diurnal variations or local hot spots which dynamic models could predict.
- (ii) Not following the basic sequence of designing a monitoring system; identifying network objectives, transforming these to technical objectives and then selecting the solution algorithm.
- (iii) Difficulties in estimating the error-covariance matrices to be used in the Kalman Filter algorithm.

- (iv) Model predictions being affected by the values assigned for the kinetic coefficients.

The above comments are a summary of the reviews that were received when this proposal was submitted to the National Science Foundation for possible funding.

In attempting to answer these criticisms the following points are made:

- (a) The aim of the research is to verify the basic hypothesis of 'designing a monitoring system for an estuary using a water quality model.' The concept must give acceptable results from a coarse data set, before one can embark on collecting a finer data set. Hence, paucity of data base is not a major concern.
- (b) The method is not applicable where a monitoring system does not exist. As a network already exists, the technical objective is to determine the number of monitoring locations using a water quality model. Kalman filter algorithm is the solution technique used to achieve the technical objective. Therefore, this follows a logical sequence.
- (c) It is difficult to estimate the error-covariance matrices to be used in the filter algorithm. However, an approach to estimate the model error is discussed later on. In whatever scientific discipline researchers are, some assumptions have to be made based on ones own judgement. Structural engineering which is considered a highly developed discipline, people work in well defined boundaries. Even in such a case structural engineers do make assumptions and approximations in the analysis of structures. There is no reason why scientists in environmental engineering

should not make prudent assumptions and approximations when necessary.

- (d) The implications in assigning values to kinetic coefficients are critiqued later on and no comments will be made here.

6.3 Water Quality Model

6.3.1 Why Wasn't an Existing Model Used?

The literature revealed that hundreds of models were developed during the past three decades. If this is so, then the logical question is, why wasn't an existing model used?

The major agency that distributes and maintains models and user manuals for water quality models is the U. S. Environmental Protection Agency. If one does not have the means of accessing the "Bulletin Board System" maintained by the EPA, it will take several weeks or even several months before obtaining the model and the user's manual. The duration will also depend on whether the agency is revising the model at the time of request. A delay of 3-6 months can be experienced.

Once you obtain the model, a certain time period has to be spent on understanding, installing and testing the model. This will depend on the size and clarity of the manual, the previous knowledge of the user, and errors that may appear in the user's manual. The errors can be rectified only by contacting the agency. One should also collect data that would be appropriate for input for the model. Having passed this stage, you execute the program and obtain results which are meaningless; for example the velocity of water, as 80 m/sec. Although the agency will request you to send the data to them for analysis, one may not get a reply at all.

In fairness to the agency, it may have only a limited number of staff trying to perform the following functions all at the same time.

- Distribute the model
- Try to answer users' queries
- Correct codes for errors, mistakes, etc.
- Modify programs for user friendliness
- Incorporate the latest developments in computer science
- Develop manuals for use

The agency's budget may be limited. However, if the users' queries are not answered, the models developed by the agency will not be used. Further, as the agency is not a private enterprise, customer satisfaction may not be on their agenda.

The above comments are the result of using the Water Quality Analysis and Simulation Program (WASP4) that was developed by the US EPA [2]. This is a computer program which can simulate the hydrodynamics and predict the quality of the water body. As an estuary is always in a dynamic state it was felt that this program could be used as the model to simulate water quality kinetics. However, when the program was installed and executed the program's output of velocities was nearly 10-20 times that observed in the nature. Inquiry from the EPA office in Athens, Georgia, indicated that the subroutine DYNHYD4, which simulates the hydrodynamics of the estuary is being revised to correct errors. Hence, further use of this program in the research was discontinued.

Obtaining an existing model is like buying a machine or equipment for which no servicing or maintenance is available. It may be worth while in the long run to develop a simple model that is appropriate for

the task at hand. As the aim was to design a monitoring system for an estuary, a model appropriate for this purpose was developed. Hence, the reason for the development of a completely stirred tank reactor (CSTR) model, which adapted several basic concepts from WASP4.

6.3.2 Completely Stirred Tank Reactor (CSTR) Model

Once you decide to develop a model, what kind of a model do you develop? A simple one or a complex one? "Different types of models are appropriate for solving different kinds of problems; there is no universal model for solving all manner of problems; comprehensiveness and complexity in a simulation are no longer equated with accuracy; and there is a healthy mood of critical questioning of the validity and credibility of water quality models" [3]. Therefore, a simple CSTR model was developed.

Is it reasonable to assume a CSTR model? In Table 6.1, dissolved oxygen concentration values are tabulated for the months of May and June for a stretch of 6.5 miles in the study area of the Potomac estuary. The table also gives the location of stations, and the depths at which the measurements were taken. The values in the table give some justification for our assumption of a completely mixed reactor. These were extracted from reference [4].

Even as recent as 1985, simple box models have been used for studying transport in the Puget Sound [5]. The characteristics of the Potomac estuary, a residence time of 85 days [6], the to and fro motion due to high and low tides, circulation etc., justify the development of the CSTR model. Further, the aim of the research was to use the physical understanding of the system as reflected by the models to

Table 6.1. DO Concentration (mg/ℓ) in the Potomac Reach
12.1 - 18.5 miles; May and June 1986.

Month	Station	PMS-44	PMS-46	PMS-48	PMS-51	XFB-2470
	Distance (miles)	12.1	12.6	13.1	13.6	18.5
May	Depth (m)					
	0.1	5.9	---	---	---	6.0
	1.0	5.5	---	---	---	---
	2.0	5.5	---	---	---	---
	3.0	5.4	---	---	---	---
	4.0	5.6	---	---	---	5.8
June	0.1	7.9	7.3	7.7	7.2	6.2
	1.0	7.7	---	---	7.3	---
	2.0	7.7	---	---	7.2	---
	3.0	7.7	---	---	6.9	---
	4.0	7.3	---	---	7.0	4.7

design a water quality monitoring program. The simplest assumptions were made to develop the CSTR model. Dispersive flow at boundaries of segments were ignored. Atmospheric reaeration and biochemical decay were the only factors considered in the oxygen budget.

The effects of some of these assumptions were reflected in the model results. On some occasions the DO concentration in segment 4 was zero. This was due to several reasons: the model assumption that there was no dispersive flow between segment boundaries; applying the Blue Plains waste water treatment plant BOD ultimate load of, 25870 kg/day into segment 4; and the volume of the segment 13.37 Mm^3 (time period 3) [7]. Neither did the model take into account the replenishment of DO due to photosynthesis, nor did it take into account the depletion of DO due to benthic and sediment oxygen demand. The complex model WASP4 [2] can handle 8 factors that contribute to the oxygen budget. However, the influence of salinity and temperature on

the saturation value of DO was considered and taken into account. The segments 10, 11 and 12 were considered saline, and corrections were made. However, corrections for change in atmospheric pressure were not made.

When segments were combined and the number of sampling locations were reduced, the DO concentration did not reduce to zero in any of the segments. This was due to the biochemical oxygen demand being met by a larger volume of water.

6.3.3 Parameters Used in the Model

Parameters are constants incorporated in the model. The CSTR model embodied two parameters, reaeration rate coefficient (k_2) and biochemical decay rate (k_d). The values assigned to these parameters will affect the model predictions. The implications in assigning values to these parameters, and the method of determining the values for these constants are described in the following pages. For the present discussion, the determination of k_2 , the reaeration rate coefficient, is analyzed.

"Very little original research on estuarine reaeration has been completed to date... reaeration formulas are most applicable for which they are developed and outside that range, errors might be quite large" [8]. A value of 0.05/day was assumed for the Potomac estuary based on depth using Covar's method [8].

If a model off the shelf, say WASP4 is used [2], the reaeration rate k_2 is determined using the Covar's method. However, Covar's method is a compilation of equations developed by O'Connor-Dobbins, Churchill et al., and Owens et al. These equations expressed to the base 'e', at 20°C are as follows.

$$\text{O'Connor-Dobbins} \quad k_2 = 12.9 V^{0.50} D^{-1.50} \quad \text{Eqn. (6.1)}$$

$$\text{Churchill et al.} \quad k_2 = 11.7 V^{0.97} D^{-1.67} \quad \text{Eqn. (6.2)}$$

$$\text{Owens et al.} \quad k_2 = 21.7 V^{0.67} D^{-1.85} \quad \text{Eqn. (6.3)}$$

Depending on the depth and velocity, WASP4, will use the appropriate equation. But, the water in an estuary is nearly stagnant. Can these equations be used?

What did the scientists who developed these equations say?

- O'Connor-Dobbins [9]

$$k_2 = 12.9 V^{0.5} D^{-1.50} \quad \text{Eqn. (6.1)}$$

O'Connor-Dobbins considered two types of turbulence, isotropic and non isotropic. For isotropic turbulence

$$k_2 = \frac{(D_L U)^{1/2}}{2.31 H^{3/2}} \quad \text{Eqn. (6.4)}$$

and for non isotropic turbulence

$$k_2 = \frac{480 D_L^{1/2} S^{1/4}}{H^{5/4}} \quad \text{Eqn. (6.5)}$$

were developed, and

U : velocity

H : depth

S : slope of the river channel

D_L : coefficient of molecular diffusion (diffusivity)

In contributing a discussion to this paper, Camp, expressed the slope of the hydraulic grade line in terms of mean velocity, U and Chezy's coefficient, C. He expressed Equation (6.5) as,

$$k_2 = 480 \frac{D_L^{1/2} U^{1/2}}{C^{1/2} H^{3/2}} \quad \text{Eqn. (6.6)}$$

which is similar to Equation (6.4). Hence, the development of Equation (6.1).

However, except under uniform flow conditions, the slope of the hydraulic grade line is not equal to the slope of the river channel. Then in Equation (6.6), k_2 incorporates two more parameters, the Chezy coefficient 'C' and diffusivity D_L . In trying to develop a formula for k_2 , two more parameters have been included, diffusivity and Chezy's coefficient.

- Churchill et al. [10]

$$k_2 = 11.7 V^{0.97} D^{-1.67} \quad \text{Eqn. (6.2)}$$

The authors expressed the following limitations in the use of this equation.

- (i) The equation is not applicable to turbulent reaches where air bubbles are entrained.
- (ii) It is not applicable where vertical stratification occurs.
- (iii) It is applicable only for clean waters and has to be adjusted for polluted waters.
- (iv) Photosynthesis is not included.

How many model users are aware of these limitations?, and what is the definition of clean waters?

- Owens et al. [11]

$$k_2 = 21.7 V^{0.67} D^{-1.85} \quad \text{Eqn. (6.3)}$$

The above equation, developed by Owens et al., was based on data obtained by Churchill et al., Gameson et al., and Owens et al. The equation is limited to water velocities of 0.1 - 5.0 ft/sec, and depths of 0.4 - 11.0 ft. However, the model WASP4 selects Owens et al. formula if the depth is less than 2 ft., and either O'Connor-Dobbins or, Churchill et al. formula, if the depth is greater than 2 ft. It should be noted that Owens et al. equation was based on a regression analysis of data obtained by Churchill et al. too.

Summarizing,

- (i) O'Connor-Dobbins equation for k_2 incorporates two more parameters, diffusivity D_L , and Chezy coefficient, C .
- (ii) There are limitations in using Churchill et al. equation for k_2 .
- (iii) Owens et al., formula for k_2 incorporates data obtained by Churchill et al., too.

Mind you that all these comments are for one parameter, reaeration rate coefficient, k_2 . If we had incorporated other factors in the oxygen budget, the number of parameters would have increased; the model would have become more complex; and the uncertainty in model prediction would have increased. The uncertainty in using water quality models is reviewed in an excellent paper by Beck [12] and he explains the implications in increasing the number of parameters. How many model users have the time and desire to review original sources to understand and verify the intended use of the equations; especially, those developed for the parameters?, is a logical question that arises in the mind of the author.

6.3.4 Unsteady hydrodynamics of the estuary

The CSTR model is deficient in an important aspect of not taking into account the hydrodynamics of the estuary. The mean high water predictions calculated from the tide tables together with depths obtained from Nautical Chart 12285, were used to obtain the volume of a segment. In reality this volume is never constant for a month, and changes with time. A hydrodynamics model which takes into account the estuarine flows can be developed, which will predict instantaneous volumes. These values of the volumes of segments can then be used as input to the CSTR model for water quality determination. As our primary aim was attempting to design a monitoring system for an estuary using the physical understanding of the system, developing a hydrodynamic model was beyond our scope.

The reasons for not using an existing model was described. The development of a simple CSTR model, and the implications in using equations for evaluating parameters that appear in model equations were then analyzed. Model predictions, and the peculiarity in some results were also stated. The deficiency of the CSTR model of not incorporating the hydrodynamics of the estuary was commented. The next section portrays the assumptions involved in using the Kalman filter algorithm and the predictions from this approach.

6.4 Kalman Filter Algorithm and Predictions

6.4.1 Assumptions in the Filter

In order to use the algorithm certain assumptions have to be made. They are,

- Initial state of the system.
- Error associated with this estimate of the initial state.

- Error-covariance structure of the model predictions.
- Error-covariance structure of the measurements.

As field measurements were available for the month of May 1982, they were taken as representing the initial state of the system. Variances of $2 \text{ mg}^2/\ell^2$ and $4 \text{ mg}^2/\ell^2$ were assumed for field measurements and initial state of the system, respectively. As the model did not incorporate all of the factors that affect DO, a larger variance of $24 \text{ mg}^2/\ell^2$ was assumed. As measurements are more accurate than the model predictions a smaller value for measurements is appropriate. However, it is felt that the model error can be scientifically calculated.

The final step in the development of a model is model validation. At this step, the model prediction can be compared with the field measurements, and the mean squared error for the entire estuary can be calculated. This value can be used as the model prediction error. But, as model development was not the aim, this step was not done. In reality, this can be done.

How do we evaluate the error covariance of measurements? As sampling and laboratory technology develops the error associated with field measurements will become smaller and smaller. A reasonable value can be assumed, based on the user's experience. Measurement error is not only due to instruments, but also due to several other factors such as, recording the measurements incorrectly and, using a wrong method. In all the scientific disciplines, at some stage or other, judgement comes into play, and assumptions are made. There is nothing wrong in making assumptions or assuming values for certain variables; the important fact is to be aware of such assumptions.

6.4.2. Field Measurements and Filter Prediction

A check on whether the filter algorithm behaves properly can be done as follows. Let us consider only one segment, so that the 'j' subscript used in section 4.2.4 can be omitted.

As shown in the appendix, the weighting factor, Kalman gain, is given by

$$k_{t + \Delta t} = \frac{\sigma_{t(+)}^2 + \sigma_{\text{model}}^2}{\sigma_{t(+)}^2 + \sigma_{\text{model}}^2 + \sigma_{\text{measurement}}^2} \quad \text{Eqn. (6.7)}$$

Predicted variance is given by

$$\sigma_{t + \Delta t(+)}^2 = [1 - k_{t + \Delta t}] [\sigma_{t(+)}^2 + \sigma_{\text{model}}^2] \quad \text{Eqn. (6.8)}$$

The expression 6.7 indicates two major facts; the weighting factor k is always less than unity, and that when the measurement noise is small relative to model error $k \rightarrow 1.0$ and when it is large, k is small. This was tested by using three different values of σ_{model}^2 , keeping $\sigma_{\text{measurement}}^2$ constant. The results are as follows:

$\sigma_{\text{measurement}}^2$	σ_{model}^2	k
2	24	0.93
2	12	0.87
2	2	0.61

This confirms the fact that the algorithm works correctly.

The graphs of field measurements for 12 locations, and the filter predictions as the number of segments are reduced show excellently how the algorithm works. Even with a simple model, by combining the field observations with the predictive model, one is able to track the DO variation effectively as indicated in Figure 5.8 when only seven segments are used. The filter tracks efficiently until a reduction of

five segments. However, when sampling locations are further reduced, the estuary is not well represented.

6.4.3 The Variation of Trace (TOE) with the Number of Sampling Locations

For the initial assumptions, the variation of the predicted variance of DO for the entire estuary (TOE) with the number of locations show a clear, distinct fact.

The graph is flat until you reduce the number of locations from 12 to 5. However, when the number of locations are reduced still further, the slope changes dramatically, and becomes very steep. In this particular case we should not reduce the sampling locations to any number less than five.

An explanation for this behavior is appropriate. In Chapter 4, the fundamental assumption of "conservation of mass" was used to develop Equation (4.11), which recursively estimates the mass of dissolved oxygen in segment 'j'.

$$\left(M_j \right)_{t + \Delta t} = \left(M_j \right)_t + \left(r_j \right)_t + \left(\xi_j \right)_t$$

The error term ' ξ ' is also expressed in mass units, kilograms. The variance-covariance term will be having kilograms², as the units.

Then, the predicted variance for the 'j' th segment can be written as

$$\left(\sigma_j^2 \right)_{t + \Delta t} = \left[1 - \left(k_j \right)_{t + \Delta t} \right] \left[\left(\sigma_t^{2(+)} \right)_t + \sigma_j^2 \text{ model} \right]$$

from Equation (6.8) expressed in units of kilograms².

However, the initial state of the system and the model prediction are expressed as mg/ℓ , and the errors associated with these are usually specified in units of mg^2/ℓ^2 . In order to execute the Kalman filter algorithm they have to be expressed in mass units.

Let us consider five segments of volume $V_1, V_2, V_3, V_4,$ and V_5 liters. The initial values of DO are $C_1, C_2, C_3, C_4,$ and C_5 mg/ℓ respectively and the error is b^2 mg^2/ℓ^2 , assumed constant for all of the segments. For the purposes of discussion let us omit the contribution of model error to the predicted variance. Then Equation (6.8) can be written as

$$\left(\sigma_j^2\right)_{t+\Delta t}^{(+)} = A \left(\sigma_j^2(+)\right)_t \quad \text{Eqn. (5.9)}$$

where A is a constant.

The following table illustrates the values of TOE as the segments are reduced one by one

No of segments	at $t + \Delta t$, TOE (mg^2)
5	$A \left[V_1^2 + V_2^2 + V_3^2 + V_4^2 + V_5^2 \right] b^2$
4	$A \left[\left[V_1^2 + V_2^2 + V_3^2 + V_4^2 + V_5^2 \right] b^2 + 2V_1V_2b^2 \right]$
3	$A \left[\left[V_1^2 + V_2^2 + V_3^2 + V_4^2 + V_5^2 \right] b^2 + 2 \left[V_1V_2 + V_3V_4 \right] b^2 \right]$

where,

$$TOE = \sum_{j=1}^n A \left(\sigma_j^2\right)_t$$

n = number of segments

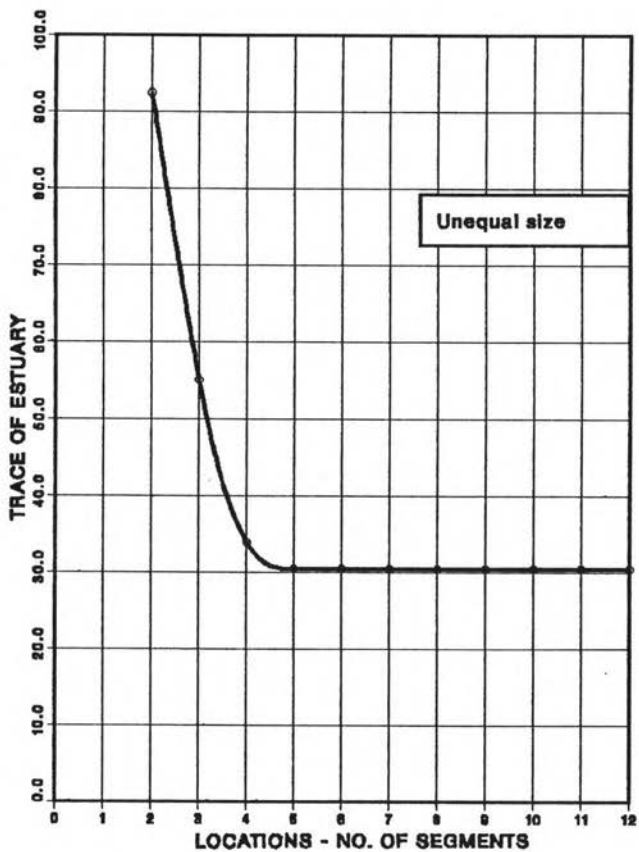
$$\sigma_j = V_j b \quad mg$$

The above formulation explains the reason for the increase in the predicted variance as the segments are combined, or as the sampling locations are reduced. The increase will depend on the sizes of segments, that is, the values of 'V'.

When volumes of segments are of the same order or magnitude, the change in TOE with the reduction in sampling locations is gradual. However, if they are not of the same order of magnitude, the change is dramatic. In our case study the volume of the first eight segments were of the same order of magnitude ($4.1-25 \text{ Mm}^3$), while the last four segments were of a different order of magnitude ($720-1700 \text{ Mm}^3$). Initially when we were analyzing the variation of TOE with the reduction in segments the smaller segments were combined. The variation of TOE was gradual. However, when we reached five segments for the estuary, further reduction could be achieved only by combining the larger segments. As we started combining the larger segments the variation of TOE was dramatic. This explains why the graph of TOE vs the number of locations is flat initially and rises sharply when larger segments are combined.

Figure 6.1 illustrates this fact clearly. The case where all 12 segments of differing magnitudes are used for the analysis is illustrated on the left hand side of Figure 6.1, a nearly horizontal line and a sharp increase of TOE. However, on the right hand side of Figure 6.1 the case where all the segments are of similar size is portrayed. This confirms our first hypothesis that the TOE increases with the reduction in the number of sampling locations. The physical representation of the segments is shown in Figure 6.2.

TRACE OF ESTUARY VS LOCATIONS



TRACE OF ESTUARY VS LOCATIONS

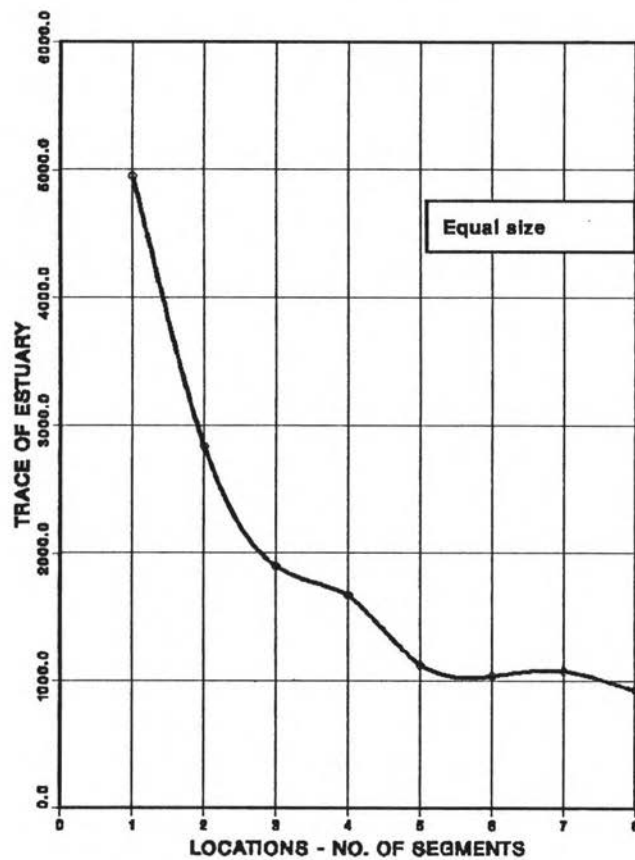


Figure 6.1. TOE vs. Locations. A Comparison of Similar Sized vs. Unequal Sized Segments.

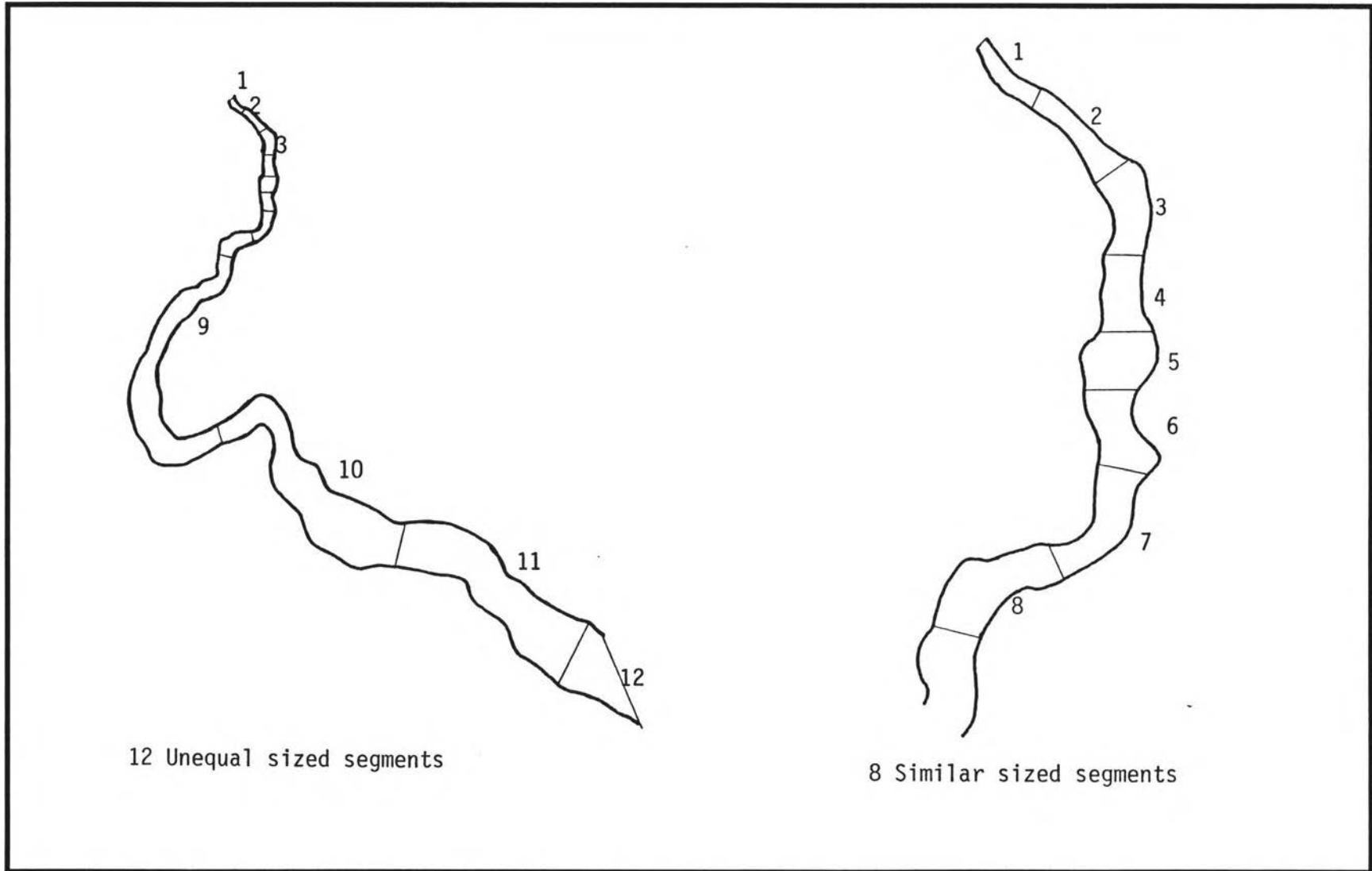


Figure 6.2. Physical Representation of Segments, Corresponding to Figure 6.1.

The results indicate that when TOE is used as a measure to determine the reduction of sampling locations, an acceptable TOE has to be defined where the sampling locations represent segments of nearly equal magnitude. However, when segments are of a different order of magnitude, the graph will indicate the maximum reduction. Or one could define an acceptable TOE as a percentage of the value of TOE if all the sampling locations were retained.

Further, at present statistical analysis of water quality data is performed without much attention being given to either the sizes of segments the stations represent or the processes that take place within the segment. In the present research we assumed that each segment was completely mixed. Such assumptions are generally not used in statistical analysis water quality data.

Therefore three major conclusions are:

- (1) Sampling locations must represent segments of equal or nearly equal size.
- (2) The processes that take place within each segment must be identical.
- (3) It is not prudent to statistically analyze data, which represent different sizes of segments.

A reduction in the values for model variance did not alter the shapes of the curves. However, the value for the TOE reduced. Figures 6.3 and 6.4 illustrate the case of TOE for different values of model variance. A further conclusion is that the shape of the variation of TOE is insensitive to model variance, depending on whether they are of similar size or unequal size segments. This is also portrayed in Figures 6.3 and 6.4.

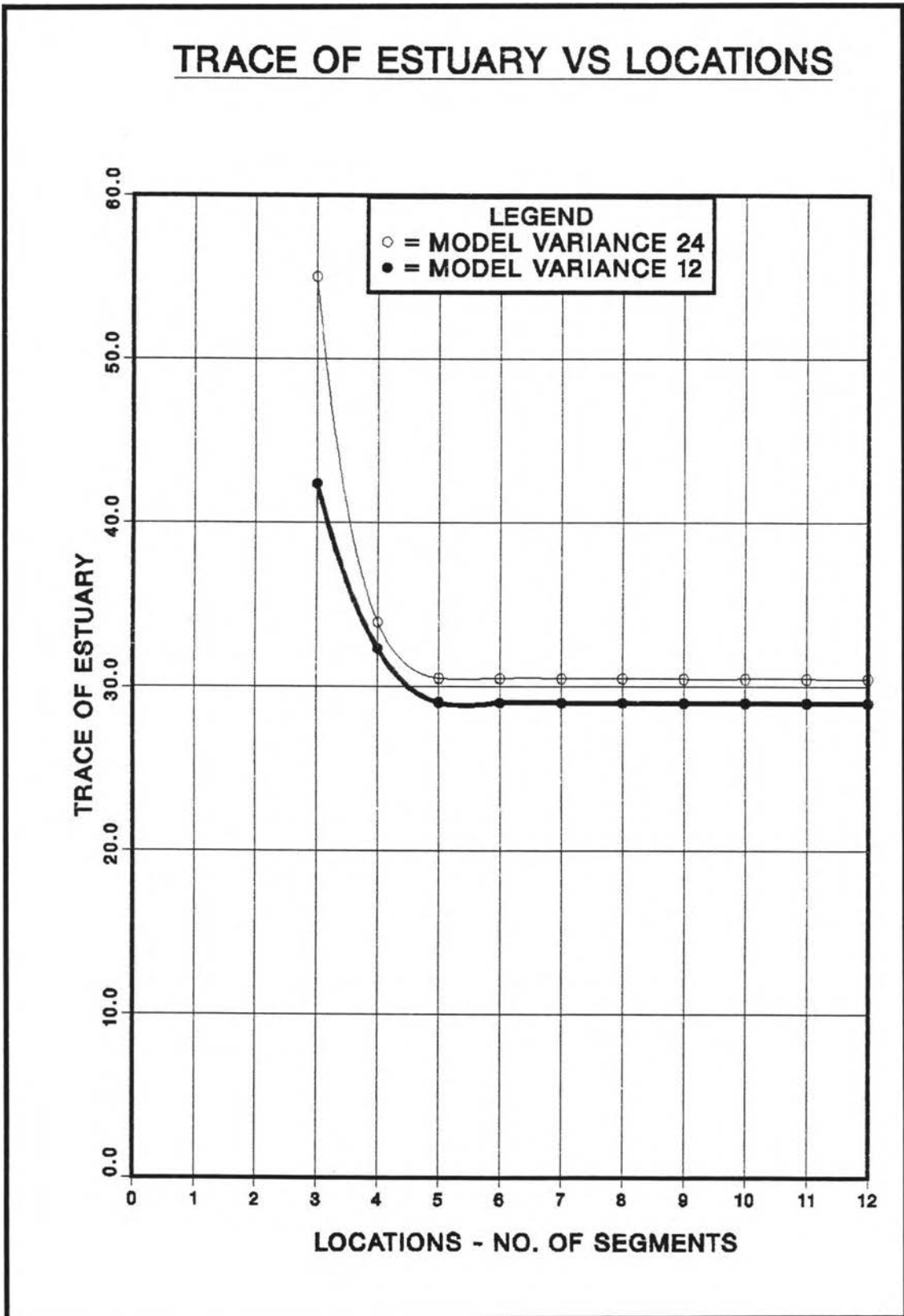


Figure 6.3. Variation of TOE for Differing Model Variances I - Unequal Sized Segments.

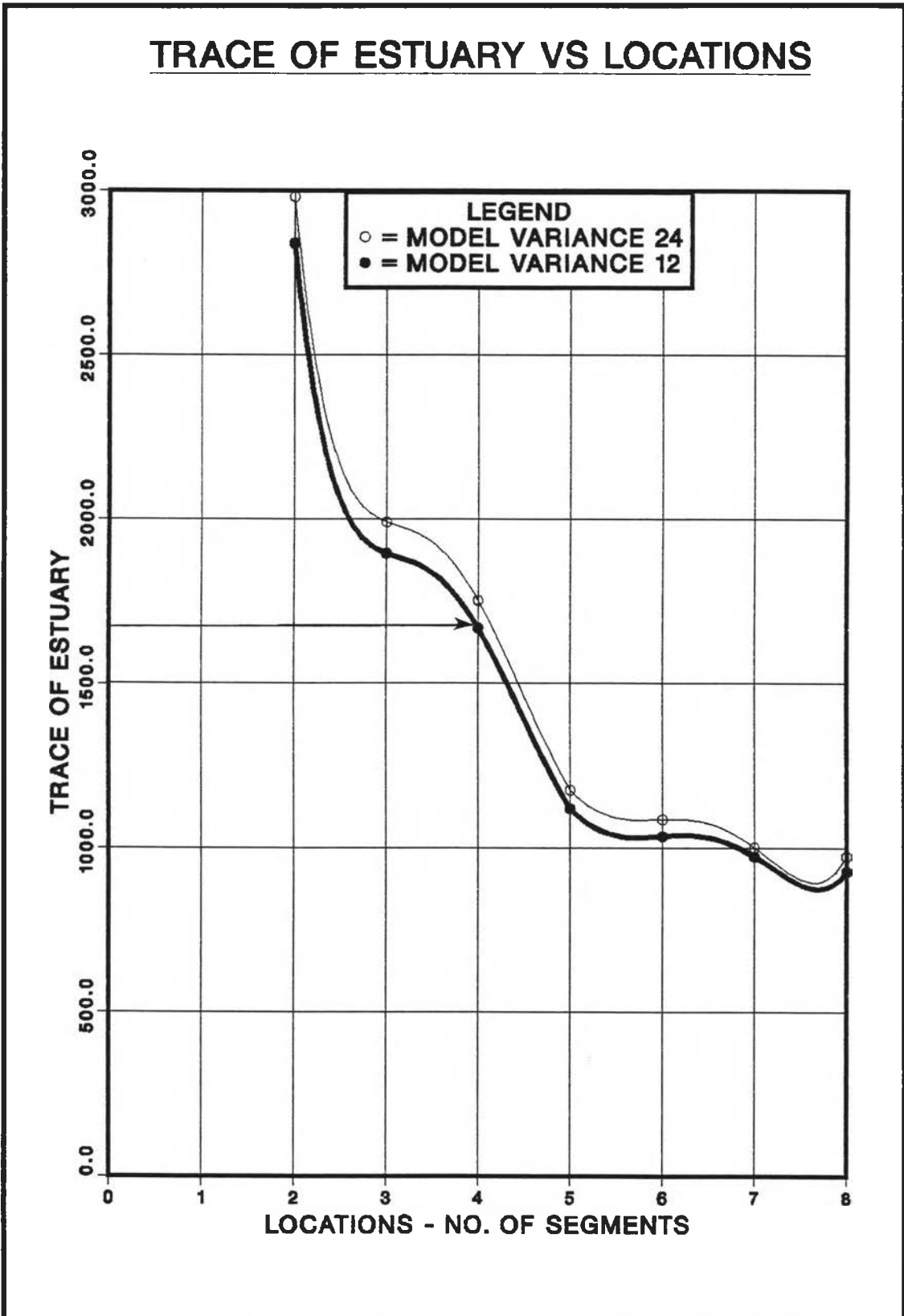


Figure 6.4. Variation of TOE for Differing Model Variances - Similar Sized Segments.

Let us consider the case of similar sized segments, Figure 6.4. One obvious fact is that, when the model variance reduces the curve of TOE vs. Locations moves downwards. This confirms our second hypothesis that the curve of TOE vs Sampling locations shifts down when an accurate model is used. Or in other words, the TOE reduces. This is to be expected because, predicted variance of a segment denoted by $\sigma_{t+\Delta t}^2 (+)$ is given by the expression

$$\sigma_{t+\Delta t}^2 (+) = [1 - k_{t+\Delta t}] [\sigma_t^2 (+) + \sigma_{\text{model}}^2]$$

and if σ_{model}^2 reduces, $\sigma_{t+\Delta t}^2 (+)$ also reduces. One can argue that the reduction in the predicted variance is not significant by looking at the graphs.

In order to answer this question let us consider Figure 6.4. If we define an acceptable TOE as $1700 \times 10^7 \text{ kg}^2$, it is sufficient to have 4 locations when the model variance is 12; but, you need 5 locations if the model variance is 24. This shows that there is a reduction in the sampling locations when a better model is used. It also shows that if an accurate model is used the number of places to be sampled is less than the one where a less accurate model is used. The third hypothesis that for a predetermined value of TOE different models give different number of sampling locations is hereby confirmed. This leads us to conclude that the selection of a model for water quality management determines the sampling locations.

6.5 Summary

This chapter answered some criticism levelled by the scientific community. It then discussed the experiences in using an existing

model. The results from the case study were analyzed and the three hypotheses which formed the basis of the research were confirmed.

CHAPTER 7

SUMMARY, CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER RESEARCH

Water quality models and water quality monitoring have been evolving independently during the past three decades. Several hundreds of models were developed and enormous amounts of data were collected during this period. In water quality management, neither of the models nor data are used effectively. One way of using the water quality models effectively is to use the model to determine the number of sampling locations required for management purposes. This approach achieves two goals;

- (i) Uses a water quality model effectively.
- (ii) Uses a valid, scientific approach to design a monitoring system.

Therefore, the research objective of this study was to use the water quality behavior of an estuary as represented in a model to determine the number of sampling locations. The next section summarizes the several steps to achieve this objective.

7.1 Summary

The steps taken to achieve our objective were:

- (i) Dissolved oxygen was chosen as the indicator of water quality for the estuary.

- (ii) The water quality behavior of the estuary as indicated by dissolved oxygen was modeled as a recursive estimation equation, and was known as the model equation.
- (iii) Field measurements of dissolved oxygen were expressed as an equation, where

$$y_t = M_t + \eta_t$$

where t : time at which measurements are taken

y : observed value of DO

M : actual value of DO

η : error in the observed DO value, y

This was described as the measurement equation.

- (iv) The model equation and the measurement equation were then combined using the Kalman filter algorithm to obtain the best estimate of the dissolved oxygen in the estuary at specified time intervals, and limits were put on these estimated values.
- (v) Trace of estuary (TOE), which was used as a measure of variability to design the monitoring network, was defined. Hypotheses about the behavior of TOE when sampling locations are reduced, and when models of differing accuracy are used, were formulated.
- (vi) The Potomac estuary used as the case study was idealized, and divided into twelve segments so that each segment had a sampling station in it.

- (vii) The values of TOE for different combinations of segments were calculated and the variations of TOE with the number of segments were plotted.

This exercise confirmed our hypotheses:

- (i) TOE reduces with an increase in the number of sampling locations.
- (ii) When two models of differing accuracy are used to evaluate TOE, the better model will give a lesser value of TOE.
- (iii) For a predetermined value of TOE, the number of sampling locations is less when an accurate model is used, and is more when a less accurate model is used.

The significance of these in water quality management are:

- (i) A scientific approach is used to determine the number of sampling locations where water quality measurements have to be made.
- (ii) This in effect guides the selection of a model and monitoring strategy for water quality management. When a measure of variability, an acceptable TOE, is defined, a model of certain accuracy and an optimum number of sampling locations corresponding to that model are chosen.
- (ii) Unlike in the past where modeling and monitoring were used independently, they will be used in an integrated fashion in the future.

7.2 Conclusions

Having summarized the various steps and illustrated the significance of the research we can arrive at the following conclusions.

- (i) Water quality behavior of the estuary can be used to determine the optimum number of sampling locations to design a monitoring network, where a network already exists. In the case study, the number of sampling locations for the Potomac estuary was reduced from twelve to five with no loss in information. The model knowledge, in effect, enabled a reduction of monitoring locations from twelve to five.
- (ii) The water quality model, which simulates the physical behavior, influences the number of sampling locations needed to obtain estimates of DO within given error bounds. We developed the measure TOE which could be used to compare the accuracy of models for the estuary. When an acceptable TOE is defined, an accurate model will give less number of sampling locations, than a less accurate model. The term "acceptable TOE" can be considered as equivalent to an acceptable error in predicting the DO in the estuary.
- (iii) The users of off-the-shelf water quality models should be aware that the models are mere idealizations of the physical behavior. There is no single model which can be used on every occasion, or for every problem. The users must be aware of the assumptions made in developing the models. They must be aware of the restrictions and comments made by the researchers who developed the various equations that have been incorporated in the model as constants.

7.3 Future Considerations

- (i) The concept of TOE should be tested for other water quality variables, such as nitrates, phosphates, and toxic chemicals.
- (ii) It is a fact that CSTR model is the crudest form in simulation models. The assumptions should be relaxed and checked to see whether there is any improvement in the value of TOE.
- (iii) The term trace of estuary was defined and it was assumed that the updated variances were spatially independent. This assumption should be checked and methods formulated to define an acceptable TOE.

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APPENDIX A-1

DO VALUES USED FOR MANN-KENDALL TEST

Table A1-1

Mean Values of DO for Mann-Kendall Test - July mg/ℓ

Year	Section										
	1	2	3	4	5	6	7	8	9	10	11
1977	6.99	6.78	5.60	5.06	4.67	5.31	6.28	8.25	6.04		
1978	9.58	9.06	8.80	8.44	7.67	7.16	6.84	8.51	5.09		
1979				5.90				8.50	2.63	4.73	
1980	7.08	6.75	6.00	5.84	5.58	4.16	5.74	8.03	4.04	5.05	4.54
1981	7.48	7.62	7.12	6.75	5.98	5.73	5.53	7.06	2.93	3.51	4.13
1982	6.63			4.90	4.22	7.23	4.60	7.70	3.20		4.35
1983	6.80	7.05	6.70	6.50	5.20	4.98	5.13	7.06	4.40		
1984		7.40	6.90	7.54	8.90	6.76	6.64	9.34	4.44		3.95
1985	6.30	5.67	7.50	7.46	6.13	6.87	8.51	7.48	3.63		4.46
1986	7.70	5.30	5.93	5.92	7.04	6.47	6.60	6.53	3.44	3.51	3.29

Table A1-2

Mean Values of DO for Mann-Kendall Test - September mg/ℓ

Year	Section										
	1	2	3	4	5	6	7	8	9	10	11
1977	7.84	4.51	3.63	3.53	3.95	4.72	4.43	8.49	5.76		
1978	8.13	7.38	6.47	6.35	5.65	6.49	7.75	7.99	5.35		
1979								5.18	5.48	5.45	
1980	7.70	6.95	5.75	5.64	4.90	4.85	4.80	6.58	4.97	3.93	5.39
1981		6.45	6.00	5.73	5.90	5.21	6.10	6.03	4.82	4.59	5.87
1982		5.47		5.84	6.10	7.00	7.26	7.70	6.95		7.80
1983	7.50	6.73	6.58	6.83	7.20	10.24	10.75	7.95	4.29		7.70
1984		7.94	7.00	7.90	6.50	6.48	6.63	7.67	3.84		5.29
1985	7.30	8.89	7.72	7.40	7.47	7.18	7.72	5.51	3.67		6.04
1986	7.10	5.98	5.39	5.20	5.17	5.29	6.30	7.00	5.15	5.40	6.39

Table A1-3

Mean Values of DO for Mann-Kendall Test - August mg/ℓ

Year	Section										
	1	2	3	4	5	6	7	8	9	10	11
1977	7.44	5.57	4.18	4.81	4.84	7.00	8.19	9.11	5.87		
1978	7.94	6.98	7.13	6.58	6.00	5.66	5.79	6.84	4.98		
1979				5.95			5.75		4.05	3.67	3.97
1980	6.45	6.22	5.53	6.20	5.09	4.26	5.61	6.73	5.27	3.97	5.00
1981	6.57	7.47	7.15	7.80	7.99	7.13	6.13	7.15	3.84	3.52	5.29
1982	6.64	5.20		4.95	4.49	5.22	5.96	6.57	5.10		8.10
1983	6.10	6.17	6.30	5.90	5.96	6.29	8.58	8.86	4.11		2.27
1984		8.27	8.00	7.28	7.70	8.06	6.00	8.09	4.90		3.38
1985	8.20	6.17	5.46	5.00	5.50	6.07	7.13	6.12	5.57	4.45	4.09
1986	6.20	5.23		5.10	4.90	5.68	6.42	6.03	4.81	4.84	4.78

APPENDIX A-2

SUMMARY OF SEGMENT DATA

SOURCE: NAUTICAL CHART 12285, NOAA, FEBRUARY 1988

Table A2-1

Summary of Segment Data: Area, Length, Width & Depth

Segment	Area 10^6 sq meter	Length 10^3 meter	Width 10^3 meter	Depth meter
1	0.75	3.99	0.19	4.74
2	3.06	6.49	0.47	4.55
3	4.80	4.45	1.08	2.70
4	4.30	3.71	1.16	2.23
5	4.83	2.04	2.36	1.66
6	8.60	4.36	1.97	1.36
7	8.25	6.49	1.27	6.03
8	11.14	6.49	1.72	1.73
9	182.99	45.7	4.0	3.31
10	267.99	48.21	5.56	2.67
11	395.67	40.78	9.70	9.67
12	111.32	11.12	10.00	14.64

APPENDIX A-3

**TRACE FOR ESTUARY FOR 18 PERIODS AS
SAMPLING LOCATIONS ARE REDUCED**

Trace for Estuary (TOE) $\text{kg}^2 \times 10^{12}$

Time Period	No. of Segments				
	2	3	4	5	6
1	92.497978	55.029178	33.939778	30.518948	30.496771
2	91.898454	54.677754	33.718754	30.320924	30.298968
3	91.730059	54.579659	33.665959	30.274369	30.252557
4	91.949566	54.701466	33.740066	30.339106	30.317098
5	92.181106	54.827506	33.822606	30.411126	30.388898
6	91.952578	54.702778	33.741478	30.340328	30.31832
7	91.126564	54.277964	33.437864	30.079654	30.058486
8	90.280641	53.826641	33.123541	29.805421	29.785055
9	91.175508	54.039708	33.353108	29.848608	29.828708
10	91.545353	54.215153	33.513353	29.950753	29.93051
11	92.584084	54.743584	33.856384	30.258584	30.237566
12	93.33693	55.10453	34.12313	30.47143	30.449694
13	93.49924	55.191941	34.18284	30.52394	30.502075
14	93.425241	55.147941	34.156741	30.499041	30.477175
15	93.499241	55.19561	34.18321	30.52394	30.502076
16	93.826447	55.360147	34.301747	30.62001	30.597971
17	94.069524	55.490224	34.390724	30.698947	30.676553
18	93.517461	55.212961	34.192761	30.538224	30.516242

Time Period	No. of Segments					
	7	8	9	10	11	12
1	30.486882	30.484498	30.478725	30.477838	30.476977	30.476714
2	30.289187	30.286826	30.281112	30.280236	30.279383	30.279124
3	30.242863	30.240508	30.252849	30.233985	30.233132	30.232872
4	30.307305	30.304939	30.299206	30.298329	30.297474	30.297214
5	30.378967	30.376585	30.370795	30.369903	30.369039	30.368777
6	30.308518	30.306151	30.300418	30.299541	30.298686	30.298426
7	30.049137	30.046852	30.041348	30.040522	30.039704	30.03945
8	29.776143	29.773935	29.768648	29.767871	29.767087	29.772292
9	29.82005	29.817885	29.812741	29.81199	29.811227	29.810983
10	29.921663	29.919467	29.91421	29.912678	29.912663	29.912417
11	30.228309	30.226023	30.22068	30.219068	30.219037	30.218782
12	30.44005	30.437692	30.432037	30.431137	30.430331	30.436161
13	30.492344	30.489991	30.484299	30.483411	30.48258	30.482321
14	30.467444	30.465091	30.459399	30.458525	30.45768	30.457421
15	30.492344	30.489991	30.484299	30.483411	30.48258	30.482321
16	30.588177	30.585802	30.580062	30.579187	30.578329	30.576662
17	30.666541	30.66413	30.658327	30.65742	30.656545	30.656281
18	30.506446	30.491094	30.498414	30.497479	30.496626	30.496366

APPENDIX A-4
LINEAR KALMAN FILTER ALGORITHM
A BRIEF EXPLANATION

Kalman Filter Algorithm

A large portion of the material in this appendix is reproduced from Beck [1], and his permission to quote is greatly appreciated.

A system can be defined as "a set of interacting elements" [2], and state variables are used to characterize a system. These state variables represent the changes that take place in a system and are used as a measure to determine the operation of the system. State variables will be denoted by 'x' in the following discussion, and determining the values for these variables is known as state estimation. Hence, linear Kalman filter algorithm is explained.

Prologue

The function of the Kalman filter algorithm in state estimation can be succinctly stated as follows

$$\hat{x}(t_k^+) = \hat{x}(t_k^-) + k(t_k) \epsilon(t_k)$$

where

$k(t_k)$: weighting factor

$\epsilon(t_k)$: difference between the measurement made at time t_k , and the prediction before this measurement was made. Suppose $y(t_k)$ was the measurement made at time t_k then

$$\epsilon(t_k) = y(t_k) - \hat{x}(t_k^-)$$

That is, it weights the difference between the measurement and the prediction, and adds it on to the prediction.

Prediction

Internally descriptive process models take into account the physical, chemical, biological and other changes that take place in the

system. Such a model is used for predicting the values of the state variables.

If continuous time behavior is of interest, it can be represented as

$$\frac{dx}{dt} = F \underline{x}(t) + G \underline{u}(t) + L \underline{\xi}(t) \quad \text{Eqn. (A-1)}$$

and if discrete time behavior is of interest

$$\underline{x}(t_k) = \phi \underline{x}(t_{k-1}) + \Gamma \underline{u}(t_{k-1}) + \Lambda \underline{\xi}(t_{k-1}) \quad \text{Eqn. (A-2)}$$

where

\underline{x} : state vector; represents the values of the different variables that describe the State of the system - 'n' dimensional vector.

\underline{u} : measured input disturbances; represents the measured changes that take place in the system - 'm' dimensional vector.

$\underline{\xi}$: stochastic, unmeasured disturbances (system noise) - 'p' dimensional vector.

F,G,L : nxn, nxm, and nxp time invariant matrices

$$\phi : \exp\left[F(t_k - t_{k-1})\right]$$

$$\Gamma \underline{u}(t_{k-1}) = \int_{t_{k-1}}^{t_k} \phi(t_k, \tau) G(\tau) \underline{u}(\tau) d\tau$$

$$\Lambda \underline{\xi}(t_{k-1}) = \int_{t_{k-1}}^{t_k} \phi(t_k, \tau) L(\tau) \underline{\xi}(\tau) d\tau$$

Further, it is assumed that the sampling interval is constant.

Measurements

The measurements when influenced by errors can be represented as

$$\underline{y} (t_k) = H \underline{x} (t_k) + \underline{\eta} (t_k) \quad \text{Eqn. (A-3)}$$

where

\underline{y} : measurements or observations 'l' dimensional vector

$\underline{\eta}(t_k)$: errors associated with the measurements 'l' dimensional vector

H : lxn observation matrix

Algorithm

The aim is to estimate the mean of the state variable and assign an upper and lower bound to this value by estimating the error-covariance matrix. In other words, knowing A-2 and A-3, and denoting 'E' as the expectation operator, estimate $\hat{\underline{x}}(t)$ for the state variable $\underline{x}(t)$,

$$\hat{\underline{x}} (t) = E \{ \underline{x} (t) \}$$

and the variance-covariance matrix P(t) of the estimation error

$$P (t) = E \left\{ (\hat{\underline{x}} (t) - \underline{x} (t)) (\hat{\underline{x}} (t) - \underline{x} (t))^T \right\}$$

Using the recursive least squares algorithm for estimating the state and the error-covariance update, and assuming certain statistical characteristics for the noise (errors), it can be shown that

Prediction between t_{k-1} and t_k

$$\hat{\underline{x}} (t_k/t_{k-1}) = \phi \hat{\underline{x}} (t_{k-1}/t_{k-1}) + \Gamma \underline{u} (t_{k-1}) \quad \text{Eqn. (A-4)}$$

$$P \left[t_k/t_{k-1} \right] = \phi P \left[t_{k-1}/t_{k-1} \right] \phi^T + \Lambda Q \Lambda^T \quad \text{Eqn. (A-5)}$$

Correction across t_k on measuring $y(t_k)$

$$\hat{x} \left[t_k/t_k \right] = \hat{x} \left[t_k/t_{k-1} \right] + k \left[t_k \right] \left\{ y \left[t_k \right] - H \hat{x} \left[t_k/t_{k-1} \right] \right\} \quad \text{Eqn. (A-6)}$$

$$P \left[t_k/t_k \right] = \left[I - k \left[t_k \right] H \right] P \left[t_k/t_{k-1} \right] \quad \text{Eqn. (A-7)}$$

$$K \left[t_k \right] = P \left[t_k/t_{k-1} \right] H^T \left[H P \left[t_k/t_{k-1} \right] H^T + R \right]^{-1} \quad \text{Eqn. (A-8)}$$

provided the initial conditions $\hat{x}(t_0/t_0)$, $P(t_0/t_0)$ and Q and R are known.

The behavior of the algorithm can be analyzed by considering, A-5, A-7 and A-8. Assuming $H = 1$, and taking only one state variable, the three expressions can be rearranged to give

$$p \left[t_k/t_k \right] = \left[1 - k \left[t_k \right] \right] \phi^2 p \left[t_{k-1}/t_{k-1} \right] + \left[1 - k \left[t_k \right] \right] \lambda^2 q \quad \text{Eqn. (A-9)}$$

and

$$k \left[t_k \right] = \frac{\phi^2 p \left[t_{k-1}/t_{k-1} \right] + \lambda^2 q}{\phi^2 p \left[t_{k-1}/t_{k-1} \right] + \lambda^2 q + r} \quad \text{Eqn. (A-10)}$$

APPENDIX A-5
LISTING OF PROGRAM EULER


```

C
C
C
C *****
C *
C * PROGRAM EULER
C * -----
C *
C * THIS PROGRAM SOLVES A SECOND ORDER DIFFERENTIAL
C * EQUATION USING THE EULER METHOD. THE SPECIFIC
C * APPLICATION IS IN RELATION TO CALCULATING DISSOLVED
C * OXYGEN MASS IN THE SEGMENTS OF THE ESTUARY.
C *
C * THE REAERATION RATE, DEOXYGENATION RATE ARE TO THE
C * BASE 'E', AND ARE INCORPORATED IN THE PROGRAM. THE
C * TIME PERIOD, NUMBER OF SEGMENTS ARE ALSO INCORPORATED*
C * IN THE PROGRAM AS PARAMETER STATEMENTS.
C *
C * THE PROGRAM READS THE DATA FROM THE DATA FILE
C * 'PODATA' IN THE SPECIFIED FORMAT. IT CREATES AN
C * OUTPUT FILE 'PORESLT' AND STORES THE RESULT. THE
C * DATA READ IN ARE ALWAYS PRINTED TO MAKE SURE THAT
C * IT IS BEING READ CORRECTLY. IN ORDER TO OBTAIN A
C * CONCISE SET OF RESULTS THAT CAN BE ATTACHED TO THE
C * DISSERTATION, SOME STATEMENTS HAVE BEEN COMMENTED
C * ANYONE INTERESTED SHOULD GO INTO THE PROGRAM AND
C * REMOVE THEM IF EXTRA DETAILS ARE TO BE OBTAINED IN
C * THE RESULT.
C *
C *****
C
C
C
C PROGRAM TO SOLVE A SECOND ORDER DIFFERENTIAL EQUATION
C BY THE EULER METHOD
C *****
C
C PROGRAM EULER
C *****
C
C PARAMETER (ITIME=24,NSEG=12)
C
C DIMENSION VOL(50,50),DO(50,50),BODU(50,50),SK6(50,50),R(50,50),
C * TEMP(50),DOSAT(50),DOSAL(50),SATDO(50,50)
C
C REAL K2,KD,DELT,M(50,50)
C
C OPEN DATA FILES
C *****
C
C OPEN(UNIT=5,FILE='PODATA',STATUS='OLD',FORM='FORMATTED')
C OPEN(UNIT=6,FILE='PORESLT',STATUS='UNKNOWN',FORM='FORMATTED')
C
C READ INPUT DATA
C *****
C
C WRITE(6,1)
C DATA K2,KD,DELT/0.05,0.30,30/
C WRITE(6,2) K2,KD,DELT
C WRITE(6,3)
C DATA ITIME,NSEG/12,18/
C WRITE(6,4) ITIME,NSEG
C
C READ THE VOLUME OF THE SEGMENTS AT DIFFERENT TIME PERIODS
C *****
C
C WRITE(6,5)
C DO 100 J=1,NSEG
C READ (5,7)(VOL(I,J),I=1,12)
C WRITE(6,6) J,(VOL(I,J),I=1,12)

```

```

100 CONTINUE
    DO 110 J=1,NSEG
        READ(5,7)(VOL(I,J),I=13,24)
        WRITE(6,6)J,(VOL(I,J),I=13,24)
110 CONTINUE
C
C
C   READ THE ULTIMATE BOD LOADING FOR THE SEGMENTS DURING
C   THE DIFFERENT MONTHS
C   *****
C
    WRITE(6,10)
    WRITE(6,11)
    WRITE(6,5)
    DO 150 J=1,NSEG
        READ(5,7)(BODU(I,J),I=1,12)
        WRITE(6,6)J,(BODU(I,J),I=1,12)
150 CONTINUE
C
C
    DO 155 J=1,NSEG
        READ(5,7)(BODU(I,J),I=13,24)
        WRITE(6,6)J,(BODU(I,J),I=13,24)
155 CONTINUE
C
C
C   READ THE DO SATURATION VALUES
C   *****
C
    WRITE(6,12)
    WRITE(6,13)
        READ(5,7)(DOSAT(I),I=1,ITIME)
        WRITE(6,23)(DOSAT(I),I=1,12)
        WRITE(6,23)(DOSAT(I),I=13,24)
        WRITE(6,24)
        WRITE(6,25)
        READ(5,7)(DOSAL(I),I=1,ITIME)
        WRITE(6,23)(DOSAL(I),I=1,12)
        WRITE(6,23)(DOSAL(I),I=13,14)
C
C
C   INITIALIZE THE SATURATION VALUES ACCORDING TO
C   TIME, SEGMENTS, AND SALINITY
C   *****
C
    DO 175 I=1,ITIME
        DO 200 J=1,9
            SATDO(I,J)=DOSAT(I)
            WRITE(6,6) J,SATDO(I,J)
200    CONTINUE
175 CONTINUE
C
    DO 225 I=1,ITIME
        DO 250 J=10,12
            SATDO(I,J)=DOSAL(I)
            WRITE(6,6) J,SATDO(I,J)
250    CONTINUE
225 CONTINUE
C
C
C   READ THE INITIAL VALUE OF DO CONCENTRATION IN THE SEGMENTS
C   *****
C
    WRITE(6,14)
    WRITE(6,15)
    READ(5,7)(DO(5,J),J=1,12)
    WRITE(6,23) (DO(5,J),J=1,12)
275 CONTINUE
C
C
C   INITIAL MASS OF DO IN SEGMENTS
C   *****

```

```

C
  WRITE(6,18)
  WRITE(6,19)
    DO 300 J=1,NSEG
      M(5,J)=VOL(5,J)*DO(5,J)*1000.0
      WRITE(6,20) J,M(5,J)
300 CONTINUE
C
C
C  MASS DERIVATIVE AND EULER INTEGRATION
C  *****
C
  WRITE(6,21)
  DO 400 I=5,ITIME
    DO 500 J=1,NSEG
      SK6(I,J)=(K2*VOL(I,J)*(SATDO(I,J)-DO(I,J))-KD*BODU(I,J))*1000.
      R(I,J) =SK6(I,J)*DELTA
      M(I+1,J)=M(I,J)+R(I,J)
      DO(I+1,J)=M(I+1,J)/(VOL(I,J)*1000.0)
      IF(DO(I+1,J).LE.0.0) THEN
        DO(I+1,J)=0.0
      ENDIF
      WRITE(6,22) J,M(I+1,J),M(I,J),R(I,J),DO(I+1,J)
500    CONTINUE
C
  IF(I.EQ.ITIME) THEN
    GO TO 1000
  ENDIF
400  CONTINUE
C
1000 STOP
C
C
C
C
C  FORMAT STATEMENTS
C  *****
C
1  FORMAT(// ' REAERATION-K2    DEOXYGENATION-KD    TIME-DELTA')
2  FORMAT(//F14.3,F20.3,F13.2)
3  FORMAT(// ' TIME PERIOD    NUMBER OF SEGMENTS')
4  FORMAT(//I12,I21)
5  FORMAT(// 'SEGMENT    JAN    FEB    MAR    APR    MAY    JUN
*   JUL    AUG    SEP    OCT    NOV    DEC')
6  FORMAT(//I7,12F8.2)
7  FORMAT(12F7.2)
8  FORMAT(// 'SEGMENT NUMBERS AND VOLUMES')
9  FORMAT('*****')
10 FORMAT(// 'SEGMENT NUMBERS AND ULTIMATE BOD LOADING')
11 FORMAT('*****')
12 FORMAT(// 'DISSOLVED OXYGEN - DO SATURATION VALUES')
13 FORMAT('*****')
14 FORMAT(// 'INITIAL DO CONCENTRATION VALUES MG/L')
15 FORMAT('*****')
C 16 FORMAT(// ' SEGMENT    DO MG/L')
C 17 FORMAT(//I8,F10.1)
18 FORMAT(// 'INITIAL MASS OF DO IN SEGMENTS - KG')
19 FORMAT('*****')
20 FORMAT(//I8,F12.2)
21 FORMAT(// 'SEGMENT    MASS(T+1)    MASS(T)    R(T)    DO(T+1)')
22 FORMAT(//I7,4F11.2)
23 FORMAT(//I2F8.2)
24 FORMAT(// 'DO SATURATION VALUES - SALINE SEGMENTS')
25 FORMAT('*****')
C
C
C  END

```

APPENDIX A-6
TYPICAL OUTPUT FROM PROGRAM EULER

REAERATION-K2 DEOXYGENATION-KD TIME-DELT
.050 .300 30.00

TIME PERIOD NUMBER OF SEGMENTS
 24 12

SEGMENT	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
1	4.08	4.11	4.17	4.21	4.22	4.21	4.21	4.21	4.23	4.22	4.16	4.11
2	16.08	16.19	16.42	16.58	16.64	16.61	16.61	16.63	16.69	16.63	16.41	16.19
3	16.35	16.52	16.88	17.13	17.22	17.18	17.13	17.21	17.29	17.21	16.85	16.52
4	12.60	12.77	13.10	13.32	13.40	13.37	13.33	13.37	13.46	13.37	13.07	12.77
5	11.33	11.59	11.97	12.22	12.30	12.26	12.22	12.27	12.36	12.27	11.93	11.59
6	17.72	18.06	18.75	19.17	19.32	19.25	19.17	19.26	19.44	19.26	18.66	18.06
7	54.83	55.11	55.10	56.16	56.31	56.24	55.91	56.29	56.44	56.29	55.69	55.11
8	25.46	25.83	26.68	27.26	27.46	27.36	27.26	27.43	27.63	27.43	26.61	25.83
9	723.32	723.99	725.43	726.67	726.92	726.88	726.42	726.92	727.32	726.92	725.37	723.99
10	1228.28	1234.36	1248.03	1257.47	1260.52	1258.99	1257.47	1260.17	1263.36	1260.17	1246.86	1234.35
11	3339.60	3347.59	3363.07	3374.05	3377.43	3375.73	3374.05	3376.98	3380.55	3376.98	3362.86	3347.59
12	1664.02	1665.71	1669.45	1671.83	1672.51	1672.17	1669.49	1671.83	1673.52	1671.83	1669.11	1665.71
1	4.09	4.10	4.18	4.20	4.21	4.21	4.21	4.22	4.25	4.22	4.18	4.10
2	16.07	16.16	16.40	16.55	16.59	16.59	16.59	16.65	16.74	16.62	16.40	16.13
3	16.32	16.46	16.85	17.09	17.14	17.14	17.14	17.23	17.38	17.18	16.85	16.42
4	12.60	12.73	13.07	13.29	13.33	13.33	13.33	13.42	13.56	13.37	13.07	12.69
5	11.40	11.54	11.93	12.17	12.22	12.22	12.22	12.17	12.46	12.27	11.93	11.49
6	17.72	17.97	18.66	19.09	19.18	19.18	19.18	19.35	19.61	19.26	18.66	17.89
7	54.78	55.03	55.69	56.10	56.18	56.18	56.18	56.18	56.35	56.27	55.61	54.95
8	25.29	25.73	25.84	27.16	27.29	27.29	27.29	27.52	27.74	27.40	26.51	25.62
9	769.20	772.04	778.01	782.67	783.14	783.14	783.14	785.45	785.86	782.61	778.01	771.04
10	1227.44	1232.47	1245.64	1256.75	1258.37	1257.92	1258.37	1262.23	1265.62	1258.37	1245.64	1231.30
11	3343.41	3348.52	3364.71	3375.28	3378.08	3376.79	3378.08	3383.20	3387.51	3379.24	3364.70	3347.36
12	1666.46	1667.57	1672.03	1674.25	1675.37	1674.25	1675.37	1676.48	1677.59	1675.37	1672.03	1667.57

SEGMENT NUMBERS AND ULTIMATE BOD LOADING

SEGMENT	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
1	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
2	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
3	1.38	2.19	2.29	2.19	1.74	.94	.64	.87	1.12	1.22	1.65	2.09

	4	24.23	19.35	60.42	47.65	40.90	25.87	35.03	31.90	30.74	28.65	17.45	16.19
	5	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	6	4.55	4.41	5.65	5.26	5.06	3.77	4.00	3.52	3.97	6.26	5.68	5.42
	7	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	8	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
.90	9	1.16	1.13	1.23	1.61	1.39	1.16	1.09	1.16	.81	1.39	1.03	
	10	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	11	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	12	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	1	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	2	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	3	1.38	2.19	2.29	2.19	1.74	.94	.64	.87	1.12	1.22	1.65	2.09
	4	24.23	19.35	60.42	47.65	40.90	25.87	35.03	31.90	30.74	28.65	17.45	16.19
	5	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	6	4.55	4.41	5.65	5.26	5.06	3.77	4.00	3.52	3.97	6.26	5.68	5.42
	7	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	8	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
.90	9	1.16	1.13	1.23	1.61	1.39	1.16	1.09	1.16	.81	1.39	1.03	
	10	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	11	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
	12	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00

DISSOLVED OXYGEN - DO SATURATION VALUES

13.38	13.20	11.49	9.66	8.91	7.92	8.44	8.28	8.78	9.37	12.08	12.32
14.03	12.48	11.81	11.08	9.64	8.83	8.22	8.22	8.53	9.54	11.87	11.87

DO SATURATION VALUES - SALINE SEGMENTS

10.10	10.20	9.07	7.71	7.15	6.40	6.77	6.66	6.87	7.49	9.51	9.69
10.93	9.80										

INITIAL DO CONCENTRATION VALUES MG/L

7.80	8.30	8.60	7.90	7.20	5.60	7.90	6.30	7.40	6.60	6.60	6.60
------	------	------	------	------	------	------	------	------	------	------	------

INITIAL MASS OF DO IN SEGMENTS - KG

1	32916.00
2	138112.00

3 148092.00
 4 105860.00
 5 88560.00
 6 108192.00
 7 444849.00
 8 172998.00
 9 5379208.00
 10 8319432.00
 11 22291038.00
 12 11038566.00

SEGMENT	MASS(T+1)	MASS(T)	R(T)	DO(T+1)
1	-5057.70	32916.00	-37973.70	.00
2	108337.60	138112.00	-29774.40	6.51
3	140439.30	148092.00	-7652.70	8.16
4	-241939.00	105860.00	-347799.00	.00
5	75109.50	88560.00	-13450.50	6.11
6	158575.80	108192.00	50383.80	8.21
7	485158.65	444849.00	40309.65	8.62
8	235503.90	172998.00	62505.90	8.58
9	7013171.80	5379208.00	1633963.80	9.65
10	9314361.00	8319432.00	994929.00	7.39
11	25032417.75	22291038.00	2741379.75	7.41
12	2373386.75	11038566.00	1334820.75	7.40
1	-42.90	-5057.70	5014.80	.00
2	98450.98	108337.60	-9886.62	5.93
3	125908.09	140439.30	-14531.21	7.33
4	-315933.40	-241939.00	-73994.40	.00
5	63460.44	75109.50	-11649.06	5.18
6	116333.93	158575.80	-42241.87	6.04
7	381456.54	485158.65	-103702.11	6.78
8	163571.29	235503.90	-71932.61	5.98
9	5118887.37	7013171.80	-1894284.43	7.04
10	7401081.94	9314361.00	-1913279.06	5.88
11	19864698.90	25032417.75	-5167718.85	5.88
12	9824911.65	2373386.75	-2548475.10	5.88
1	8255.70	-42.90	8298.60	1.96

2	116057.11	98450.98	17606.13	6.99
3	148701.41	125908.09	22793.33	8.68
4	-462445.60	-315933.40	-146512.20	.00
5	78285.55	63460.44	14825.12	6.41
6	149250.44	116333.93	32916.51	7.79
7	475449.74	381456.54	93993.21	8.50
8	219222.73	163571.29	55651.44	8.04
9	6632082.68	5118887.37	1513195.32	9.13
10	9037470.06	7401081.94	1636388.11	7.19
1124300957.40	19864698.90	4436258.50	7.20	
1212019834.82	9824911.65	2194923.17	7.20	
1	3160.35	8255.70	-5095.35	.75
2	103306.43	116057.11	-12750.68	6.21
3	130525.80	148701.41	-18175.61	7.58
4	-583490.20	-462445.60	-121044.60	.00
5	67770.15	78285.55	-10515.41	5.52
6	131852.92	149250.44	-17397.51	6.85
7	411549.74	475449.74	-63900.01	7.31
8	184018.55	219222.73	-35204.18	6.71
9	5695017.69	6632082.68	-937064.99	7.83
10	7996255.82	9037470.06	-1041214.24	6.35
1121508897.34	24300957.40	-2792060.06	6.37	
1210621393.33	12019834.82	-1398441.49	6.35	
1	9106.40	3160.35	5946.05	2.15
2	122595.00	103306.43	19288.57	7.35
3	151456.28	130525.80	20930.48	8.76
4	-682882.00	-583490.20	-99391.80	.00
5	83150.49	67770.15	15380.34	6.73
6	152519.93	131852.92	20667.01	7.85
7	490894.90	411549.74	79345.16	8.70
8	224865.23	184018.55	40846.68	8.14
9	6719304.88	5695017.69	1024287.19	9.24
10	8945434.26	7996255.82	949178.44	7.08
1124003011.64	21508897.34	2494114.30	7.10	
1211873821.69	10621393.33	1252428.36	7.10	
1	9791.19	9106.40	684.79	2.32

2	128098.24	122595.00	5503.24	7.70
3	156229.58	151456.28	4773.30	9.08
4	-752816.65	-682882.00	-69934.65	.00
5	86787.80	83150.49	3637.31	7.07
6	140217.67	152519.93	-12302.27	7.28
7	502665.47	490894.90	11770.57	8.93
8	230537.57	224865.23	5672.34	8.40
9	6850241.22	6719304.88	130936.34	9.42
10	9674173.82	8945434.26	728739.57	7.68
1125931886.7324003011.64		1928875.10		7.68
1212819085.3311873821.69		945263.64		7.67
1	25692.42	9791.19	15901.23	6.18
2	190842.02	128098.24	62743.78	11.63
3	217259.24	156229.58	61029.66	12.89
4	-673038.25	-752816.65	79778.40	.00
5	131385.02	86787.80	44597.21	11.01
6	223442.59	140217.67	83224.93	11.97
7	720807.00	502665.47	218141.53	12.94
8	332242.05	230537.57	101704.48	12.49
9	9731223.78	6850241.22	2880982.55	13.42
1013057639.90	9674173.82	3383466.07		10.47
1135122896.1125931886.73		9191009.38		10.44
1217386595.6912819085.33		4567510.36		10.42
1	18569.79	25692.42	-7122.63	4.52
2	162607.96	190842.02	-28234.05	10.04
3	184232.37	217259.24	-33026.87	11.15
4	-582758.65	-673038.25	90279.60	.00
5	109107.32	131385.02	-22277.70	9.41
6	184024.48	223442.59	-39418.12	10.19
7	624289.89	720807.00	-96517.11	11.33
8	280825.54	332242.05	-51416.51	10.87
9	8533393.46	9731223.78-1197830.32		11.79
1011563972.2413057639.90-1493667.66				9.37
1131290000.4935122896.11-3832895.62				9.35
1215525922.1117386595.69-1860673.58				9.32
1	31924.70	18569.79	13354.91	7.81

2	213697.04	162607.96	51089.07	13.30
3	242263.84	184232.37	58031.47	14.84
4	-535661.65	-582758.65	47097.00	.00
5	143042.31	109107.32	33934.99	12.55
6	245151.87	184024.48	61127.39	13.83
7	801307.55	624289.89	177017.66	14.63
8	355621.66	280825.54	74796.12	14.06
9	11111367.78	8533393.46	2577974.32	14.45
10	14393996.88	11563972.24	2830024.65	11.73
11	139183812.54	31290000.49	7893812.04	11.72
12	19503164.63	15525922.11	3977242.52	11.70
1	15672.57	31924.70	-16252.13	3.82
2	148871.47	213697.04	-64825.57	9.21
3	164171.92	242263.84	-78091.92	9.97
4	-471506.05	-535661.65	64155.60	.00
5	96872.66	143042.31	-46169.65	8.39
6	168944.43	245151.87	-76207.43	9.40
7	579022.42	801307.55	-222285.13	10.52
8	249574.02	355621.66	-106047.64	9.70
9	8825197.69	11111367.78	-2286170.09	11.43
10	10786831.52	14393996.88	-3607165.36	8.75
11	29496506.12	39183812.54	-9687306.42	8.81
12	14697210.61	19503164.63	-4805954.02	8.81
1	20753.71	15672.57	5081.14	4.97
2	167773.82	148871.47	18902.36	10.23
3	189967.01	164171.92	25795.09	11.27
4	-783751.00	-471506.05	-312244.95	.00
5	112992.83	96872.66	16120.18	9.47
6	185509.16	168944.43	16564.73	9.94
7	641620.42	579022.42	62597.99	11.52
8	286368.14	249574.02	36794.12	11.08
9	9256413.60	8825197.69	431215.91	11.90
10	11802731.61	10786831.52	1015900.08	9.48
11	32031470.58	29496506.12	2534964.46	9.52
12	15922411.45	14697210.61	1225200.84	9.52
1	14278.20	20753.71	-6475.51	3.40

2	143872.31	167773.82	-23901.51	8.69
3	165283.65	189967.01	-24683.35	9.67
4	-991721.20	-783751.00	-207970.20	.00
5	97359.31	112992.83	-15633.52	8.00
6	170768.93	185509.16	-14740.24	8.95
7	559486.20	641620.42	-82134.22	9.97
8	241272.06	286368.14	-45096.07	8.88
9	8282114.72	9256413.60	-974298.88	10.58
10	10428275.66	11802731.61	-1374455.95	8.30
11	28190136.19	32031470.58	-3841334.39	8.35
12	13986842.09	15922411.45	-1935569.36	8.35
1	8686.51	14278.20	-5591.69	2.06
2	122433.65	143872.31	-21438.66	7.38
3	148817.22	165283.65	-16466.43	8.68
4	-1167069.40	-991721.20	-175348.20	.00
5	82421.55	97359.31	-14937.76	6.74
6	145210.70	170768.93	-25558.23	7.57
7	486422.94	559486.20	-73063.26	8.66
8	227245.11	241272.06	-14026.95	8.33
9	7163176.82	8282114.72	-1118937.90	9.15
10	9519129.69	10428275.66	-909145.97	7.56
11	25551074.56	28190136.19	-2639061.64	7.56
12	2649895.28	13986842.09	-1336946.82	7.55
1	6418.20	8686.51	-2268.31	1.52
2	113517.72	122433.65	-8915.93	6.84
3	144150.69	148817.22	-4666.53	8.41
4	-1223343.55	-1167069.40	-56274.15	.00
5	75643.13	82421.55	-6778.42	6.19
6	147503.75	145210.70	2293.05	7.69
7	455892.63	486422.94	-30530.31	8.11
8	202833.49	227245.11	-24411.62	7.43
9	6780660.89	7163176.82	-382515.93	8.66
10	8578520.50	9519129.69	-940609.19	6.82
11	23106260.30	25551074.56	-2444814.26	6.84
12	1448385.97	2649895.28	-1201509.31	6.84
1	3700.20	6418.20	-2717.99	.88

2	102795.84	113517.72	-10721.89	6.20
3	133500.86	144150.69	-10649.83	7.79
4	-1374254.65	-1223343.55	-150911.10	.00
5	67851.04	75643.13	-7792.09	5.55
6	126737.52	147503.75	-20766.23	6.61
7	419753.08	455892.63	-36139.55	7.47
8	190068.95	202833.49	-12764.54	6.96
9	6255975.75	6780660.89	-524685.14	7.99
10	8156750.62	8578520.50	-421769.88	6.48
11	21932963.68	23106260.30	-1173296.61	6.49
12	10855743.41	11448385.97	-592642.55	6.48
1	5169.32	3700.20	1469.11	1.22
2	108338.92	102795.84	5543.08	6.51
3	136813.98	133500.86	3313.12	7.94
4	-1495886.05	-1374254.65	-121631.40	.00
5	71547.02	67851.04	3695.98	5.88
6	141851.75	126737.52	15114.22	7.33
7	437822.86	419753.08	18069.77	7.79
8	196884.27	190068.95	6815.32	7.15
9	6518491.08	6255975.75	262515.33	8.30
10	8373037.83	8156750.62	216287.21	6.63
11	22533829.99	21932963.68	600866.30	6.66
12	1163786.14	10855743.41	308042.73	6.66
1	6738.97	5169.32	1569.65	1.59
2	114140.42	108338.92	5801.50	6.82
3	142103.51	136813.98	5289.53	8.18
4	-1599045.85	-1495886.05	-103159.80	.00
5	76094.84	71547.02	4547.83	6.11
6	141395.05	141851.75	-456.70	7.21
7	455099.55	437822.86	17276.69	8.08
8	209130.27	196884.27	12246.00	7.54
9	6783439.24	6518491.08	264948.16	8.63
10	8720010.80	8373037.83	346972.97	6.89
11	23400877.42	22533829.99	867047.44	6.91
12	11574092.99	1163786.14	410306.84	6.90
1	12090.07	6738.97	5351.10	2.86

2	136989.31	114140.42	22848.89	8.24
3	166266.93	142103.51	24163.42	9.68
4	-1665571.15	-1599045.85	-66525.30	.00
5	94276.81	76094.84	18181.97	7.68
6	152358.51	141395.05	10963.46	7.91
7	533643.08	455099.55	78543.53	9.48
8	246373.73	209130.27	37243.46	8.99
9	7836999.83	6783439.24	1053560.59	10.01
10	10053091.50	8720010.80	1333080.70	7.99
11	26964968.08	23400877.42	3564090.65	7.98
12	13340407.07	11574092.99	1766314.08	7.96
1	23551.76	12090.07	11461.69	5.63
2	181227.35	136989.31	44238.04	11.05
3	206821.37	166266.93	40554.44	12.27
4	-1589909.80	-1665571.15	75661.35	.00
5	124193.84	94276.81	29917.03	10.41
6	212061.60	152358.51	59703.09	11.36
7	687703.29	533643.08	154060.21	12.37
8	315827.66	246373.73	69453.94	11.91
9	9993794.23	7836999.83	2156794.40	12.85
10	2569789.40	10053091.50	2516697.91	10.09
11	3886938.94	26964968.08	6921970.86	10.07
12	6799990.61	13340407.07	3459583.54	10.05
1	16900.75	23551.76	-6651.02	4.12
2	156056.41	181227.35	-25170.94	9.67
3	178054.32	206821.37	-28767.05	10.84
4	-1509674.35	-1589909.80	80235.45	.00
5	104353.27	124193.84	-19840.57	9.08
6	176846.65	212061.60	-35214.95	9.89
7	601775.98	687703.29	-85927.31	10.95
8	269154.83	315827.66	-46672.83	10.51
9	8857668.00	9993794.23	-1136126.24	11.49
10	11174615.33	2569789.40	-1395174.07	9.08
11	30270419.72	3886938.94	-3616519.22	9.04
12	5034906.35	16799990.61	-1765084.26	9.02

APPENDIX A-7
LISTING OF PROGRAM EULKAL

```

C
C
C
C *****
C *
C * PROGRAM EULKAL
C * -----
C *
C * THIS PROGRAM IS MODIFICATION OF THE PREVIOUS PROGRAM
C * 'EULER'. THE PROGRAM 'EULKAL' USES THE KALMAN FILTER
C * ALGORITHM TO COMPARE THE MODEL PREDICTION AND FIELD
C * MEASUREMENTS, AND CALCULATES THE CONCENTRATION OF THE
C * DISSOLVED OXYGEN CONCENTRATION. IT ALSO CALCULATES THE
C * FORECAST VARIANCE UPDATE OF THE FILTER ALGORITHM.
C *
C * THE LISTING IN THIS PROGRAM CORRESPONDS TO TWO
C * ESTUARINE SEGMENTS. IT ALSO SHOWS HOW THE SEGMENTS ARE
C * COMBINED AND HOW THE BOD LOADING AND DO COCENTRATION
C * ARE ASSIGNED.
C *
C *****
C
C
C
C PROGRAM TO SOLVE THE COMBINED MONITORING AND MODELLING PROBLEM
C BY THE EULER KALMAN ALGORITHM - 02 SEGMENTS
C *****
C
C PROGRAM EULKAL
C *****
C
C PARAMETER (ITIME=24,NSEG=12,NSEG1=2)
C
C
C DIMENSION VOL(50,50),DO(50,50),BODU(50,50),SK6(50,50),R(50,50),
* TEMP(50),DOSAT(50),DOSAL(50),SATDO(50,50),
* VAR1(50,50),VAR2(50,50),Y(50,50),XK(50,50),
* VARMD1(50,50),VARME1(50,50)
C
C REAL K2,KD,DELT,M(50,50),M1(50,50),MY(50,50)
C
C OPEN DATA FILES
C *****
C
C OPEN(UNIT=5,FILE='KALDATA',STATUS='OLD',FORM='FORMATTED')
C OPEN(UNIT=6,FILE='KALRLT',STATUS='UNKNOWN',FORM='FORMATTED')
C
C READ INPUT DATA
C *****
C
C WRITE(6,1)
C DATA K2,KD,DELT/0.05,0.30,30/
C WRITE(6,2) K2,KD,DELT
C WRITE(6,3)
C DATA ITIME,NSEG/12,18/
C WRITE(6,4) ITIME,NSEG1
C
C READ THE VOLUME OF THE SEGMENTS AT DIFFERENT TIME PERIODS
C *****
C
C WRITE(6,5)
C DO 100 J=1,NSEG
C READ (5,7)(VOL(I,J),I=1,12)
C WRITE(6,6) J,(VOL(I,J),I=1,12)
100 CONTINUE
C DO 110 J=1,NSEG
C READ(5,7)(VOL(I,J),I=13,24)
C WRITE(6,6)J,(VOL(I,J),I=13,24)
110 CONTINUE
C
C
C READ THE ULTIMATE BOD LOADING FOR THE SEGMENTS DURING

```

```

C THE DIFFERENT MONTHS
C *****
C
C WRITE(6,10)
C WRITE(6,11)
C WRITE(6,5)
C DO 150 J=1,NSEG
C READ(5,7)(BODU(I,J),I=1,12)
C WRITE(6,6)J,(BODU(I,J),I=1,12)
150 CONTINUE
C
C DO 155 J=1,NSEG
C READ(5,7)(BODU(I,J),I=13,24)
C WRITE(6,6)J,(BODU(I,J),I=13,24)
155 CONTINUE
C READ THE DO SATURATION VALUES
C *****
C
C WRITE(6,12)
C WRITE(6,13)
C WRITE(6,5)
C READ(5,7)(DOSAT(I),I=1,ITIME)
C WRITE(6,6) J,(DOSAT(I),I=1,ITIME)
C READ(5,7)(DOSAL(I),I=1,ITIME)
C WRITE(6,6) J,(DOSAL(I),I=1,ITIME)
C
C
C
C READ THE FIELD MEASUREMENTS OF DISSOLVED OXYGEN
C *****
C
C DO 160 J=1,NSEG
C READ(5,7)(Y(I,J),I=1,12)
C WRITE(6,6) J,(Y(I,J),I=1,12)
160 CONTINUE
C
C DO 162 J=1,NSEG
C READ(5,7)(Y(I,J),I=13,24)
C WRITE(6,6)J,(Y(I,J),I=13,24)
162 CONTINUE
C
C
C REASSIGN VOLUMES AND MEASUREMENTS TO
C SUIT THE REDUCTION IN SEGMENTS
C *****
C
C WRITE(6,35)
C
C DO 165 I=1,ITIME
C VOL(I,1)=VOL(I,1)+VOL(I,2)+VOL(I,3)+VOL(I,4)
C VOL(I,2)=VOL(I,5)+VOL(I,6)+VOL(I,7)+VOL(I,8)
C VOL(I,1)=VOL(I,1)+VOL(I,2)
C VOL(I,2)=VOL(I,9)+VOL(I,10)+VOL(I,11)+VOL(I,12)
C BODU(I,1)=(BODU(I,1)+BODU(I,2)+BODU(I,3)+BODU(I,4))
C BODU(I,2)=(BODU(I,5)+BODU(I,6)+BODU(I,7)+BODU(I,8))
C BODU(I,1)=(BODU(I,1)+BODU(I,2))
C BODU(I,2)=(BODU(I,9)+BODU(I,10)+BODU(I,11)+BODU(I,12))
C Y(I,1) =Y(I,1)
C Y(I,2) =Y(I,9)
C WRITE(6,36)(VOL(I,L),BODU(I,L),Y(I,L),L=1,2)
C DO 164 K=4,NSEG1+1
C VOL(I,K-1)=VOL(I,K+7)
C BODU(I,K-1)=BODU(I,K+7)
C Y(I,K-1)=Y(I,K+7)
C WRITE(6,36) VOL(I,K-1),BODU(I,K-1),Y(I,K-1)
C 164 CONTINUE
165 CONTINUE
C
C QUANTITY OF OXYGEN IN THE SEGMENTS AS REFLECTED
C BY THE FIELD MESUREMENTS

```



```

C *****
C
C DO 170 J=1,NSEG1
C   DO 172 I=1,ITIME
C     MY(I,J)=VOL(I,J)*Y(I,J)*1000.0
172 CONTINUE
170 CONTINUE
C
C WRITE(6,23)((MY(I,J),I=1,ITIME),J=1,NSEG1)
C
C
C INITIALIZE THE SATURATION VALUES ACCORDING TO
C TIME, SEGMENTS, AND SALINITY
C *****
C
C DO 175 I=1,ITIME
C   DO 200 J=1,NSEG1-3
C     SATDO(I,1)=DOSAT(I)
C     WRITE(6,6) J,SATDO(I,J)
C 200 CONTINUE
175 CONTINUE
C
C DO 225 I=1,ITIME
C   DO 250 J=NSEG1-2,NSEG1
C     SATDO(I,2)=DOSAL(I)
C     WRITE(6,6) J,SATDO(I,J)
C 250 CONTINUE
225 CONTINUE
C
C READ THE INITIAL VALUE OF DO CONCENTRATION IN THE SEGMENTS
C *****
C
C WRITE(6,14)
C WRITE(6,15)
C WRITE(6,16)
C DO 275 J=1,NSEG1
C   DO(5,J)=Y(5,J)
C   WRITE(6,17) J,DO(5,J)
275 CONTINUE
C
C
C INITIAL MASS OF DO IN SEGMENTS
C *****
C
C WRITE(6,18)
C WRITE(6,19)
C   DO 300 J=1,NSEG1
C     M(5,J)=VOL(5,J)*DO(5,J)*1000.0
C     WRITE(6,20) J,M(5,J)
300 CONTINUE
C
C
C
C INITIAL VALUES OF VARIANCES
C *****
C
C DO 350 J=1,NSEG1
C   VAR1(5,J)=((VOL(5,J)*1000.)**2.0)*4.0
C   M1(5,J) =0.0
C   VAR2(5,J)=0.0
C   XK(5,J) =0.0
350 CONTINUE
C
C
C VARIANCE OF THE MODEL PREDICTION AND
C THE VARIANCE OF MEASUREMENTS
C *****
C
C WRITE(6,24)
C READ(5,34)VARMD,VARME
C WRITE(6,25) VARMD,VARME
C

```

```

C
C   CALCULATE THE ERRORS IN PREDICTION AND MEASUREMENTS FOR
C   EACH SEGMENT AND TIME PERIOD
C   *****
C
C   DO 360 I=1,ITIME
C     DO 362 J=1,NSEG1
C       VARMD1(I,J)={(VOL(I,J)*1000.0)**2.0}*VARMD
C       VARME1(I,J)={(VOL(I,J)*1000.0)**2.0}*VARME
362   CONTINUE
360   CONTINUE
C
C   WRITE(6,30)
C   WRITE(6,31)((VARMD1(I,J),I=1,ITIME),J=1,NSEG1)
C   WRITE(6,32)
C   WRITE(6,33)((VARME1(I,J),I=1,ITIME),J=1,NSEG1)
C
C
C   MASS DERIVATIVE AND EULER INTEGRATION
C   COMBINED WITH KALMAN FILTER ALGORITHM
C   *****
C
C   WRITE(6,26)
C   WRITE(6,27)
C
C
C   WRITE(6,21)
C     DO 400 I=5,ITIME
C       DO 500 J=1,NSEG1
C         SK6(I,J)=(K2*VOL(I,J)*(SATDO(I,J)-DO(I,J))-KD*BODU(I,J))*1000.
C         R(I,J) =SK6(I,J)*DELT
C
C   PRIOR FORECAST
C   *****
C
C     M(I+1,J)=M(I,J)+R(I,J)
C
C   FORECAST ERROR
C   *****
C
C     VAR1(I+1,J)=VAR1(I,J)+VARMD1(I,J)
C
C   FORECAST ERROR
C   *****
C
C     XK(I+1,J)=VAR1(I+1,J)/(VARME1(I,J)+VAR1(I+1,J))
C
C   FORECAST UPDATE
C   *****
C
C     M1(I+1,J)=M(I+1,J)+XK(I+1,J)*(MY(I+1,J)-M(I+1,J))
C     DO(I+1,J)=M1(I+1,J)/(VOL(I,J)*1000.0)
C
C
C   VARIANCE UPDATE
C   *****
C
C     VAR2(I+1,J)=(1-XK(I+1,J))*VAR1(I+1,J)
C
C
C   THE UPDATED FORECAST AND THE VARIANCE ARE USED TO
C   MAKE A PRIOR FORECAST AND THE VARIANCE OF THE
C   FORECAST
C   *****
C
C     M(I+1,J)=M1(I+1,J)
C     VAR1(I+1,J)=VAR2(I+1,J)
C
C     IF(DO(I+1,J).LE.0.0) THEN
C       DO(I+1,J)=0.0

```

```

      ENDIF
      WRITE(6,22) J,M(I+1,J),M(I,J),R(I,J),DO(I+1,J)
C
C      IF((I+1).EQ.ITIME) THEN
      GO TO 1000
      ENDIF
500    CONTINUE
C
C 400    CONTINUE
C
C 1000  WRITE(6,28)
      WRITE(6,29) ((M(I,J),VAR1(I,J),M1(I,J),VAR2(I,J),
      *           XK(I,J),I=5,ITIME),J=1,NSEG1)
C
C
C
C
C 1000  STOP
C      FORMAT STATEMENTS
C      *****
C
1    FORMAT(// ' REAERATION-K2    DEOXYGENATION-KD    TIME-DELT')
2    FORMAT(/F14.3,F20.3,F13.2)
3    FORMAT(// ' TIME PERIOD    NUMBER OF SEGMENTS')
4    FORMAT(/I12,I21)
5    FORMAT(// 'SEGMENT    JAN    FEB    MAR    APR    MAY    JUN
      *    JUL    AUG    SEP    OCT    NOV    DEC')
6    FORMAT(/I7,12E8.2)
7    FORMAT(12F7.2)
8    FORMAT(// 'SEGMENT NUMBERS AND VOLUMES')
9    FORMAT('*****')
10   FORMAT(// 'SEGMENT NUMBERS AND ULTIMATE BOD LOADING')
11   FORMAT('*****')
12   FORMAT(// 'DISSOLVED OXYGEN - DO SATURATION VALUES')
13   FORMAT('*****')
14   FORMAT(// 'INITIAL DO CONCENTRATION VALUES MG/L')
15   FORMAT('*****')
16   FORMAT(// ' SEGMENT    DO MG/L')
17   FORMAT(/I8,F10.1)
18   FORMAT(// 'INITIAL MASS OF DO IN SEGMENTS - KG')
19   FORMAT('*****')
20   FORMAT(/I8,F12.2)
21   FORMAT(// 'SEGMENT    MASS(T+1)    MASS(T)    R(T)    DO(T+1)')
22   FORMAT(/I7,4F11.2)
23   FORMAT(/12E10.2)
24   FORMAT(/ ' VARM    VARME')
25   FORMAT(/2F7.2)
26   FORMAT(// ' RESULTS FROM KALMAN FILTER ALGORITHM')
27   FORMAT(' *****')
28   FORMAT(// '    M(I,J)    VAR1(I,J)    M1(I,J)    VAR2(I,J)
      *    XK(I,J)')
29   FORMAT(/5E15.5)
30   FORMAT(// 'MODEL VARIANCES - KG')
31   FORMAT(/12E10.2)
32   FORMAT(// 'MEASUREMENT VARIANCES - KG')
33   FORMAT(/12E10.2)
34   FORMAT(2F7.2)
35   FORMAT(// 'RECALCULATED VALUES TO SUIT REDUCTION IN SEGMENTS')
36   FORMAT(/3F8.2)
C
C
C      END

```

APPENDIX A-8

TYPICAL OUTPUT FROM PROGRAM EULKAL

REAERATION-K2 DEOXYGENATION-KD TIME-DELT
 .050 .300 30.00

TIME PERIOD NUMBER OF SEGMENTS
 24 2

SEGMENT	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
1	.41E+01	.41E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.41E+01
2	.16E+02	.16E+02	.16E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.16E+02	.16E+02
3	.16E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02
4	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02
5	.11E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02
6	.18E+02	.18E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.18E+02
7	.55E+02	.55E+02	.55E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.55E+02
8	.25E+02	.26E+02	.27E+02	.27E+02	.27E+02	.27E+02	.27E+02	.27E+02	.28E+02	.27E+02	.27E+02	.26E+02
9	.72E+03	.72E+03	.73E+03	.73E+03	.73E+03	.73E+03	.73E+03	.73E+03	.73E+03	.73E+03	.73E+03	.72E+03
10	.12E+04	.12E+04	.12E+04	.13E+04	.13E+04	.13E+04	.13E+04	.13E+04	.13E+04	.13E+04	.12E+04	.12E+04
11	.33E+04	.33E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.33E+04
12	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04
1	.41E+01	.41E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.42E+01	.43E+01	.42E+01	.42E+01	.41E+01
2	.16E+02	.16E+02	.16E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.16E+02	.16E+02
3	.16E+02	.16E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.17E+02	.16E+02
4	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.13E+02	.14E+02	.13E+02	.13E+02	.13E+02
5	.11E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.12E+02	.11E+02
6	.18E+02	.18E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.19E+02	.20E+02	.19E+02	.19E+02	.18E+02
7	.55E+02	.55E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.56E+02	.55E+02
8	.25E+02	.26E+02	.26E+02	.27E+02	.27E+02	.27E+02	.27E+02	.28E+02	.28E+02	.27E+02	.27E+02	.26E+02
9	.77E+03	.77E+03	.78E+03	.78E+03	.78E+03	.78E+03	.78E+03	.79E+03	.79E+03	.78E+03	.78E+03	.77E+03
10	.12E+04	.12E+04	.12E+04	.13E+04	.13E+04	.13E+04	.13E+04	.13E+04	.13E+04	.13E+04	.12E+04	.12E+04
11	.33E+04	.33E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.34E+04	.33E+04
12	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04	.17E+04

SEGMENT NUMBERS AND ULTIMATE BOD LOADING

SEGMENT	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
1	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
2	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
3	.14E+01	.22E+01	.23E+01	.22E+01	.17E+01	.94E+00	.64E+00	.87E+00	.11E+01	.12E+01	.17E+01	.21E+01

4	.24E+02	.19E+02	.60E+02	.48E+02	.41E+02	.26E+02	.35E+02	.32E+02	.31E+02	.29E+02	.17E+02	.16E+02
5	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
6	.46E+01	.44E+01	.57E+01	.53E+01	.51E+01	.38E+01	.40E+01	.35E+01	.40E+01	.63E+01	.57E+01	.54E+01
7	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
8	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
9	.12E+01	.11E+01	.12E+01	.16E+01	.14E+01	.12E+01	.11E+01	.12E+01	.81E+00	.14E+01	.10E+01	.90E+00
10	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
11	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
12	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
1	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
2	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
3	.14E+01	.22E+01	.23E+01	.22E+01	.17E+01	.94E+00	.64E+00	.87E+00	.11E+01	.12E+01	.17E+01	.21E+01
4	.24E+02	.19E+02	.60E+02	.48E+02	.41E+02	.26E+02	.35E+02	.32E+02	.31E+02	.29E+02	.17E+02	.16E+02
5	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
6	.46E+01	.44E+01	.57E+01	.53E+01	.51E+01	.38E+01	.40E+01	.35E+01	.40E+01	.63E+01	.57E+01	.54E+01
7	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
8	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
9	.12E+01	.11E+01	.12E+01	.16E+01	.14E+01	.12E+01	.11E+01	.12E+01	.81E+00	.14E+01	.10E+01	.90E+00
10	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
11	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
12	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01	.50E+01
1	.00E+00	.00E+00	.00E+00	.00E+00	.78E+01	.96E+01	.70E+01	.70E+01	.90E+01	.11E+02	.11E+02	.14E+02
2	.00E+00	.00E+00	.00E+00	.00E+00	.83E+01	.95E+01	.66E+01	.66E+01	.72E+01	.90E+01	.96E+01	.12E+02
3	.00E+00	.00E+00	.00E+00	.00E+00	.86E+01	.88E+01	.65E+01	.52E+01	.55E+01	.82E+01	.80E+01	.11E+02
4	.00E+00	.00E+00	.00E+00	.00E+00	.79E+01	.87E+01	.57E+01	.47E+01	.57E+01	.87E+01	.78E+01	.10E+02
5	.00E+00	.00E+00	.00E+00	.00E+00	.72E+01	.86E+01	.49E+01	.42E+01	.59E+01	.91E+01	.75E+01	.10E+02
6	.00E+00	.00E+00	.00E+00	.00E+00	.56E+01	.85E+01	.42E+01	.45E+01	.61E+01	.84E+01	.69E+01	.10E+02
7	.00E+00	.00E+00	.00E+00	.00E+00	.79E+01	.85E+01	.11E+02	.54E+01	.73E+01	.10E+02	.88E+01	.11E+02
8	.00E+00	.00E+00	.00E+00	.00E+00	.63E+01	.88E+01	.46E+01	.60E+01	.73E+01	.10E+02	.93E+01	.11E+02
9	.00E+00	.00E+00	.00E+00	.00E+00	.74E+01	.72E+01	.77E+01	.66E+01	.77E+01	.11E+02	.10E+02	.11E+02
10	.00E+00	.00E+00	.00E+00	.00E+00	.66E+01	.59E+01	.32E+01	.51E+01	.70E+01	.10E+02	.94E+01	.11E+02
11	.00E+00	.00E+00	.00E+00	.00E+00	.66E+01	.61E+01	.38E+01	.66E+01	.74E+01	.93E+01	.10E+02	.11E+02
12	.00E+00	.00E+00	.00E+00	.00E+00	.66E+01	.63E+01	.44E+01	.81E+01	.78E+01	.85E+01	.11E+02	.11E+02
1	.13E+02	.14E+02	.11E+02	.13E+02	.66E+01	.77E+01	.66E+01	.65E+01	.78E+01	.84E+01	.12E+02	.12E+02
2	.13E+02	.13E+02	.11E+02	.11E+02	.92E+01	.58E+01	.68E+01	.61E+01	.75E+01	.82E+01	.13E+02	.15E+02
3	.12E+02	.13E+02	.11E+02	.12E+02	.84E+01	.85E+01	.67E+01	.60E+01	.68E+01	.84E+01	.10E+02	.12E+02

4	.12E+02	.12E+02	.11E+02	.12E+02	.84E+01	.92E+01	.67E+01	.63E+01	.66E+01	.84E+01	.10E+02	.12E+02
5	.11E+02	.13E+02	.11E+02	.12E+02	.84E+01	.96E+01	.65E+01	.59E+01	.68E+01	.81E+01	.10E+02	.12E+02
6	.11E+02	.12E+02	.11E+02	.12E+02	.84E+01	.86E+01	.52E+01	.60E+01	.72E+01	.82E+01	.98E+01	.13E+02
7	.12E+02	.13E+02	.11E+02	.11E+02	.77E+01	.75E+01	.50E+01	.59E+01	.75E+01	.80E+01	.10E+02	.12E+02
8	.13E+02	.13E+02	.11E+02	.12E+02	.76E+01	.74E+01	.51E+01	.86E+01	.10E+02	.89E+01	.10E+02	.12E+02
9	.13E+02	.13E+02	.13E+02	.11E+02	.86E+01	.66E+01	.70E+01	.96E+01	.80E+01	.85E+01	.10E+02	.12E+02
10	.12E+02	.11E+02	.96E+01	.85E+01	.70E+01	.43E+01	.44E+01	.40E+01	.43E+01	.69E+01	.93E+01	.10E+02
11	.12E+02	.11E+02	.11E+02	.98E+01	.82E+01	.54E+01	.44E+01	.32E+01	.60E+01	.85E+01	.96E+01	.10E+02
12	.12E+02	.11E+02	.13E+02	.11E+02	.94E+01	.64E+01	.44E+01	.23E+01	.77E+01	.10E+02	.99E+01	.10E+02

RECALCULATED VALUES TO SUIT REDUCTION IN SEGMENTS

158.45	55.16	.00
6955.22	16.16	.00
160.18	50.95	.00
6971.65	16.13	.00
163.07	93.36	.00
7005.98	16.23	.00
166.05	80.10	.00
7030.02	16.61	.00
166.87	72.70	7.80
7037.38	16.39	7.40
166.48	55.58	9.60
7033.77	16.16	7.20
165.84	64.67	7.00
7027.43	16.09	7.70
166.67	61.29	7.00
7035.90	16.16	6.60
167.54	60.83	9.00
7044.75	15.81	7.70
166.68	61.13	10.80
7035.90	16.39	10.60
163.38	49.78	10.80
7004.20	16.03	10.30
160.18	48.70	13.70
6971.64	15.90	10.50
158.27	55.16	13.20
7006.51	16.16	12.50

159.72	50.95	13.80
7020.60	16.13	13.30
162.62	93.36	11.00
7060.39	16.23	12.90
165.65	80.10	12.60
7088.95	16.61	10.80
166.14	72.70	6.60
7094.96	16.39	8.60
166.14	55.58	7.70
7092.10	16.16	6.60
166.14	64.67	6.60
7094.96	16.09	7.00
166.74	61.29	6.50
7107.36	16.16	9.60
168.09	60.83	7.80
7116.58	15.81	8.00
166.59	61.13	8.40
7095.59	16.39	8.50
163.21	49.78	12.40
7060.38	16.03	10.20
159.29	48.70	12.20
7017.27	15.90	11.80

.00E+00	.00E+00	.00E+00	.00E+00	.13E+07	.16E+07	.12E+07	.12E+07	.15E+07	.18E+07
.18E+07	.22E+07								
.21E+07	.22E+07	.18E+07	.21E+07	.11E+07	.13E+07	.11E+07	.11E+07	.13E+07	.14E+07
.20E+07	.19E+07								
.00E+00	.00E+00	.00E+00	.00E+00	.52E+08	.51E+08	.54E+08	.46E+08	.54E+08	.75E+08
.72E+08	.73E+08								
.88E+08	.93E+08	.91E+08	.77E+08	.61E+08	.47E+08	.50E+08	.68E+08	.57E+08	.60E+08
.72E+08	.83E+08								

INITIAL DO CONCENTRATION VALUES MG/L

SEGMENT	DO MG/L
1	7.8
2	7.4

INITIAL MASS OF DO IN SEGMENTS - KG

1 1301586.00

2 52076612.00

VARMD VARME

2.00 2.00

MODEL VARIANCES - KG

.50E+11	.51E+11	.53E+11	.55E+11	.56E+11	.55E+11	.55E+11	.56E+11	.56E+11	.56E+11
.53E+11	.51E+11								
.50E+11	.51E+11	.53E+11	.55E+11	.55E+11	.55E+11	.55E+11	.56E+11	.57E+11	.56E+11
.53E+11	.51E+11								
.97E+14	.97E+14	.98E+14	.99E+14	.99E+14	.99E+14	.99E+14	.99E+14	.99E+14	.99E+14
.98E+14	.97E+14								
.98E+14	.99E+14	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15
.10E+15	.98E+14								

MEASUREMENT VARIANCES - KG

.50E+11	.51E+11	.53E+11	.55E+11	.56E+11	.55E+11	.55E+11	.56E+11	.56E+11	.56E+11
.53E+11	.51E+11								
.50E+11	.51E+11	.53E+11	.55E+11	.55E+11	.55E+11	.55E+11	.56E+11	.57E+11	.56E+11
.53E+11	.51E+11								
.97E+14	.97E+14	.98E+14	.99E+14	.99E+14	.99E+14	.99E+14	.99E+14	.99E+14	.99E+14
.98E+14	.97E+14								
.98E+14	.99E+14	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15	.10E+15
.10E+15	.98E+14								

RESULTS FROM KALMAN FILTER ALGORITHM

1	1429937.14	1301586.00	-376461.45	8.57
	250304879.1352076612.00	-2786527.50		7.15
1	1018054.28	1429937.14	-662330.34	6.12
	249804711.1450304879.13	-8039858.97		7.08
1	1109022.92	1018054.28	-3706.45	6.69
	246416764.3749804711.14	-3420986.67		6.61
1	1296691.86	1109022.92	-153428.68	7.78
	251421889.3846416764.37	434136.85		7.31
1	1493924.55	1296691.86	-296158.89	8.92
	263904922.3451421889.38	-4775995.69		9.07
1	1494838.72	1493924.55	-436866.73	8.97
	262570625.9463904922.34	*****		8.89
1	2048831.92	1494838.72	314560.68	12.54
	271565678.0262570625.94	6337568.73		10.22
1	1888339.35	2048831.92	-491228.11	11.79
	279323013.8771565678.02	-5659805.08		11.38

1	2097899.38	1888339.35	35618.21	13.26
	286138858.0379323013	87-4853353.35		12.29
1	1660374.72	2097899.38	-644270.71	10.40
	279089346.4286138858	03*****		11.27
1	1731881.51	1660374.72	-495209.35	10.65
	269581659.8979089346	42*****		9.86
1	1104753.79	1731881.51	-614022.92	6.67
	259820618.4069581659	89*****		8.44
1	1245388.77	1104753.79	86051.86	7.50
	249290549.8159820618	40-6517781.74		6.95
1	1089296.47	1245388.77	-167778.86	6.56
	250046216.0849290549	81 1373022.54		7.06
1	1021934.63	1089296.47	-167468.51	6.15
	259453081.0550046216	08-4791454.19		8.38
1	1187397.29	1021934.63	-34143.69	7.12
	250669040.0659453081	05*****		7.13
1	1244329.00	1187397.29	-192274.92	7.40
	255392305.2350669040	06-3228334.67		7.78
1	1721031.04	1244329.00	-16104.40	10.33
	264954082.4555392305	23-1888308.86		9.15
1	1832372.98	1721031.04	-71234.65	11.23

M(I,J)	VAR1(I,J)	M1(I,J)	VAR2(I,J)	XK(I,J)
.13016E+07	.11138E+12	.00000E+00	.00000E+00	.00000E+00
.14299E+07	.41768E+11	.14299E+07	.41768E+11	.75000E+00
.10181E+07	.35300E+11	.10181E+07	.35300E+11	.63683E+00
.11090E+07	.34184E+11	.11090E+07	.34184E+11	.62146E+00
.12967E+07	.34314E+11	.12967E+07	.34314E+11	.61763E+00
.14939E+07	.34640E+11	.14939E+07	.34640E+11	.61704E+00
.14948E+07	.34384E+11	.14948E+07	.34384E+11	.61882E+00
.20488E+07	.33195E+11	.20488E+07	.33195E+11	.62180E+00
.18883E+07	.31928E+11	.18883E+07	.31928E+11	.62220E+00
.20979E+07	.31103E+11	.20979E+07	.31103E+11	.62083E+00
.16604E+07	.31470E+11	.16604E+07	.31470E+11	.61680E+00
.17319E+07	.32509E+11	.17319E+07	.32509E+11	.61464E+00
.11048E+07	.33710E+11	.11048E+07	.33710E+11	.61425E+00
.12454E+07	.34059E+11	.12454E+07	.34059E+11	.61695E+00

.10893E+07	.34110E+11	.10893E+07	.34110E+11	.61788E+00
.10219E+07	.34117E+11	.10219E+07	.34117E+11	.61801E+00
.11874E+07	.34329E+11	.11874E+07	.34329E+11	.61738E+00
.12443E+07	.34837E+11	.12443E+07	.34837E+11	.61649E+00
.17210E+07	.34381E+11	.17210E+07	.34381E+11	.61943E+00
.18324E+07	.33136E+11	.18324E+07	.33136E+11	.62198E+00
.52077E+08	.19810E+15	.00000E+00	.00000E+00	.00000E+00
.50305E+08	.74287E+14	.50305E+08	.74287E+14	.75000E+00
.49805E+08	.62977E+14	.49805E+08	.62977E+14	.63647E+00
.46417E+08	.61323E+14	.46417E+08	.61323E+14	.62087E+00
.51422E+08	.61210E+14	.51422E+08	.61210E+14	.61823E+00
.63905E+08	.61325E+14	.63905E+08	.61325E+14	.61784E+00
.62571E+08	.61210E+14	.62571E+08	.61210E+14	.61823E+00
.71566E+08	.60723E+14	.71566E+08	.60723E+14	.61888E+00
.79323E+08	.60171E+14	.79323E+08	.60171E+14	.61900E+00
.86139E+08	.60606E+14	.86139E+08	.60606E+14	.61728E+00
.79089E+08	.60878E+14	.79089E+08	.60878E+14	.61756E+00
.69582E+08	.61509E+14	.69582E+08	.61509E+14	.61695E+00
.59821E+08	.62028E+14	.59821E+08	.62028E+14	.61715E+00
.49291E+08	.62193E+14	.49291E+08	.62193E+14	.61775E+00
.50046E+08	.62175E+14	.50046E+08	.62175E+14	.61807E+00
.59453E+08	.62215E+14	.59453E+08	.62215E+14	.61797E+00
.50669E+08	.62407E+14	.50669E+08	.62407E+14	.61771E+00
.55392E+08	.62573E+14	.55392E+08	.62573E+14	.61775E+00
.64954E+08	.62282E+14	.64954E+08	.62282E+14	.61853E+00
-I	-I	-I	-I	-I

APPENDIX A-9

STATISTICAL ANALYSIS OF DO DATA FOR TRENDS-POTOMAC ESTUARY

APPENDIX A-9

STATISTICAL ANALYSIS OF DO DATA FOR TRENDS-POTOMAC ESTUARY

A9.1 Introduction

Statistical analysis for trends in water quality was outside the scope of the main dissertation. However, it forms part of the water quality management strategy formulated in Chapter 3. For completeness sake, the analysis of trends using the non-parametric Mann-Kendall test is discussed in this section.

The section covers the following topics:

- (i) Data collection effort used for trend analysis
- (ii) Choice of test and assumptions
- (iii) Water quality trends in the Potomac estuary
- (iv) Discussion of results.

A9.2 Data Collection

A9.2.1 Data for Analysis

The U. S. Environmental Protection Agency (USEPA), the U. S. Geological Survey (USGS), and the Metropolitan Washington Council of Governments (MWCOG) were involved in collecting water quality data for the Potomac estuary. It was possible to abstract 10 years (1977-1986) of data for the summer months of July, August and September from reports published by these agencies [1-7]. A brief description of the data collection effort by the agencies is given in the following sections. Details can be obtained from references [1-7].

A9.2.2 EPA's Program 1977-1978

Observations were made between 9.00 and 16.00 hours in 23 stations for a length of 67 miles. The stretch extended between Chain Bridge, Washington D. C. and Route 301 Bridge. All the stations were sampled along the main channel near the surface [2,3].

A9.2.3 U. S. Geological Survey 1979-1981

The USGS conducted an interdisciplinary study of the Potomac estuary for three years. The data collection effort was to satisfy the needs of research and water quality assessment. Altogether, 29 stations were sampled between Point Lookout and Chain Bridge, Washington D. C. At a given location measurements were taken laterally (across the river), as well as vertically (depthwise). Further measurements were taken throughout the day at predetermined intervals. Such continuous measurements lasted for 4-5 days [1,4,5,6].

A9.2.4 MWCOG Monitoring Program 1982-1986

The Metropolitan Washington Council of Governments organized a regional monitoring program in 1982 for the Potomac River. About eleven agencies were involved in the data collection program. A total of 59 stations were established within 43 miles upstream and 107 miles downstream of Chain Bridge [7]. The frequency of sampling varied; weekly, fortnightly and monthly. While on some occasions the sampling was done at various depths, on several occasions it was done just below the water surface.

A9.2.5 Selection of Stations for the Analysis

Although the names of the stations were the same in the three monitoring efforts, the distances as measured from the reference station, Chain Bridge, Washington D. C., varied. While the USGS

reports the distance from Chain Bridge to the mid point of a line joining Point Lookout and Smith Point as 116 miles, MWCOG reports it as 107.4 miles [7]. The positions of stations along the length of the river are shown in Figures A9.1 and A9.2. It was possible to select a set of stations from these figures, which would have a 10 year data set. However, when values were extracted from all the reports, observations were missing for some years in some stations. A summary of the stations selected for the analysis is given in Table A9.1.

If, for a particular year, data was not available at a given location, then data from the closest station to this point was taken. It was assumed that this station was representative of the former station. In this manner it was possible to select eleven sections which would have a 10 year data set. Owing to the manner of selection, sections may be located within a range of ± 2.5 miles.

A9.3 Choice of Statistical Test

Using dissolved oxygen (DO) as an indicator of water quality, water quality managers need to know the estuary's dissolved oxygen behavior in the past; its present state; and its behavior in the future. The statistical analysis of past data may indicate 'trends', which will help the manager make future predictions. Hence, a statistical analysis of past data to detect trends was carried out for selected months in the summer; July, August and September.

In general, data from environmental systems do not fit any particular distribution. Fitting data to distributions was not the intention; detecting trends for these months was the aim. As non-parametric tests do not assume a particular distribution of data, Mann-Kendall test for trend, a non parametric test, was selected.

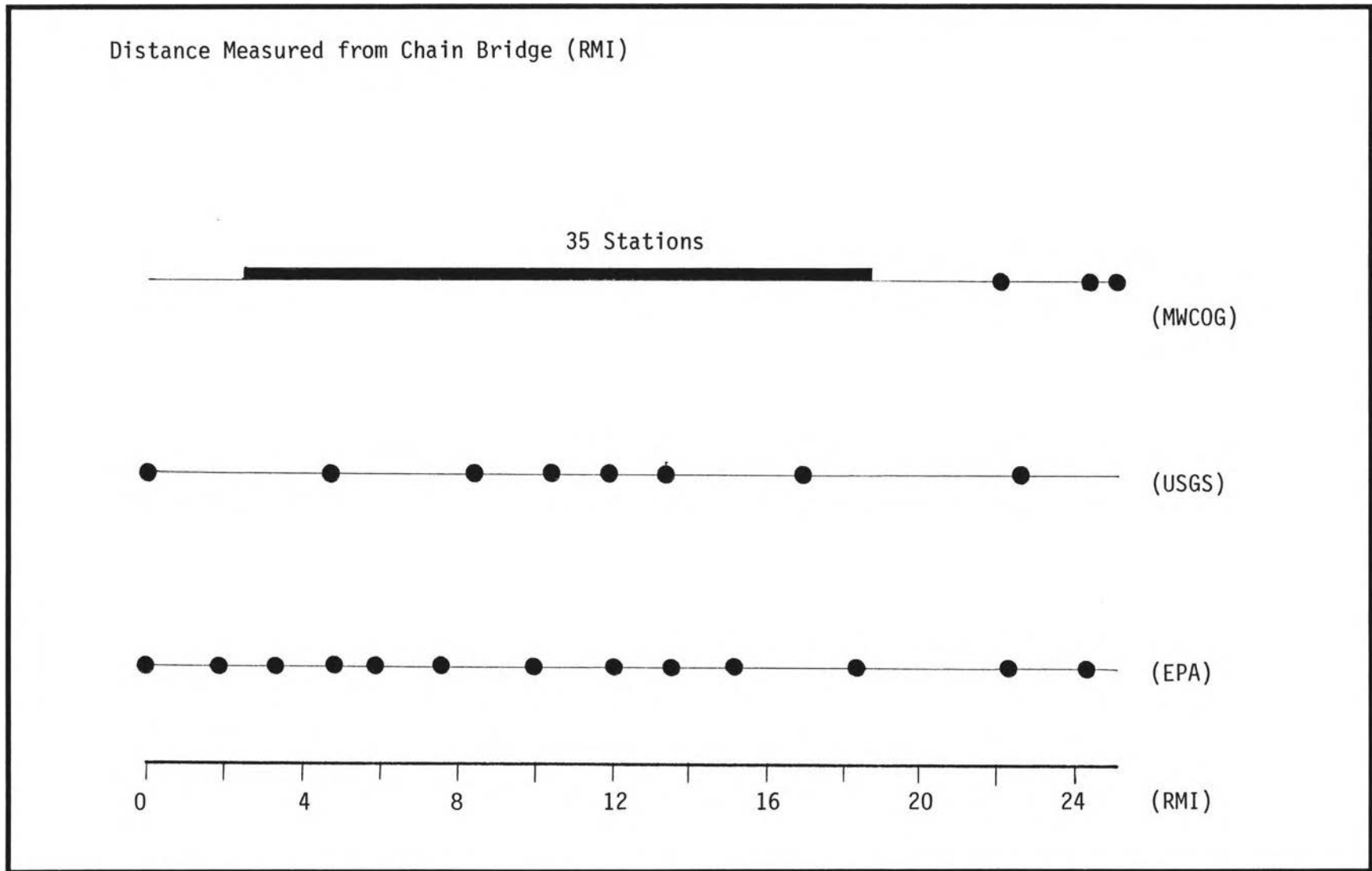


Figure A9.1. Positions of Stations (I).

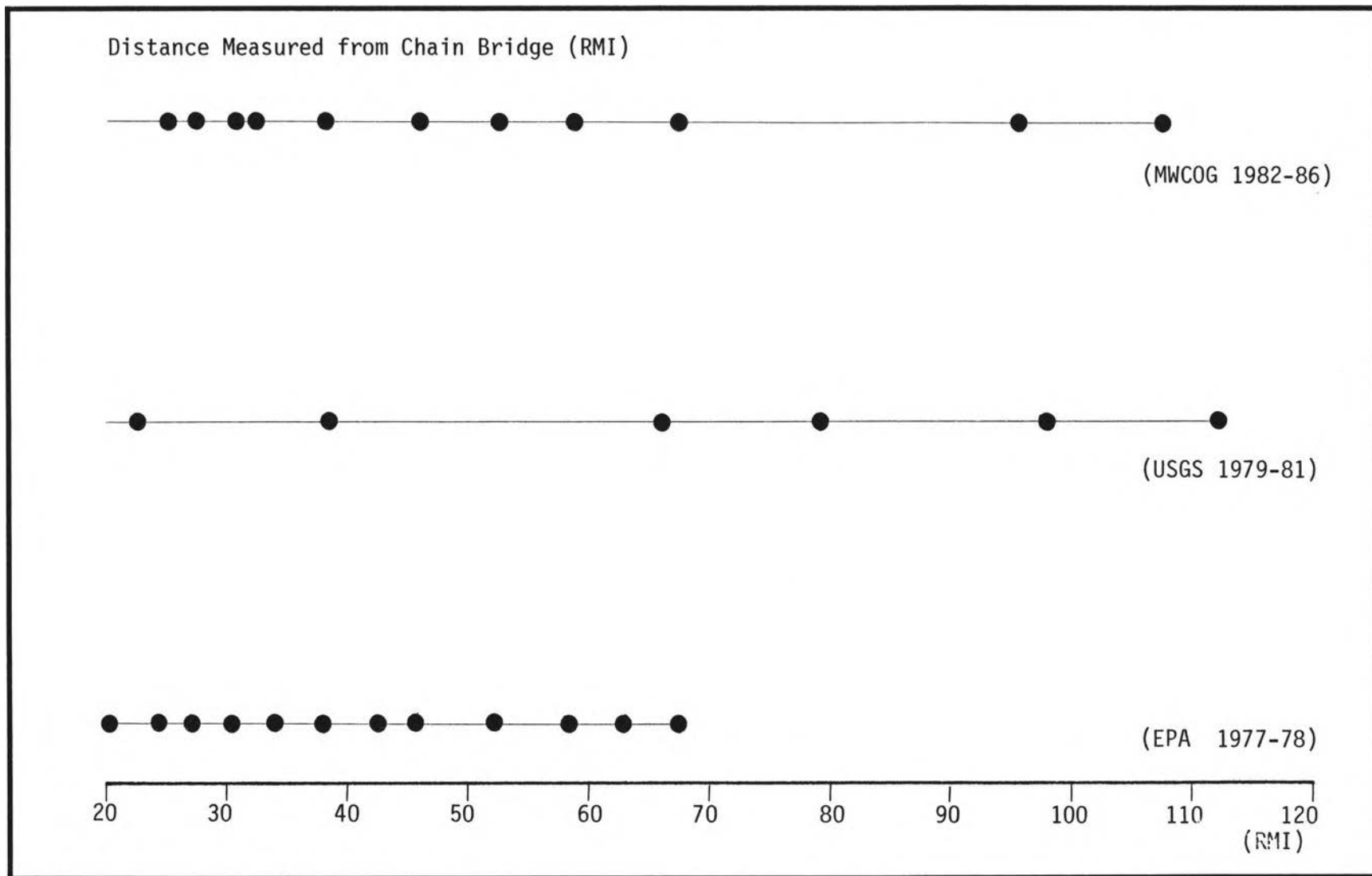


Figure A9.2. Positions of Stations (II).

Table A9-1. Agencies, Names of Stations and Distances from Chain Bridge, Washington D.C. in Miles.

STATION NAMES	AGENCY		
	EPA	USGS	MWCOG
1. Memorial Bridge Memorial Bridge Memorial Bridge	4.85	4.70	4.90
2. Hains Point Geisboro Point/Hains Point (MWCOG) Geisboro Point South	7.60	8.40	8.40 8.50
3. Bellevue Marbury Point/Naval Research Lab.	10.00	10.40	10.40
4. Alexandria Woodrow Wilson Bridge	12.10	11.90	12.10
5. Rosier Bluff	13.60	13.40	13.60
6. Hatton Point Buoy C "83" Fort Washington (Piscataway) Piscataway	18.35	16.90	17.00 18.50 18.70
7. Potomac @ Dogue Creek Dogue Creek @ Marshall Hall	22.30	22.50	22.00
8. Possum Point Quantico	38.00	38.25	38.00
9. Morgan Town Route 301 Bridge	67.40	66.37	67.40
10. Ragged Point Piney Point		97.80	95.50
11. Point Lookout Potomac Chesapeake Bay Boundary		112.00	107.40

Many reports and documents published by the various agencies usually claim to contain a complete set of data, that is, field observations. When you actually extract the data from these reports, observations are not recorded in a sequence. Some observations will be missing. These so called "missing data points" is common. The data reports of Potomac estuary are no exception. The non-parametric Mann-Kendall test for trend, takes into account missing data points, and the selection of this test is appropriate. The details of this test are explained well in reference [8]. Such tests had been previously used to detect trends [9,10].

Criticism may be leveled against the use of the mean as the test statistic. The main handicap was that, as reported in the different reports, there was no fixed pattern on the selection of the number of observations for evaluating the DO concentration. On some occasions more than 50 observations were available, both laterally and vertically, to calculate the mean, while, on other occasions there were only 1 or 2 values. In order to be consistent the mean was used.

Another shortcoming was the averaging over the depth. An examination of the raw data showed that, at depths greater than 12.0 m, the DO concentration was zero. This may have caused the trend to go down in some sections. It is possible to divide each section into three vertical segments according to depth, 0-1.5, 1.5-5.0 and >5.0 m, and carry out a statistical analysis. However, as our motive was designing monitoring systems using models, further analysis was not carried out.

A9.4 Water Quality Trends in the Potomac (Mann-Kendall Test)

The mean value of the dissolved oxygen (DO) was selected to detect trends, that is, trends in mean were studied. The results of the Mann-Kendall test for the months of July, August and September are shown in Tabular format in Table A9.2, and graphically illustrated in Figure A9.3. The mean values used for the analysis is given in Appendix A-1.

A9.5 Discussion

The results of Mann-Kendall test were presented earlier for a confidence level of 90%, in Figure A9.3 and Table A9.2.

Trend in July: The analysis showed that there was no trend except in sections 8 and 11. In section 8, there was a downward trend, while in section 11, there was an upward trend. If the analysis had shown that there had been either an upward trend, or a downward trend, in all of the sections, we could have tested the hypothesis that there was

Table A9-2 Description of Trend in the Various Sections of the Potomac Estuary.

Section	July			August			September		
	NT	UT	DT	NT	UT	DT	NT	UT	DT
1	X			X			X		
2	X			X				X	
3	X			X				X	
4	X			X				X	
5	X			X				X	
6	X			X				X	
7	X			X			X		
8			X	X			X		
9	X			X					X
10	X			X			X		
11		X			X			X	

NT: No trend; UT: Upwards trend; DT: Downwards trend

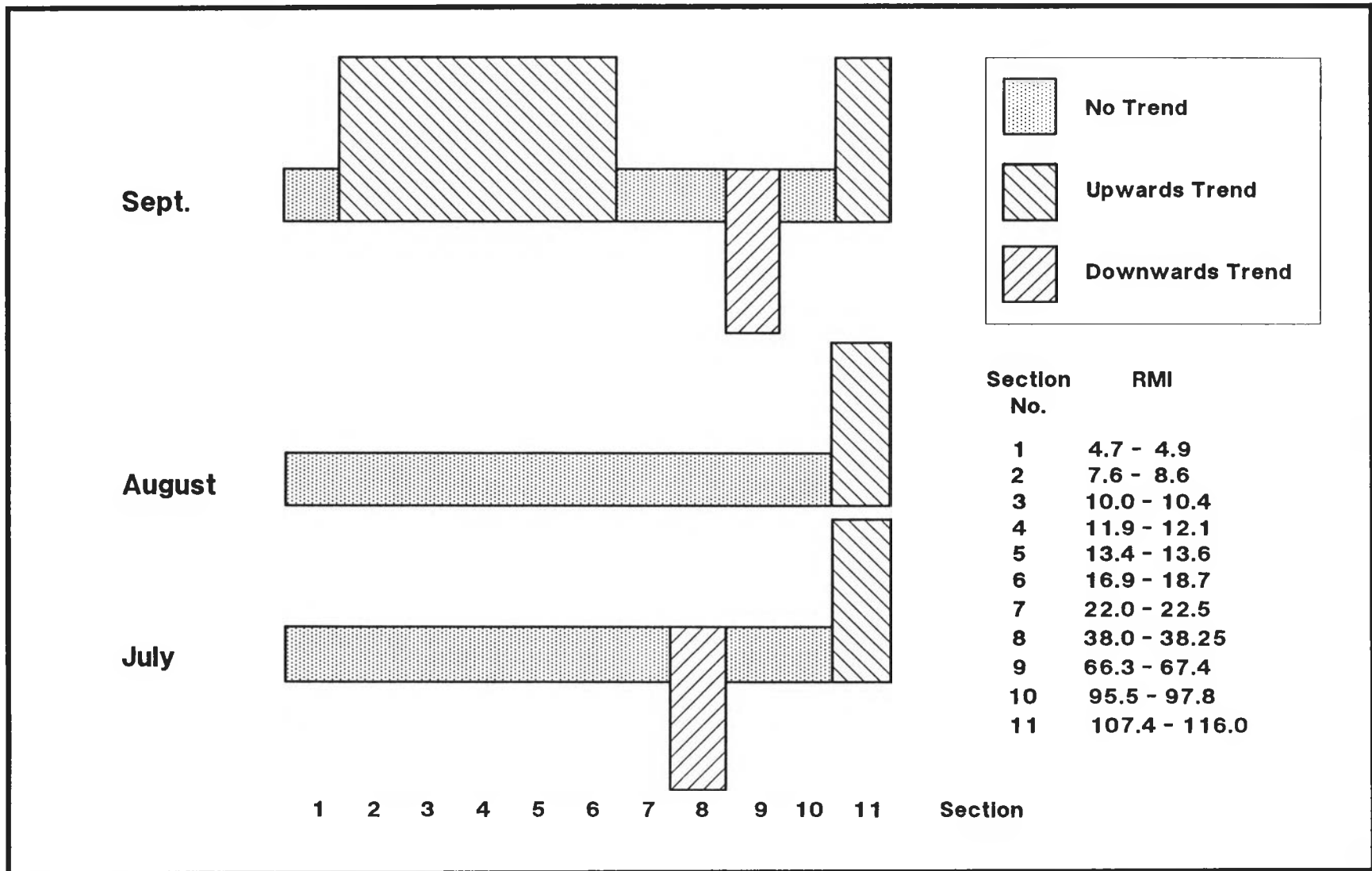


Figure A9.3. Trends in Mean - DO.

either an upward trend or a downward trend for the entire length of the estuary.

Trend in August: It was found that for the month of August, there was no trend in sections 1 to 10. However, there was an upward trend in section 11. For reasons mentioned in the previous paragraph, no comment can be made for the full length of the estuary.

Trend in September: It was interesting to find that a larger number of sections showed an upward trend for the month of September. While sections 1, 7, 8 and 10 did not show any trend, sections 2 to 6 and section 11, showed an upward trend. A downward trend was observed in section 9.

Although the present analysis did not show any trend, Haywood et al. [10], using Kendall-Tau test, concluded that there was an upward trend in the Potomac River for the period 1973-1984. It is felt that the analysis is different; in this particular research, data for 10 years for the months of July, August and September (1977-86) was considered. However, Haywood et al. considered data irrespective of months and for a different period 1973-1984. It appears that scientists still do not understand the water quality attributes of estuaries. Several billions of dollars were spent on modifying treatment plants for removing phosphorous and thus preventing algae growth in the Potomac. However, "The summer of 1983 was marked by a massive bloom of blue-green algae... Upper Potomac... for the first time in about a decade... In 1984 another algal bloom occurred" [10]. The above statements appear to corroborate the conclusion that the behavior of the estuary in relation to water quality is not well understood; or the estuary is behaving in its own way.