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APPLICATION OF MULTILEVEL CONTROL TECHNIQUES TO CLASSES OF DISTRIBUTED PARAMETER PLANTS

BY

FREDERICK DONALD CHICHESTER

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ABSTRACT

This study concerns the application of a combination of multilevel hierarchical systems analysis techniques and Pontryagin's minimum principle (multilevel control) to the problem of controlling optimally two classes of dynamic distributed parameter plants representing concentrations balances in streams, rivers and estuaries. The concentrations treated in this study are those deemed the most effective indicators of water quality, dissolved oxygen (DO) and biochemical oxygen demand (BOD).

One class of plants treated in this study consists of linear continuous distributed parameter plants represented mathematically by sets of simultaneous partial differential equations. Optimal control of a plant of this class is initiated by applying spatial discretization followed by a combination of multilevel techniques and Pontryagin's minimum principle for lumped parameter systems. This approach reduces the original problem of optimally controlling a distributed parameter plant to a hierarchy of subproblems comprised of ordinary differential and algebraic equations that can be solved iteratively.

A general two-dimensional plant representative of a class of two-step discrete dynamic distributed parameter

plants is derived from mass balances at the faces of a model of a volume element of a waterway. The resulting set of simultaneous finite-difference equations represents dynamic balances of concentrations at a finite number of spatial points in a reach of a waterway at selected time instants. Application of Pontryagin's minimum principle for discrete systems in conjunction with multilevel hierarchical systems analysis techniques reduces the problem of controlling such a plant optimally to a hierarchy of subproblems to be solved iteratively.

Implicit in the application of optimal control to a plant is the selection of a suitable performance index functional with which to measure the relative optimality of each solution iteration. A variety of performance indices based upon physical considerations is utilized in conjunction with several different control modes for a number of plants representative of the two classes treated in this study.

Subproblem hierarchies corresponding to both continuous and discrete distributed parameter plants representing concentrations balances in waterway reaches subject to multilevel optimal control are aggregated into super hierarchies. These super hierarchies possess at least one more level than those corresponding to the single reaches and represent, in this context, the concentrations balances in multireach or regional portions of waterways.

Sufficient boundary, initial and final conditions are presented for numerical solution of the subproblem hierarchies developed in this study. Flow charts for the corresponding digital computer programs also are depicted.

A proof of consistency between the ordinary differential equations of the spatially discretized plant and the partial differential equations of the continuous distributed parameter plant that it approximates is developed for a representative plant. A proof of convergence of the solutions of the equations of the same spatially discretized plant also is developed.

Stability analyses are conducted for representative continuous and discrete distributed parameter plants. The optimal control of the spatially discretized continuous distributed parameter plant is formulated as a linear regulator problem and the associated performance index is utilized as a Liapunov function. The optimal control of the discrete distributed parameter plant with time-varying mean volume flow rate is formulated as the problem of optimal control of a nonstationary system which is treated by transforming the nonstationary system to an equivalent stationary system. The z-transform is applied to the finite-difference equations of the plant to facilitate evaluation of the effect of the presence of transport lags.

The relationship between structural characteristics and computational efficiency of subproblem hierarchies is analyzed.

Multilevel hierarchical systems analysis techniques are applied to the sensitivity analysis of a spatially discretized distributed parameter plant subject to multilevel optimal control. The combination of discretization and multilevel techniques is shown to reduce the generation of trajectory sensitivity coefficients for an optimally controlled distributed parameter plant to generation of trajectory sensitivity coefficients for a series of lumped parameter plants under optimal control. A normalized performance index sensitivity function also is developed for the same plant.

Numerical results of multilevel optimization are presented for various control modes and configurations applied to plants representing: single reaches of a tidal river, four contiguous reaches of a tidal river, six contiguous reaches of a tidal river with taper and waste dischargers, and single reaches of an estuary.

The study culminates with the application of one of the single reach subproblem hierarchies for a discrete distributed parameter plant under multilevel optimal control and multilevel hierarchical systems analysis techniques to the problem of minimizing total treatment cost for a multireach portion of a tidal river. This demonstrates the feasibility and efficiency of the multilevel approach to the solution of dynamic systems optimization problems of regional scope.

APPROVAL OF DISSERTATION

APPLICATION OF MULTILEVEL CONTROL TECHNIQUES
TO CLASSES OF DISTRIBUTED PARAMETER PLANTS

BY

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FOR

DEPARTMENT OF ELECTRICAL ENGINEERING
NEW JERSEY INSTITUTE OF TECHNOLOGY

BY

FACULTY COMMITTEE

APPROVED: ______________________, Chairman

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NEWARK, NEW JERSEY

SEPTEMBER, 1976

THIS WORK IS DEDICATED WITH APPRECIATION TO MY PARENTS, MY BROTHER, MY UNCLE, THE LATE FRANK A. SAWYER SR., THE LATE JOHN G. KREER, JR. AND HIS WIFE, MABEL KREER.

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CHAPTER I

INTRODUCTION

Although research on modeling and control of water quality in streams, rivers and estuaries has been conducted for many years, it has intensified during the past decade as concern over environmental quality has become more widespread. This research has engendered the development of many diverse water quality models. Despite their diversity, however, most water quality models for streams, rivers and estuaries share certain common characteristics. In particular, most such models are derived from mass balances involving concentrations that are considered effective indicators of the level of pollution (or, conversely, cleanliness) of the water in the waterway being modeled.

One of the most widely accepted measures of pollution in a waterway is the following set of concentrations[469]: dissolved oxygen, (DO), and biochemical oxygen demand, (BOD). The equations comprising most water quality models include one or both of these concentrations as variables and at least some subset of the equations of the model represents mass balances within the waterway considered. The variation of these concentrations with both spatial location and time implies that the model incorporating them is, with few exceptions, a distributed parameter system.

Optimal control of the water quality of a waterway is a problem of increasing urgency as world population continues to increase and correspondingly increasing demands are placed upon waterways. The distributed character and complexity of realistic water quality models renders optimal control difficult to attain in many cases of practical utility.

The scope of the research represented by this dissertation is the development of classes of dynamic distributed parameter water quality models amenable to the application of various modes of multilevel optimal control and the development of specific approaches for the control of the models belonging to these classes. The contributions of this work include the following.

1.) Sequential application of several modes of multilevel optimal control to members of a class of continuous distributed parameter water quality models for a reach of a waterway,

2.) derivation, by application of the principle of conservation of mass, of a general two-dimensional model representative of a broad class of two-step discrete distributed parameter water quality models for a reach of a waterway,

3.) application of several modes of multilevel optimal control to the members of the class of discrete distributed parameter water quality models developed earlier in this work,

4.) aggregation of single reach water quality models with various modes of multilevel optimal control into regional models comprised of two or more contiguous reaches with general interface conditions,

5.) construction of proofs of consistency and convergence between a spatially discretized form of a representative water quality model and the continuous distributed parameter model that it approximates,

6.) formulation of control of a spatially discretized continuous distributed parameter water quality model as an optimal tracking problem,

7.) stability analysis of a spatially discretized water quality model under optimal control in which the performance index is used as the Liapunov function,

8.) stability analysis of a discrete distributed parameter water quality model under optimal control,

9.) application of stability analysis to a nonstationary water quality model by transformation to an equivalent stationary system,

10.) analysis of sensitivity of a system under multilevel optimal control using multilevel hierarchical systems techniques,

11.) reformulation of a river basin water treatment cost minimization problem, utilizing both a model developed earlier in the work and multilevel systems techniques to effect a substantial reduction in total treatment cost.

The nine areas from which the requisite background for this work is drawn are discussed in the following sequence in the balance of this chapter.

1.) water quality models,

2.) optimal control,

3.) optimal control of distributed parameter systems,

4.) multilevel hierarchical control,

5.) multilevel optimal control of discretized distributed parameter plants,

6.) boundary conditions,

7.) stability,

8.) sensitivity analysis,

9.) water resources management and associated economics .

1.1 Water Quality Models

The earliest water quality model commonly cited in the literature is the model of BOD and DO concentration rate balances in a river or stream presented in the pioneering work of Streeter and Phelps in 1925[459]. Until 1967 most water pollution studies utilized either this model or a variant of this model. Among the most frequently cited models between 1957 and 1967 are those by Dobbins[103], O'Connor[333, 335, 336], Thomann[477], and Young and Clark[545] for rivers and streams and those by Ketcham[219], O'Connor[332, 334], Orlob, Shubinski and Feigner[346], Stommel[457] and Thomann[479, 480] for estuaries. Analytical solutions were presented for several of these models but the scope of practical problems to which they could be applied was limited by the assumptions required in order to attain mathematical tractability. A number of transient models also were developed, e.g., O'Connor[336], to determine instantaneous concentrations distributions within the waterways.

During the years 1967 through 1969, several approaches to the treatment of distributed parameter water quality models were published. The common goal of these approaches was the development of a set of finite-difference equations representing the water quality model that could be solved numerically.

The majority of these approaches, exemplified by the works of Bigura, Ahlert and Schlanger[33], Di Toro and O'Connor[10] and Pence, Jeglic and Thomann[351], begin with a continuous distributed parameter water quality model comprised of partial differential equations which later are approximated by a set of finite-difference equations. Another approach, represented by the publications of Tarassov, Perlis and Davidson[470] and Di Toro[102], applies the method of characteristics to the partial differential equations of the water quality model to convert them to ordinary differential equations which may later be discretized to facilitate solution by a digital computer.

An approach that completely avoids formulation in terms of partial differential equations was presented by Bella and Dobbins[27]. With this approach, the principle of conservation of mass is applied to a volume element of a waterway to directly derive a discrete distributed parameter water quality model. The resulting set of finite-difference equations thus represents exactly the concentrations at a finite number of points within the space-time domain of interest.

Subsequent research with distributed parameter water quality models has emphasized the first approach over the remaining two. However, there have been recent publications utilizing the method of characteristics by Olgac, Longman and Cooper(343) and utilizing a discrete dynamic distributed model by Tamura(469) and by Young(546).

Since 1969, in addition to the models cited above, water quality models for rivers and streams have been presented by Arbabi, Elzinga and Revelle(9), Arbabi and Elzinga(10), Beck and Young(25), Donigan(104), Hsueh(192), Ozgoren, Longman and Cooper(348, 349), Keshavin, et. al.(217), Li and Kozlowski(263), Lin, Fan and Erickson(268), O'Connor and Di Toro(338), Rood and Holley(391), Dysert and Hines(111), Singh(434) and Warren and Bewtra(518). Some of these models are dynamic, e.g., Beck and Young(25), Li and Kozlowski(263) and Lin, Fan and Erickson(268), and therefore are capable of representing transient phenomena.

Due to the additional physical processes and spatial dimensions involved, water quality models of estuaries tend to be considerably more complex than those for rivers and streams. For example, dispersive effects, which frequently can be ignored in river models, usually must be represented in estuary models. Further, many rivers can be fairly accurately represented by models with a single spatial dimension while most estuaries must be represented by models with two or more spatial dimensions. Consequently, the development of practical estuary water quality models has tended to lag that of rivers and streams.

The earliest publications in estuary water quality modeling probably were those due to Ketchum[218, 219] and to Stommel[457] in the early 1950's. Additional estuarial water quality models were presented between then and 1967 by O'Connor[332, 334], Orlob, Shubinski and Feigner[346] and Shubinski, McCarty and Lindorf[430].

The preponderance of publication on estuary water quality models has occurred since 1967. It has included works by Butz, Fischl and Harper[68], Espey[127], Harleman[175], Hess[179], Hill[183], Joy[208], Lee[256], Leendertse and Liu[258], Masch and Shanker[292], Merrill[306], O'Conner, St. John and Di Toro[337], Olufeagba[344], Reid and Bodine[388], Schofield and Krutchkoff[416], Segall and Gudland[418] and Shankar[423].

In addition to the development of the water quality models themselves, an active area of research has been the evaluation of the specific processes within the DO and BOD balances utilized for the equations of the model. Details of this work are deferred to Chapter 2.

The classes of distributed parameter water quality models treated in this dissertation are restricted to deterministic models that may be described by linear or quasilinear partial differential or finite-difference equations defined over a fixed spatial domain. These models are regarded as being dynamic because they represent the spatial distribution of BOD and DO concentrations at each time instant. A class of distributed parameter water quality models represented by linear partial differential equations is treated in Chapter 2 and a class of discrete distributed parameter models represented by finite-difference equations is derived and treated in Chapter 3.

1.2 Optimal Control

A control system may be regarded as consisting of a plant (frequently represented by a mathematical model) that is acted upon by a controller. The controller usually has some means of collecting data from the plant so that the relationship between the two may be depicted as shown in Figure 1-1.

Plants and their mathematical models may be classified as follows.

1.) lumped parameter systems

2.) discrete systems

3.) distributed parameter systems

This classification is somewhat arbitrary in that discrete distributed parameter plants could belong to either the second or third category.

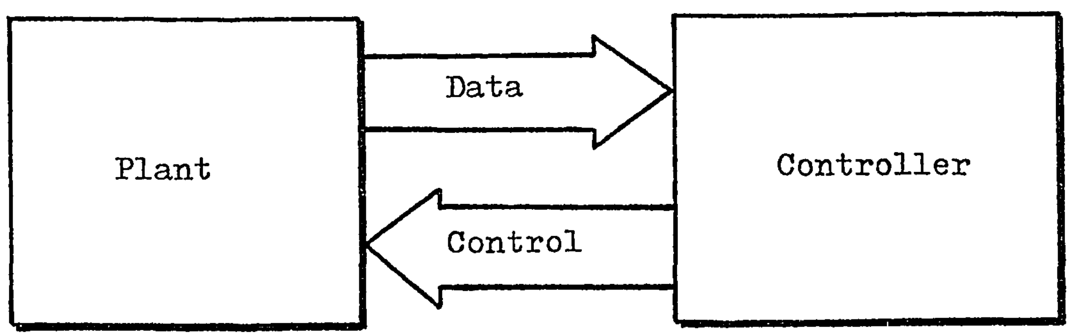


Figure 1-1: Control system

To facilitate the application of control, the ordinary differential equations of the lumped parameter plants may be expressed in the form of scalar components of a vector-matrix state equation of the following structure.

$$\dot{x}_k = g_k\ (\underline{x},\ t) \tag{1-1}$$

where $k = 1, 2, \ldots, N+1$

$$\underline{x} = (x_1,\ x_2,\ \ldots,\ x_{N+1})^T \tag{1-2}$$

and, in general, g_k may be nonlinear time-varying functions.

The corresponding formulation for the finite-difference equations of discrete plants is:

$$x_{k,i+1} = g_{k,i}(\underline{x}_i) \tag{1-3}$$

where $k = 1, 2, \ldots, N+1$; $i = 1, 2, \ldots, I_m - 1$

$$\underline{x}_i = (x_{1,i},\ x_{2,i},\ \ldots,\ x_{N+1,i})^T \tag{1-4}$$

The subscript, i, denotes the ith point on the time axis. The assignment of this subscript has the effect of eliminating temporal variation within each finite-difference equation of the set. Such variation is accommodated by construction of a different equation for each temporal point. Hence, in contrast with the lumped parameter model, each $g_{k,i}$ is, in general, nonlinear but <u>not</u> time-varying.

Most distributed parameter plant models are represented by sets of partial differential equations. Each of these partial differential equations may be approximated with a set of ordinary differential equations by discretization of the spatial variables. The spatially discretized distributed parameter plant model can then be expressed in state equation form.

A smaller class of distributed parameter models exists in discrete form as a set of finite-difference equations. These equations may be expressed in the state equation form of (1-3).

Optimal control is defined in terms of the performance index, a given functional of independent and control variables that is considered an effective criterion of the quality of performance of the control system. The objective of an optimal control problem is the determination of control variable values such that the performance index is either maximized or minimized, depending upon the specific application, while satisfying equality and inequality constraints.

Choice of the approach to be utilized in determining the optimal control variables for a specific problem depends jointly upon the nature of the plant and the specific selection of a performance index. The type of plant for which the largest assortment of optimal control approaches is available is the lumped parameter system. Applicable approaches include: calculus of variations[34,50,147,499], dynamic programming[29], Pontryagin's maximum (minimum) principle[59, 61, 378, 396, 397, 398], functional analysis[35, 232] and the method of gradients[48, 213, 378]. The common result of these approaches is a set of mathematical conditions to be satisfied in order to achieve optimal performance. Some of these approaches also may be applied to discrete plants.

The combination of plant and performance index for which the most comprehensive array of optimal control results is available is the linear lumped parameter plant with a quadratic performance index. This particular combination is the one most amenable to analytical solution. However, even for those cases in which analytic solutions are available, numerical solutions often are more useful for engineering applications. Consequently, two major areas that are subjects of continuing research in optimal control are the construction of performance indexes to measure appropriately the quality of performance of the control system and the development of approaches to numerical optimization. Literature reviews and discussions of these areas are presented in Appendix 1.

The classical Pontryagin's minimum principle approach to those optimal control problems involving a lumped parameter plant in state variable form with a quadratic performance index would be the formation of the Hamiltonian functional and the application of the Pontryagin necessary conditions for minimization of the performance index subject to the applicable constraints. These conditions yield a set of costate equations to be solved, in addition to the state equations, to attain optimal performance. The approach for optimal control problems involving discrete plants in state variable form with a quadratic performance index, following Butkovskii[59], is similar to that for lumped parameter plants except that the Pontryagin necessary conditions for minimization of the performance index are applied to the functions, $g_{k,i}$, in equation (1-3).

Earlier in this section distributed parameter plants were said to be either discrete or reducible, by spatial discretization, to the form of lumped parameter plants of large dimension. To accommodate the large dimensions associated with either of these forms, the Pontryagin approach is applied in conjunction with the techniques of multilevel hierarchical systems analysis in this dissertation.

1.3 Optimal Control of Distributed Parameter Plants

One of the earliest publications on the application of optimal control to distributed parameter systems was that by Butkovskii and Lerner in 1960[54]. Since that time, Butkovskii[55, 56, 57, 58, 60, 62, 63, 64, 65, 66, 67] has published extensively in this area. Much of his work has been directed toward extending Pontryagin's maximum principle. The earliest publications on optimal control of distributed parameter systems in this country probably were those by Wang and Tung in 1963[514] and Wang in 1964[515]. In these publications, the necessary conditions for the optimal control of distributed parameter systems were developed by applying techniques of dynamic programming. These papers also contain discussions of stability, controllability, observability, approximation methods and instrumentation.

During the next several years, publications in this area by a number of other investigators begin to appear. These included Abdikerimov[1], Egorov[118, 119, 120, 121], Gelig[148], Lure[279], Porter[379], Russell[400], Sakawa[406, 407], Sirozetdinov[441, 442], Volin and Ostrovskii[510], Vostrova[511] and Wismer[531]. Abdikerimov's work was one of the earliest published applications of optimal control to discrete distributed parameter systems. Lure utilized a Mayer-Bolza formulation of a class of distributed parameter optimal control problems. Sakawa obtained computational results for a linear one-dimensional diffusion equation with optimal boundary control.

Wismer treated a broad class of distributed parameter systems represented by scalar parabolic or elliptic partial differential equations. His approach to the problem of applying optimal control to this class of systems began with the discretization of the spatial domain. This leads to the approximation of the partial differential equations of the mathematical model of the original plant by a large set of ordinary differential equations effectively reducing the original distributed parameter system optimal control problem to a set of coupled lumped parameter system optimal control problems. Wismer then applied a combination of multilevel hierarchical systems analysis techniques and lumped parameter systems optimal control techniques to the set of ordinary differential equations of the spatially discretized system. This combination of techniques yielded a hierarchy of subproblems of much smaller dimension than would have resulted from direct application of the lumped parameter systems optimal control techniques alone. Wismer also applied this approach to a representative selection of distributed parameter plants in conjunction with both boundary and distributed control obtaining numerical solutions in each case.

Wismer's dissertation, published in 1966, marked the first application of multilevel hierarchical systems analysis techniques to a distributed parameter plant. It also presented one of the broadest selections of numerical results for optimal control of distributed parameter systems available at that time. This dissertation provides the principal background for the work reported in the present dissertation.

Since 1966 an extensive array of publications on the application of optimal control to distributed parameter plants has appeared. This has included: Ajinka[3], Andreev[5], Axelband[13], Ball and Hewit[16], Barnes[19], Brogan[44], Butkovskii[60, 64, 65, 66, 67], Combot[82], Cornick and Michel[84], Deans[93], Degtyarev and Sirazetdinov[95], Egorev[122], Falterini[130], Gal'chuk[146], Golub[149], Grainger[151], Hullett[195], Johnson and Athans[206], Kadymov and Listengarten[211], Kim and Erzberger[220], Kim and Gajwani[221], M.C.Y.Kuo[242], Kusic[243], Kwakernaak et. al.[244], Lin et. al.[270], Lukes and Russell[277], Makavov et. al.[286], Malanowski[285], McGlothin[299], Narasimha[326], Ozgoren et. al.[348, 349], Perlis and Cook[363], Perlis[367], Prabhu[381], Pulvirenti[385], G. A. Russell[401], Samoilenko[408], Santgati[411], Schmaedeke[414], Seinfeld[419], Shih[427], Singh[434], Sirazetdinov[443,444,445], Tamura[469], Tarassov et. al.[470], Vidyasager[504], Weigand[520], J. K. Wong[534], Yang and Chang[540], K. G. Yang[514], Yavin and Sivan[543], Yeh and Tou[544], and Zone and Chang[553].

Brogan presented computational results for a linear one-dimensional diffusion equation with distributed control and many of the remaining publications of the past decade also have presented computational results. Butkovskii presented many of his results in a book on the subject of optimal control of distributed parameter plants[60]. The paper by Tarassov, Perlis and Davidson in 1969 marked the first application of the techniques developed for distributed parameter systems optimal control to control problems in the water pollution area. Other investigators who have published results for such application since then include Hullett[195], Olufeagha[344], Ozgoren et. al.[348, 349], Perlis and Cook[363], Perlis[367], Singh[434] and Tamura[469].

1.4 Multilevel Hierarchical Control

The control of large-scale multivariable systems is a class of control problems that arises in many areas of practical application. Examples of such systems include mathematical models of large-scale industrial, economic, biological and social systems. Direct application of control to a large-scale system often severely taxes or exceeds available computer capacity due to the high dimensionality of the overall control problem to be solved. Application of multilevel systems analysis techniques to the large overall control problem decomposes it into a multilevel hierarchy of subproblems of smaller dimension.

The roles of the subproblems are correlated with the levels that they occupy in the hierarchy. Each of the infimal subproblems on the lowest level of the hierarchy pertains to control of a portion of the original system to be controlled. For example, decomposition of the overall control problem into control of N portions of the original system yields N infimal subproblems. Each of the subproblems on a level above the lowest one pertains to coordination of the solutions of the subproblems on the next lower level. The number of subproblems per level decreases for each higher level in the hierarchy until the top (or supremal) level is occupied by a single overall coordination subproblem.

A two level subproblem hierarchy corresponding to decomposition of the original control problem into N infimal subproblems is depicted in Figure 1-2. The subproblems of this hierarchy may be solved in the following sequence. The second level coordination subproblem provides coordination or intervention variables which are held fixed

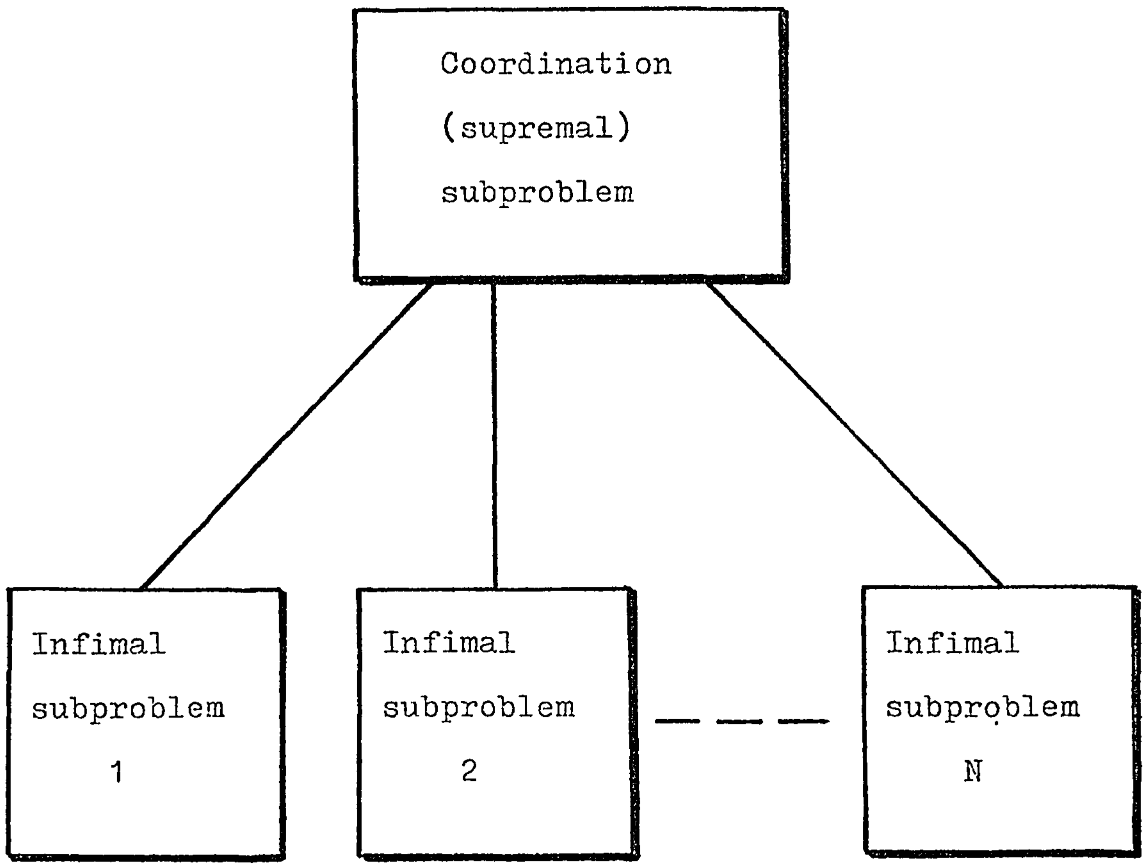


Figure 1-2: Two level subproblem hierarchy

while the optimal solution is determined for each infimal subproblem independently. After the optimal solution is obtained for each infimal subproblem, numerical responses are sent to the coordination subproblem on the second level. The coordination subproblem now adjusts the coordination variables and sends their adjusted values to the infimal subproblems on the lower level. The infimal subproblems are again solved independently with the adjusted values of the coordination variables. This procedure continues iteratively until the overall coordination subproblem at the top of the hierarchy is satisfied. The result sought is an optimized collection of subsystems, with interconnections restored, which is equivalent to the original system optimized. This procedure may be readily extended to subproblem hierarchies with more than two levels.

A special class of large-scale systems consists of those which are inherently multilevel, e.g., composites of smaller subsystems. Such systems are referred to as "structurally multilevel" to distinguish them from large-scale systems that become multilevel as a result of decomposition.

The term, "multilevel control", as used by Wismer[531] and others, denotes the combination of multilevel hierarchical systems analysis techniques with various (usually optimal) control techniques. The resulting hybrid procedure is an efficient means for applying control to large-scale systems. Details on the hybrid procedure for lumped parameter systems appear in Chapter 2. Details on the corresponding procedure for discrete systems appear in Chapter 3. Both procedures are initiated by decomposing the original large control problem into a series of smaller control subproblems to be solved.

An extensive review of the literature on multilevel hierarchical systems analysis techniques appears in Appendix 2. An area of application of these techniques in which publication has been abundant since 1971, water quality modeling and control, is treated in detail in this section because it is especially pertinent to the work reported in this dissertation.

Recent contributors to the literature on applications of multilevel hierarchical systems techniques to water quality problems include: Foley and Haimes(141), Haimes, Foley and Yu(166), Haimes, Kaplan and Husar(167), Haimes and Macko(168), Haimes(171), Koide et. al.(229), Mesarovic, Klabbers and Richardson(314), Nainis and Haimes(325), Singh, Drew and Coales(438), Tamura(469) and Yu and Haimes(548).

Many of the papers with which Haimes was involved have treated multilevel control of water quality models on a regional basis. The models so treated generally have been static models.

In Foley and Haimes[141] the interdependence of temperature and DO concentration distribution is modelled for a regional water quality system. The authors have developed and applied a BOD-DO temperature-dependent model for the Chatahoochee River in Georgia. The multilevel approach to control of this model permits inclusion of simulation of a regional decision authority, effluent dumping charges and decentralized decision making.

In Haimes[171] four principal bases for water resources systems decompositions are presented:

1.) temporal,

2.) physical-hydrological,

3.) political-geographical,

4.) goal or functional.

These bases are illustrated with a two level hierarchical structure directed toward management of water and related land resources for pollution control and maintenance of ecological equilibrium. The paper includes a tutorial summary of water resources problems for which hierarchical modeling is deemed applicable.

Publications by Singh[434, 438] in this area have emphasized the utilization of dynamic water quality models. Singh, Drew and Coales[438] begins with a survey of methods for control of large interconnected dynamic systems. The survey of optimization methods in this paper stresses infeasible methods such as:

1.) goal coordination and the Takahara-Sage algorithm,

2.) Tamura's three-level method,

3.) Tamura's time-delay method,

4.) Pearson's pseudo-model coordination.

Sub-optimal methods for control of serially connected dynamic systems models are developed. These methods are applied to water quality control of serially connected portions of a river.

Tamura's paper[469] presents a discrete dynamic model of multi-dimensional high-order difference equations representing the dynamics of biochemical oxygen demand and dissolved oxygen concentrations in a multiple-reach river system. In this paper high order difference equations represent the distributed transport delays between contiguous reaches in a river to allow for dispersion of BOD and DO concentrations. A hierarchical optimization technique, based on duality and decomposition, is applied to the high order discrete model, having state and control variable constraints, for minimizing departure of water quality variables from their specified levels.

Tamura shows that the distributed delay model is the most realistic one by comparing the transient responses to input disturbances for no delay, pure delay and distributed delay models. As an example, he solves a water quality problem involving a four-reach model. Included in the a priori information necessary for the solution of this problem is the distribution of delay magnitudes for the distributed delay model.

This is the one publication in the applications literature that the approaches of Chapters 2 and 3 of the present dissertation most closely resemble. The resemblence lies in the application of multilevel hierarchical control techniques to a water quality model of distributed nature.

In particular, Chapter 3 more closely resembles the contents of Tamura's paper because in this chapter multilevel control is applied to a discrete distributed parameter model instead of a discretized continuous distributed parameter model. The principal distinctions between Tamura's model and the corresponding model of Chapter 3 (the regional tidal river model) lie in their respective representations of dispersive effects and in the number of longitudinal axis increments per reach. Tamura's model represents dispersive effects with insertion of delay models for each interreach coupling term with each reach corresponding to one longitudinal axis increment. Except for these terms, the Tamura model is a lumped parameter system. The discrete distributed parameter regional tidal river model of Chapter 3 was derived directly from conservation of mass considerations and the second order dispersive terms are an inherent part of the derived model. Further, the regional tidal river model of Chapter 3 provides for the possibility of having many longitudinal axis increments for each reach. This model is therefore capable of generating a more detailed representation of the concentration distributions within each reach while obviating the need for a priori data on the distribution of lags at reach interfaces.

1.5 Multilevel Control of Discretized Distributed Parameter Plants

Wismer's dissertation[531] appears to represent the pioneering work in combining spatial discretization with multilevel hierarchical systems techniques in the control of distributed parameter systems. Despite the fact that the dissertation was published approximately ten years ago, few publications, other than those by Wismer, appear to have followed this approach. One of the principal objectives of the present work has been the extension of concepts presented by Wismer to classes of distributed parameter plants representing water quality models of streams, rivers and estuaries. The derivation and optimal control of these classes of models are presented in Chapters 2 and 3 of the present dissertation. In both of these chapters, Wismer's approach is extended to aggregations of distributed parameter plants.

The class of distributed parameter systems treated in Wismer's dissertation was restricted to those that could be represented by sets of partial differential equations of certain general forms. Such mathematical models are designated as continuous distributed parameter systems in the present dissertation to distinguish them from a class of discrete distributed parameter models which is derived in Chapter 3.

The spatial discretization step in Wismer's approach to optimal control of continuous distributed parameter plants engenders the questions of consistency and convergence. If the original distributed parameter model and the approximating semidiscrete model jointly satisfy the consistency conditions given by Wismer, then the ordinary differential equations of the semidiscrete model actually do approximate the partial differential equations of the original model. If the <u>solutions</u> of the ordinary differential equations of the semidiscrete model and the solutions of the partial differential equations of the original distributed parameter model jointly satisfy the convergence conditions given by Wismer, then the solutions of the semidiscrete model closely approximate those of the original model. Proofs of consistency and convergence following the approaches of Wismer are presented in Chapter 4 of this dissertation.

1.6 Boundary Conditions

A solution of an equation of a distributed parameter model is uniquely determined over the spatial and temporal domain of the model by specifying proper boundary, initial and final conditions[531]. Appropriate boundary and initial conditions may be obtained from the following publications: Bella and Dobbins[27], Dresnack and Dobbins[106], Okunseinde[340], Segall and Gudland[418], Tarassov, Perlis and Davidson[470], Taylor[473] and Wismer[531]. The boundary, initial and final conditions required for determining specific solutions are discussed in detail in Chapters 2, 3 and 4 of the present dissertation.

1.7 Stability Analysis

Stability analyses of both semidiscrete continuous distributed parameter and discrete distributed parameter water quality models are presented in Chapter 4 of this dissertation. These analyses are based upon the concepts and techniques of seven areas which are enumerated with representative references in the sequel.

1.) Matrix theory: Barrett and Storey[20], Hohn[187], and Kenschaft[214];

2.) discrete systems theory: Freeman[145], Grujic and Siljak[155, 157], Jury[210], and Lindorff[271];

3.) linear, time-varying systems theory: Lun'kov and Tonkov[278], Taft and Kheyfels[465], Vanyurikhin[510], Wu[538] and Wu and Horowitz[539];

4.) numerical stability: Dresnack and Dobbins[106], Leendertse[257], Lilly[265], and Okunseinde[340];

5.) Liapunov stability analysis: Grujic[159], Klimentov and Prokopov[223], Knowles[227], M.C.Y. Kuo[240], La Salle and Lefschetz[246], Nagaraja and Chalam[324], Nesbit[327], Parks[352], Prokopov[384], Schultz[417], and Srivastra and Musa[453];

6.) time-delay systems: Frankena[144], Haberland, Rao and Eisenberg[162], Mishra and Rajamani[320], Shamash[422], Truxal[493], Tamura[469] and Zahr and Slivinski[550];

7.) optimal control for which a literature review is given in Section 1.2.

Alternate approaches to stability analysis of such systems are described in two other areas:

1.) Stability analysis of interconnected (composite) systems: Cook[83], Grujic[158], Gulcur and Meyer[161], Ladde and Siljak[245], Michel[316,317], and Thompson[486].

2.) Stability analysis of distributed parameter systems: Ansari[7], Gelig[148], Lin et.al.[270], and Sirazetdinov[445].

Two approaches to stability analysis are presented in Chapter 4 of this dissertation. The first is directed toward stability analysis of the discretized water quality models developed in Chapter 2. The second is developed for application to the discrete finite-difference water quality models of Chapter 3.

The first approach begins with the equations of the spatially discretized continuous distributed parameter water quality model in state variable form and the optimal control performance index in its spatially discretized form. The work of Kuo[241] suggested the use of the performance index functional as a Liapunov function. The recasting of the original problem into the form of an optimal tracking control problem, following Kirk[222] is a necessary preliminary to utilizing the performance index as a Liapunov function. The effects of decomposition upon the stability of the system are evaluated. Then the stability analysis is extended to control systems involving a gradient controller.

The second approach begins with the finite-difference equations of a discrete distributed parameter water quality model in vector-matrix form. Matrix partitioning is introduced to facilitate later analysis. The nonstationarity of the model motivates its transformation to an equivalent stationary model following Freeman(145). Z-transformation is applied to the stationary system to facilitate stability analysis.

1.8 Sensitivity Analysis

An important consideration in the synthesis of optimal control systems is the sensitivity of the state variables and/or performance index to perturbations in the parameters of the system to be controlled (plant). Sensitivity has, in fact, been utilized directly in the synthesis of optimal control systems in some recent research: Sesak(420) and Shirokov(428).

The earliest published work in the area of sensitivity probably is that of Bode(36) which appeared in 1945. His work introduced the concept of sensitivity functions. A later, more familiar treatment of sensitivity functions appears in Truxal(493). Many publications have appeared in this area since these two works. A representative sampling of them is: Kokotovic and Rutman[230], Malek-Zavarei and Jamshid[287a], Peterson[370], Platzman and Athans[374], Rootenberg[392], Sagalov[405] and Tomovic[489]. The various definitions of sensitivity utilized in these works share in common the concept of a sensitivity coefficient which is further developed by Tomovic.

An area of sensitivity analysis that has attracted particular attention during the past five years is the application of sensitivity concepts to water quality models. Publications in this specific area include: Meier et. al.[305], O'Laoghaire and Himmelblau[341,342], Perlis and Duckworth[366] and Perlis[367].

Perlis applied the concepts of performance index sensitivity coefficient and normalized performance index sensitivity function to the analysis of water quality models. Performance index sensitivity coefficients measure the tendency of the performance index of the optimal control system to vary with changes in the parameters of the system being controlled. Generation of performance index sensitivity coefficients requires space-time contours of the optimal state variables just as generation of trajectory sensitivity coefficients does. These optimal contours could be obtained from any optimal solution of the original control problem. In contrast with the state trajectory sensitivity contours, the performance index sensitivity coefficient yields a single number which facilitates sensitivity comparisons among different systems. Both sensitivity measures vary in direct proportion with the boundary conditions imposed upon the original control problem. A normalized performance index sensitivity function was introduced which is not affected by such changes. Since it is a function of the optimal value of the performance index, its generation requires space-time contours of optimal control variables as inputs.

In Chapter 5 of this dissertation a distributed parameter water quality model is spatially discretized to permit direct application of trajectory sensitivity techniques previously developed for lumped systems. Application of the hierarchical systems analysis techniques of decomposition and coordination facilitates solution of the large set of discretized equations.

1.9 Water Resources Management and Associated Economics

Background for the application of a model developed in Chapter 3 to the optimal control of a tidal river water quality system in Chapter 7 of this dissertation is based upon the following areas of research:

1.) Water resources management: Davis[91], Dee et. al.[94], Gourishanker and Lawson[150], Kerri[216], S.H. Lin[269], Maass, et.al.[280], Marsden et. al.[290], Mickel and Montanari[318], Thomann and Sobel[478], Truitt et. al.[491], Trumbull[492], Vachtsevanos et. al.[497], and Viessman et. al.[505];

2.) Water resources economics: Boyd[41], Case[71], Davidson et. al.[90], Hass[176], Howe[191], E. L. Johnson[205], Jordening[207], Kerri[215], Kneese[224, 225], Krishna and Rajamani[235], K-S Lee[255], Major[287], McCuen[294], Parks[353], Stevens[454], Upton[496] and Whipple[524];

3.) Mathematical programming: Bayer[24], Cohon and Marks[80], Drobny[108], Ecker[115], Graves et. al.[154], Kenschaft[214], Masqati[293], Penamalli[362], Loucks et. al.[275], Pingry and Whinston[372, 373], Shih and Meier[426] and Sobel[448];

4.) Regional water resources models: Foster et.al.[142], Fox[143], Haimes and Scott[170], Hufschmidt[194], Hwang et. al.[197], Laura[250], Law[251], Rossman[395], Shojalashkari[429], Walker et. al.[512], and Yao[542];

5.) Water quality modelling: in addition to most of the references listed in Section 1.1 of this chapter, Ippen[199], Shieh[425], Smith[446] and D-S Wu[537];

6.) Measurement and control: in addition to many of the publications listed in Section 1.2 of this chapter, Amberg and McCormick[4], Burns and Eckenfelder[53], Hullett[195], Liptak[272], Ozgoren[349], Perlis and Cook[363], Thackston and Speece[476], Thomann[483], Whipple and Yu[523] and Wiley et. al.[527].

Kerri's paper[215] presented an economic model which is used to generate the minimum cost of attaining a water quality objective by optimizing effluent treatment costs for multiple waste dischargers taking into account the natural purification capacity of the receiving waters.

The construction of this economic model for minimization of effluent treatment costs for dischargers into a river is based upon maintenance of specified water quality levels in a critical reach of the river downstream from the outfalls of all of the dischargers. Therefore, an important early step in the development of the model is the identification of the critical reach, the reach for which it is most difficult to maintain the specified water quality levels without treatment of the dischargers' effluent.

One major component of Kerri's model is a cost matrix displaying the cost of effluent treatment for each discharger affecting the critical reach. This cost matrix is constructed in a form to facilitate minimization of the total collective cost for all dischargers by techniques of linear programming. The minimization is predicated upon the assumption that once the total amount of effluent that the critical reach can assimilate without violating minimum water quality standards is calculated, it remains fixed.

The other major component of Kerri's economic model is a concentrations balance model of the portion of the river between the discharger located furthest upstream and the downstream end of the critical reach. Since this model includes at least one reach in addition to the critical reach, it actually is a regional model for which a hierarchical structure is especially appropriate.

The concentration balances in the reaches between the dischargers and the upstream end of the cricitcl reach are represented by a steady-state model developed by O'Connor[334]. This model is used to calculate the relationships between the waste loads introduced by the dischargers and the resulting waste load delivered to the critical reach.

In Chapter 7 of this dissertation, the following modifications are made in Kerri's model.

1.) The discrete distributed parameter tidal river water quality (concentrations) model with aeration control of Chapter 3 represents the critical reach.

2.) An instream treatment cost minimization subproblem is constructed around the discrete tidal river concentrations model with optimal aeration control to supplement its natural assimilative capacity.

3.) An economic subproblem hierarchy is constructed that coordinates the dischargers' treatment cost minimization subproblem with the instream treatment cost minimization subproblem.

The present chapter has laid the foundation for the work reported in this dissertation in nine areas; namely, water quality models, optimal control, optimal control of distributed parameter plants, multilevel hierarchical control, multilevel optimal control of discretized distributed parameter plants, boundary conditions, stability analysis, sensitivity analysis and water resources management and associated economics. It also has presented the scope of the research represented by this dissertation, listed the contributions of the work and previewed the subsequent material in the dissertation.

Chapter 2 presents a development of a class of continuous distributed parameter water quality models, reviews approaches to the evaluation of their parameters and presents a detailed application of multilevel optimal control, in a sequence of different modes, to this class of models.

Chapter 3 presents an original derivation of a two-dimensional model representative of a class of discrete distributed parameter water quality models, derives several additional models belonging to this class, develops multilevel control techniques appropriate for discrete models and applies them to the water quality models developed within it.

Chapter 4 presents an approach to evaluation of supplemental boundary values, proofs of consistency and convergence between a representative discretized water quality model and the distributed parameter model that it approximates and an approach to stability analysis of water quality models representative of the classes of models developed in Chapters 2 and 3. The chapter concludes with a development of the relationships between the structural characteristics and the computational efficiency of subproblem hierarchies.

Chapter 5 presents a sensitivity analysis of a system under multilevel optimal control.

Chapter 6 presents numerical results for water quality control problems representative of those developed analytically in Chapters 2 and 3.

Chapter 7 formulates a river basin water treatment problem utilizing a combination of multilevel control techniques and linear programming.

Chapter 8 presents the conclusions reached in this work and suggests areas suitable for further research.

CHAPTER 2

CONTINUOUS DYNAMIC DISTRIBUTED PARAMETER WATER QUALITY MODELS AND THEIR OPTIMAL CONTROL

The waterways to be modeled in this dissertation consist of estuaries, rivers and streams. Their utilization for fresh water supply, transportation, recreation and other purposes attracts to their boundaries municipal and industrial complexes which discharge pollutional loads into their waters. These waterways' principal role as receiving waters for municipal and industrial wastes motivates the development of mathematical models of the physical and chemical processes involved. These models determine the distributions of water quality variables of interest in these waterways.

The intended uses of a particular reach of a water system determine the choice of specific water quality variables with which to define the corresponding mathematical models. Many water quality models emphasize the depletion of dissolved oxygen content of the water resulting from the biodegradable organic content of the municipal and industrial discharges and urban runoff and this emphasis will be followed in this chapter.[114, 340] For this type of water quality evaluation the critical variables are the dissolved oxygen (DO) and the biochemical oxygen demand (BOD) concentrations.

This chapter presents a class of linear distributed parameter models representing the mass balance of dissolved oxygen and biochemical oxygen demand concentrations in specified tapered waterways, i.e., waterways whose cross sectional areas vary with location along the axis of principal flow. The specific tapered waterway models derived from the general distributed parameter model for this class are:

1.) a three-dimensional estuary

2.) a two-dimensional stratified estuary

3.) a one-dimensional tidal river

4.) a non-dispersive stream or river

Included with the presentation of these models is a review of currently available methods of measuring some of the critical water quality variables and parameters. The choice of the variables most critical for the proper management of polluted waterways is a subject of extensive debate among researchers in this field due to the multiple utilizations of the waterways and the extent of variation of the pollutants introduced to them.[340] This review is limited to the variables and parameters appearing in the water quality models presented in this chapter.

Except for the steady-state model, all of the models derived from the general distributed parameter water quality model at the beginning of this chapter may be classified as linear continuous dynamic distributed parameter systems. Optimal aeration control of continuous distributed parameter models of sufficient complexity for practical utility is a class of problem for which relatively few analytic solutions are available. Each of the original distributed parameter models is therefore discretized spatially to reduce it to a series of lumped models to which optimal control methods may be more easily applied. The resulting, usually substantial, increase in dimension may severely tax the capacity of available computers in the numerical solution of the large set of associated optimal control problems.

Multilevel hierarchical systems analysis combined with Pontryagin's minimum principle is especially effective for the application of optimal control to dynamic systems of large dimension[309, 531]. In Section 2.8 of this chapter this approach, in conjunction with three modes of optimal control:

1.) aeration

2.) waste dumping

3.) flow augmentation,

is applied, in turn, to spatially discretized dynamic water quality models of the tapered tidal river and the tapered stream to produce a total of six combinations of waterway models and optimal control modes.

Each model with multilevel control consists of a hierarchy of subproblems to be solved. These subproblems are discretized with respect to time and provided with appropriate boundary, initial and final conditions to support generation of numerical solutions on a digital computer. The solutions consist of space-time distributions of concentrations and the control variable for a reach of the waterway which minimize specified performance indexes.

Analysis of entire river basins, watersheds or other regions often requires water quality models extending over more than one reach. In Section 2.9 of this chapter, each of the six single reach models with multilevel control developed earlier is aggregated into a regional multireach model. Between the j_m contiguous reaches of each regional model interface conditions sufficiently general to include:

1.) addition of volume flow rate from tributaries and flow augmentation

2.) addition of BOD and DO concentrations due to dischargers,

are incorporated.

The equations derived for the water quality models presented in this chapter are assigned to specific models in the text of the chapter and also in tables at the end of the chapter.

The contributions by the author in this chapter are the following:

1.) derivation of six concentrations models for tapered waterways from the general distributed parameter dynamic water quality model;

2.) presentation of the advantages of full decomposition over standard decomposition for this class of models;

3.) combined application of multilevel hierarchical systems analysis and Pontryagin's minimum principle to effect optimal control of discretized dynamic continuous distributed parameter water quality models for six combinations of model and control mode;

4.) aggregation of each of the six water quality models with multilevel control for a single reach into a regional multireach hierarchical model with general interface conditions between its contiguous reaches.

2.1 General Distributed Parameter Water Quality Model

The class of distributed parameter water quality models treated in this dissertation may be defined by equations resulting from application of the principle of conservation of matter which may be described as[546]:

time rate of accumulation of constituent in a fluid element	=	net rate of flow of constituent into fluid element	+	time rate of net production of constituent in fluid element	(2-1)

The general partial differential equation expressing the distribution of each constituent in a three-dimensional model may be written, following Butz et. al.[68], as:

$$\frac{\partial \hat{c}}{\partial t}(x,y,z,t) = -\nabla\cdot(\hat{\underline{v}}\hat{c}) + \nabla\cdot D_m\nabla\hat{c} + r_s \qquad (2\text{-}2)$$

where $\hat{c}$ is the instantaneous concentration, $\hat{\underline{v}}$ is the instantaneous velocity vector and r_s is the net rate of production of the constituent. The first term on the right side of the equation represents the effects of local fluid velocity, while the second term represents molecular diffusion effects.

In general, both c and $\underline{v}$ are stochastic variables due to turbulence in the fluid. Each of them may be represented in terms of their deterministic and stochastic components as follows:

$$\hat{c} = c + c' \qquad (2\text{-}3)$$

$$\hat{\underline{v}} = \underline{v} + \underline{v}' \qquad (2\text{-}4)$$

Although c' and $\underline{v}'$ each may be considered as having an ensemble mean of zero, the ensemble mean of the product of these two random variables is not necessarily zero.

Taking the ensemble average of (z) yields.

$$\frac{\partial c}{\partial t} = -\nabla\cdot(\underline{v}c) - \nabla\cdot(\underline{v}'c') + \nabla\cdot D_m\nabla c + r_s \qquad (2\text{-}5)$$

Applying Fick's approximation for diffusion,

$$- \nabla \cdot (\underline{v}'c') = \frac{\partial}{\partial x}(D_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(D_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(D_z \frac{\partial c}{\partial z}) \tag{2-6}$$

where D_x, D_y and D_z are eddy diffusion coefficients associated with each spatial axis. Since the magnitude of molecular diffusion is several orders of magnitude smaller than that of eddy diffusion, $D_m \approx 0$.

Equation (2-5) then reduces to

$$\frac{\partial c}{\partial t} = - \nabla \cdot (\underline{v}c) + \frac{\partial}{\partial x}(D_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(D_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(D_z \frac{\partial c}{\partial z}) + r_s \tag{2-7}$$

$$\underline{v} = \frac{1}{A} \underline{Q} \tag{2-8}$$

where $\underline{Q}$ is the volume flow rate vector and A is the effective cross sectional area over which the flow occurs. Substitution of (2-8) in the first term on the right side of equation (2-7) yields

$$\nabla \cdot (\underline{v}c) = \nabla \cdot \left[\frac{c}{A} \underline{Q}\right] \tag{2-9}$$

But $\nabla \cdot \left[\frac{c}{A} \underline{Q}\right] = \frac{c}{A} (\nabla \cdot Q) + \left[\nabla (\frac{c}{A})\right] \cdot \underline{Q}$

Due to incompressibility of the fluid

$$\nabla \cdot \underline{Q} = 0 \text{ and } \nabla \cdot (\underline{v}c) = \left[\nabla (\frac{c}{A})\right] \cdot \underline{Q}$$

$$= (\frac{1}{A}\nabla c) \cdot \underline{Q} + (c \nabla \frac{1}{A}) \cdot \underline{Q} \tag{2-10}$$

Assuming negligible variation of flow cross-section for transverse axes implies $(\frac{1}{A}) = 0$ for the y- and zdirections. Hence,

$$\nabla \cdot (\underline{v}c) = Q \frac{\partial}{\partial x}\left(\frac{c}{A}\right) + V_y \frac{\partial c}{\partial y} + V_z \frac{\partial c}{\partial z} \tag{2-11}$$

where Q represents the mean volume flow rate along the x-axis which is the principal flow axis and A represents the cross sectional area normal to that axis which may vary as a function of x.

2.2 Three-Dimensional Tapered Estuarine Water Quality Model

The general equation which may represent the distributions of BOD and DO concentrations in a three-dimensional estuarine water quality model with cross sectional variation (taper) along the axis of principal flow is as follows,

$$\frac{\partial c}{\partial t} = -Q \frac{\partial}{\partial x}\left(\frac{c}{A}\right) - V_y \frac{\partial c}{\partial y} - V_z \frac{\partial c}{\partial z} + \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z}\right) + r_s \tag{2-12}$$

where $Q = A \cdot V_x$ (2-13)

If A is constant, the concentration model expressed by equation (2-12) reduces to the form of the equation presented by Okunseinde[340]. The general concentrations model with these simplifications closely resembles the BOD and DO concentrations models for estuaries in which a strong dependence of density upon salinity and temperature exists.

Major sources of DO are natural reaeration and photosynthesis. Reaeration is the transfer of oxygen from air to water at their common interface. Surface turbulence and natural mixing are the principal vehicles for this process[103]. Reaeration may be represented as follows,

$$r_s = K_a(C_s - C) \qquad (2\text{-}14)$$

where K_a is the coefficient of reaeration, C is the instantaneous DO concentration and C_s is the saturation level of DO in the estuary. In some of the literature on water quality analysis, the expression, C_s-C, is represented by a single composite variable defined as the DO deficit. In general K_a, the coefficient of reaeration, is a function of space, time and ambient temperature. For a fixed temperature it may be related to mean advective (non-tidal) velocity and depth by the following empirical equation[72],

$$K_a = b_1 \frac{v^{b_2}}{d^{b_3}} \qquad (2\text{-}15)$$

where v = mean advective velocity, d = mean depth and b_1, b_2 and b_3 are constants. Researchers have evaluated the numerical values of the constants in this equation for numerous specific streams, rivers and estuaries[102,234,330].

Investigations of variation of K_a as a function of temperature[33,117], show that it increases exponentially with increases in temperature. A representative empirical equation expressing this functional dependence is:

$$K_a = .430 \exp\left[.025 \ (T-273)\right] \qquad (2\text{-}16)$$

where T is temperature in degrees Kelvin. An empirical equation combining equations of the form of (2-15) and (2-16) appears in[76]. From equation (2-16) it is evident that diurnal thermal variations could elicit temporal variations in K_a.

Since photosynthesis is a process transferring oxygen between suspended algae and water, it varies diurnally with exposure to sunlight[338]. It also increases with increase in temperature and the nutrient supply for the algae. Its effect is represented by the term, P.

Principal consumers of DO include deoxygenation, nitrification, respiration demand and benthal deposit demand. Deoxygenation and nitrification result from the presence of two classes of soluble organic material in the water[85]:

1.) carbonaceous organic material which serves as nutrients for aerobic organisms;
2.) oxidizable nitrogen which serves as food for specific organisms.

Oxidation occurs in two steps during self-purification of the water. During the first stage, deoxygenation, between 70 and 80% of the organic carbon present is oxidized. During the second stage, nitrification, biochemical oxidation of ammonia occurs concurrently with oxidation of the remaining 20 to 30% of carbonaceous organic material.

Since deoxygenation is a first order reaction proportional to the concentration of BOD present, it may be represented as follows,

$$r_s = -K_d L \qquad (2\text{-}17)$$

where L is the BOD concentration and K_d is the coefficient of deoxygenation. K_d increases with increasing longitudinal mixing and increasing bottom growth[340].

Nitrification may be represented as a first order decay with a time lag.[128] It can be a significant oxygen consumer close to sources of large concentrations of oxidizable nitrogenous organic material[85]. After introduction of waste to the water, a lag that typically lasts several days occurs before increases in oxygen demand due to nitrification may be observed. Extensive experimentation has established an empirical relationship between this lag and mean water temperature[551].

Respiration by plankton and fixed plants produces an additional oxygen demand[103]. This demand is a function of both turbulence and the nutrient supply. It is represented by R.

Benthal deposits on the bottom produce oxygen demand in two principal ways:

1.) diffusion of partly decomposed products of anaerobic reactions within the deposits into the water above;

2.) purging action of gases rising from the benthal layer.

The term BD is used to represent the effect of all oxygen demands other than the flowing BOD load, nitrification, and respiration.

The BOD rate balance has associated with it a source, L_a, due to runoff and a first order decay reaction, with coefficient K_r, which may include the effects of oxidation, flocculation and sedimentation.

The following dynamic water quality model for a three-dimensional tapered estuary includes terms representing all of the above described transport and reaction processes.

$$\frac{\partial L}{\partial t} = -Q \frac{\partial}{\partial x}\left(\frac{L}{A}\right) - V_y \frac{\partial L}{\partial y} - V_z \frac{\partial L}{\partial z} + \frac{\partial}{\partial x}\left(D_x \frac{\partial L}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial L}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial L}{\partial z}\right) - K_r L + L_a \qquad (2\text{-}18)$$

$$\frac{\partial C}{\partial t} = -Q \frac{\partial}{\partial x}\left(\frac{C}{A}\right) - V_y \frac{\partial C}{\partial y} - V_z \frac{\partial C}{\partial z}$$

$$+ \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right)$$

$$- K_d L - K_a C + K_a C_s + P - R - BD \qquad (2\text{-}19)$$

Although they provide a more detailed representation of estuarine conditions, three-dimensional models often prove to be quite cumbersome computationally. They have been employed extensively only comparatively recently[179,258].

2.3 Two-Dimensional Water Quality Models

In many applications, two-dimensional models represent concentration distributions in waterways in sufficient detail. Such models may be classified as either stratified or non-stratified.

Stratification in an estuary, for example, is the variation in density with depth resulting from salinity intrusion. The important axis, in addition to the one in the direction of principal flow, is therefore the vertical axis.

2.3.1 Non-stratified estuaries. Non-stratified waterways are those in which complete vertical mixing occurs so that variations along the vertical axis may be neglected. An estuary with this characteristic may be represented in plan view. Under this assumption, the three-dimensional tapered estuary equations, (2-18) and

(2-19) reduce to:

$$\frac{\partial L}{\partial t} = -Q\frac{\partial}{\partial x}\left(\frac{L}{A}\right) - V_y\frac{\partial L}{\partial y} + \frac{\partial}{\partial x}\left(D_h\frac{\partial L}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_h\frac{\partial L}{\partial y}\right) - K_r L + L_a \quad (2\text{-}20)$$

$$\frac{\partial C}{\partial t} = -Q\frac{\partial}{\partial x}\left(\frac{C}{A}\right) - V_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial x}\left(D_h\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_h\frac{\partial C}{\partial y}\right) - K_d L - K_a C + K_a C_s + P - R - BD \quad (2\text{-}21)$$

where D_h is the horizontal diffusivity coefficient. D_h usually is smaller in magnitude than the eddy coefficients of the three-dimensional model(383). Plan view models appear in(37,109,188,292,346).

2.3.2 <u>Stratified estuaries</u>. In general stratified estuaries are shallow with vertical mixing at about the same rate as tidal action(339,418). Corresponding to the elimination of the lateral horizontal axis, lateral distributions of density, velocity and concentrations are averaged laterally.

The three-dimensional tapered estuary concentrations equations then reduce to:

$$\frac{\partial L}{\partial t} = -Q\frac{\partial}{\partial x}\left(\frac{L}{A}\right) - V_z\frac{\partial L}{\partial z} + \frac{\partial}{\partial x}\left(D_x\frac{\partial L}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial L}{\partial z}\right) - K_r L + L_a \quad (2\text{-}22)$$

$$\frac{\partial C}{\partial t} = -Q\frac{\partial}{\partial x}\left(\frac{C}{A}\right) - V_z\frac{\partial C}{\partial z} + \frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right) - K_d L - K_a C + K_a C_s + P - R - BD \quad (2\text{-}23)$$

Such a model is described as a two-dimensional side elevation model. Models of this type appear in many works[183,256,306,382,546].

2.4 One-Dimensional Water Quality Models

2.4.1 Tidel river. In portions of a waterway where it may be regarded as laterally and vertically homogeneous a one-dimensional model is appropriate. Along such a stretch of an estuary, for example, the single axis of the model extends downstream in the direction of principal flow. Physically, the homogeneity condition corresponds to minimal salinity intrusion in this stretch. The mathematical model reflecting this condition may be obtained from the three-dimensional estuary model by spatially averaging its equations, (2-18) and (2-19), over the cross-section of the estuary. If it is assumed that cross-sectional area is time-invariant, the resulting model for a tapered tidal river is:

$$\frac{\partial}{\partial t} L(x,t) = -\frac{1}{A}\frac{\partial}{\partial x}(QL) + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial L}{\partial x}\right) - K_r L + L_a \qquad (2\text{-}24)$$

$$\frac{\partial}{\partial t} C(x,t) = -\frac{1}{A}\frac{\partial}{\partial x}(QC) + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) - K_d L - K_a C + K_a C_s + P - R - BD \qquad (2\text{-}25)$$

where $A(x)$ is the spatially-dependent cross-sectional area and D is the logitudinal dispersion coefficient.

Many researchers have investigated properties and effects of longitudinal dispersion[472,418,92,100,135,136,137,262,138,173,182,475]. Longitudinal dispersion results from spatial variation in velocity and concentration over the cross section. D is several orders of magnitude larger than the coefficients of eddy diffusion appearing in the three-dimensional estuary model equations (2-18) and (2-19).

One-dimensional tidal river-type models have been used in many studies of estuaries, rivers and streams[332,68,334,418,208,425] estuaries,[212,335,296,106,349,484,545] rivers and streams. The effect of dispersion reduces with distance upstream from the mouth of the estuary. It is most pronounced in the tidal saline portion, less pronounced in the tidal non-saline portion and, beyond the tidal portion, negligible. Dobbins[103] presents a comparison of the magnitudes of the dispersive and advective terms of the model.

2.4.2 Tapered stream. If dispersion is negligible in comparison with advection, the one-dimensional tidal river model equations reduce to the following form for a tapered stream.

$$\frac{\partial L}{\partial t} = -\frac{Q}{A}\frac{\partial L}{\partial x} - \frac{L}{A}\frac{\partial Q}{\partial x} - K_r L + L_a \qquad (2\text{-}26)$$

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} - \frac{C}{A}\frac{\partial Q}{\partial x} - K_d L - K_a C + K_a C_s + \bar{P} - \bar{R} - \overline{BD} \qquad (2\text{-}27)$$

$\bar{P}$, $\bar{R}$ and $\overline{BD}$ are used in some studies to represent the daily average of photosynthesis, respiration and benthal deposit terms(470). This tapered stream model with temporally averaged terms has been applied to a number of practical problems by the author(75, 365).

2.4.3 Stream with uniform cross-section. If the stream being modeled has a uniform cross section (i.e. no taper), equations (2-26) and (2-27) reduce to the transient version of the Streeter-Phelps model presented by O'Conner(336), and others(340, 470).

2.5 Steady-state Water Quality Models

The models presented in the preceding sections are dynamic in the sense that they yield instantaneous values of the variables and are capable of portraying transient responses to disturbances. If less information is required, steady state models may be capable of supplying the necessary results at a considerable reduction in complexity of analysis compared with their dynamic counterparts. The models of the class considered herein may be reduced to their steady-state forms by setting their temporal partial derivative terms to zero.

For the estuary this step corresponds to assuming that the concentration distributions do not change from one point in the tidal period to the next. With this assumption, equations (2-24) and (2-25) become:

$$-\frac{1}{A}\frac{\partial}{\partial x}(QL) + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial L}{\partial x}\right) - K_r L + L_a = 0 \qquad (2\text{-}28)$$

$$-\frac{1}{A}\frac{\partial}{\partial x}(QC) + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) - K_d L - K_a C$$

$$+ K_a C_s + P - R - BD = 0 \qquad (2\text{-}29)$$

A model similar in form to this one was used in a study of the East River in New York[335].

2.6 Evaluation of Variables and Parameters

To obtain realistic and useful results in applying the above described models to practical problems it is necessary to be able to measure water quality variables, BOD and DO and evaluate the hydrodynamic variables, Q and the dispersion coefficients, and the biochemical parameters K_r , K_d , K_a with sufficient accuracy.

2.6.1 Measurement of water quality variables BOD and DO.

An extensive discussion of measurement of the water quality variables appears in Okunseinde[340]. A significant difference between DO measurement and BOD measurement is that DO values can be obtained very quickly, but BOD_5 requires a 5-day incubation period for evaluation. With this difference in measurement times DO concentration is acceptable for feedback control and BOD is not. To effect feedback control of BOD concentration it is necessary to employ more quickly evaluated variables that are related to BOD. The two most popular means for quickly measuring BOD indirectly are chemical oxygen demand analysis and total organic carbon analysis. Readings of both have been shown to be linearly related to the BOD concentrations of polluted water samples under controlled conditions[126].

2.6.2 Hydrodynamic variables.

2.6.2.1 Tidal velocity. Recently considerable research has been applied to the determination of tidal velocity distribution in a number of estuaries[175,418,37,183,208,256,179]. Three principal approaches have been employed:

1.) solution of the continuity and momentum equations,

2.) cubature method,

3.) direct measurement.

The first of these methods involves simultaneous solution of a pair of non-linear hyperbolic partial differential equations representing conservation of mass and momentum. An example of these equations for a one-dimensional estuary is presented in Okunseinde[340]. For estuaries field measurements of tidal elevations at the freshwater flow boundary and the ocean boundary are applied as boundary conditions in solving these equations. Since analytical solutions are difficult to obtain, in general the equations are solved by finite-difference methods.

The cubature method is employed when data on the distributions of tidal amplitude and phase are available a priori. It consists of integrating the continuity equation. This method in conjunction with assumption of harmonic tidal flow was utilized to determine tidal velocity distribution in a two-dimensional model,of Galveston Bay[388].

Tidal flow has been represented in many studies by the harmonic approximation,

$$V(x,t) = V_F(x) + V_T(x) \sin\left[\omega t - F(x)\right] \qquad (2\text{-}30)$$

where $V_F(x)$ is the mean freshwater flow, $V_T(x)$ is the maximum tidal velocity and $F(x)$ is the tidal phase. This model is especially useful when field measurements of its parameters are available.

Tidal velocity distributions resulting from density variations due to salinity intrusion have been investigated using two-dimensional estuary concentrations models recently[174,418,256,306,219]. Experimental data[174] and mathematical analysis[418] show a time-averaged velocity distribution with a logarithmic vertical profile.

2.6.2.2 Dispersion coefficient. Dispersion of pollutants results from cross sectional flow variations. Among the earliest research on dispersion was the work by Taylor [472] on determining the coefficient of longitudinal dispersion for unidirectional flow in a pipe. Subsequent research in this area has been extensive [92,100,135,136,137,173,182,188,261,339,418,484,138,67,1,192]. Fischer [138] proposed the following expression for the longitudinal dispersion coefficient.

$$D_x = -\frac{1}{A'}\int_0^w u'd\left[\int_0^y \frac{1}{\epsilon_y d}\left(\int_0^y\int_0^d u'dzdy\right)dy\right]dy \qquad (2\text{-}31)$$

where:

A' = cross-sectional flow area
w = flow width
u' = spatial variation of velocity from the cross-sectional mean value
ϵ_y = coefficient of lateral mixing
y = coordinate transverse to flow
d = mean cross-sectional depth

Usually, however, the distribution of dispersion is determined by curve-fitting of field measurements of the salinity distribution.

2.6.3 Biochemical parameters.

2.6.3.1 BOD removing coefficient (K_r). The reduction of BOD due to carbonaceous oxidation, sedimentation, flocculation, volatization and other BOD removing processes may be modelled as a first-order decay involving the BOD removal coefficient as follows:

$$\frac{dL}{dt} = - K_r L \qquad (2\text{-}32)$$

where K_r represents the combined effects of the BOD removal processes listed above. Due to cleansing effects as the water proceeds downstream, K_r may decrease spatially.

The solution of equation (2-32) may be expressed in the form:

$$\log_e L = \text{constant} - K_r t \qquad (2\text{-}33)$$

Hence, K_r may be evaluated from a best-fit logarithmic plot of BOD data obtained under steady state low-flow conditions. In order to more closely approximate steady state conditions, ultimate BOD (BOD_{20}) values are used in this analysis and adjustments are made to account for temperature changes[114].

2.6.3.2 <u>Deoxygenation coefficient</u> (K_d). Deoxygenation occurs when stream DO is decreased due to demands resulting from carbonaceous oxidation. This first-order process may be represented as:

$$\frac{dC}{dt} = -K_d L \qquad (2\text{-}34)$$

where:

C = DO concentration
L = BOD concentration

In the absence of a non-oxidation process, $K_d = K_r$. K_d also may be evaluated by the techniques listed above for K_r.

2.6.3.3 Reaeration coefficient (K_a). The reaeration coefficient may be evaluated from a number of empirical equations of the form of equation (2-15). It also may be computed directly from BOD and DO concentrations data by means of curve fitting[103].

2.6.3.4 Sources and sinks. O'Conner and DiToro[338] have shown that photosynthesis may be modelled as a summation of diurnal harmonic functions. Coefficients of each harmonic are determined by applying curve-fitting to DO field data. Respiration and benthal deposit rates may be similarly evaluated.

2.7 Spatial Discretization of Continuous Dynamic Distributed Parameter Water Quality Models

Analytical solutions have been obtained under specific conditions for continuous dynamic distributed water quality models in simplified form under specific conditions. However, for more realistic and, consequently, more complex models analytic solutions become impractical and unavailable. Hence, a more general approach to obtaining solutions for these water quality models is the application of finite-difference techniques. The first step in such application is discretization of the equations of the model along its spatial axes to convert each of its linear partial differential equations to a set of ordinary linear differential equations. For greater clarity in presentation, the spatial discretization of the one-dimensional tidal river model will be described first.

2.7.1 Spatial discretization of the tidal river model. Spatial discretization of a distributed parameter model with one spatial dimension is begun by determining the interval of practical interest along the spatial axis and dividing it into segments. For the tidal river model, such an interval could be a single reach along the river. Division of this reach into N increments defines N-1 internal spatial points plus two end points. For each partial differential equation in the original model there now corresponds a set of ordinary differential equations, one for each spatial point at the ends of the increments. In practice one or both ends of the reach may have special end conditions associated with it instead of an ordinary differential equation.

Expansion of the derivatives of products in the equation expressing the BOD concentration rate balance in the tidal river model, (2-24) yields:

$$\frac{\partial L}{\partial t} = - \frac{Q}{A} \frac{\partial L}{\partial x} - \frac{L}{A} \frac{\partial Q}{\partial x} + D \frac{\partial^2 L}{\partial x^2} + \frac{D}{A} \frac{\partial A}{\partial x} \frac{\partial L}{\partial x}$$

$$+ \frac{1}{A} \frac{\partial D}{\partial x} \frac{\partial L}{\partial x} - K_r L + L_a \qquad (2\text{-}35)$$

Similarly, the DO concentration rate balance, equation (2-25), with substitution of $\bar{B}$ for $\overline{BD}$, may be expanded to:

$$\frac{\partial C}{\partial t} = - \frac{Q}{A} \frac{\partial C}{\partial x} - \frac{C}{A} \frac{\partial Q}{\partial x} + D \frac{\partial^2 C}{\partial x^2} + \frac{D}{A} \frac{\partial A}{\partial x} \frac{\partial C}{\partial x} + \frac{1}{A} \frac{\partial D}{\partial x} \frac{\partial C}{\partial x} - K_d L - K_a C + K_a C_s + \bar{P} - \bar{R} - \bar{B} \qquad (2\text{-}36)$$

where $\bar{P}$, $\bar{R}$ and $\bar{B}$ are temporally averaged as explained earlier. If the spatial segments are sufficiently small, the spatial variation of the longitudinal diffusion coefficient is negligible and terms involving $\frac{\partial D}{\partial x}$ may be omitted just before spatial discretization.

The discretization itself is now accomplished following the methods of Dresnack and Dobbins[106]. Let the subscript k represent the kth spatial point which precedes a spatial increment h_k units in length. Then at the kth point on the spatial axis each zero order variable, such as L, is assigned the subscript k.

Since the partial derivatives with respect to time must be approximated by forward differences so that the numerical solution will advance in time, the spatial derivatives of the model must be represented by backward differences to avoid generation of false dispersive effects. This results from the fact that under pure convection, the concentrations at a given point one time increment in the future must be identical with the present concentrations one spatial increment upstream from the point if the spatial increment equals the product of the mean fluid velocity and the temporal increment. More specifically, if h_t represents the temporal segment or increment, the subscript, i, represents a specific point in time and

$$h_k = \frac{Q}{A} h_t \qquad (2\text{-}37)$$

where: Q = constant volume flow rate
A = cross sectional area

then

$$L_{k,i+1} = L_{k-1,i} \qquad (2\text{-}38)$$

and

$$C_{k,i+1} = C_{k-1,i} \qquad (2\text{-}39)$$

under pure convection.

Equation (2-37) presents an additional necessary condition for avoiding generation of false dispersive effects in the numerical solution.

First order spatial derivatives are therefore approximated as follows:

$$\frac{\partial L}{\partial x} \approx \frac{L_k - L_{k-1}}{h_k} \qquad (2\text{-}40)$$

$$\frac{\partial C}{\partial x} \approx \frac{C_k - C_{k-1}}{h_k} \qquad (2\text{-}41)$$

$$\frac{\partial A}{\partial x} \approx \frac{A_k - A_{k-1}}{h_k} \qquad (2\text{-}42)$$

$$\frac{\partial Q}{\partial x} \approx \frac{Q_k - Q_{k-1}}{h_k} \tag{2-43}$$

Second order spatial derivatives may be expressed by applying the backward differencing operation to the corresponding approximation of the first order term.

$$\frac{\partial^2 L}{\partial x^2} \approx \frac{\dfrac{L_{k+1} - L_k}{h_{k+1}} - \dfrac{L_k - L_{k-1}}{h_k}}{h_{k+1}}$$

$$= \frac{L_{k+1}}{h^2_{k+1}} - \frac{h_{k+1} + h_k}{h^2_{k+1}\ h_k} L_k + \frac{L_{k-1}}{h_{k+1}\ h_k} \tag{2-44}$$

where, from equation (2-37),

$$h_k = \frac{Q_k + Q_{k-1}}{A_k + A_{k-1}} h_t \tag{2-45}$$

Similarly,

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_{k+1}}{h^2_{k+1}} - \frac{h_{k+1} + h_k}{h^2_{k+1}\ h_k} C_k + \frac{C_{k-1}}{h_{k+1}\ h_k} \tag{2-46}$$

At the kth point in space each temporal partial derivative becomes an ordinary derivative,

$$\frac{\partial L}{\partial t} \Rightarrow \frac{dL_k}{dt} = \dot{L}_k \tag{2-47}$$

$$\frac{\partial C}{\partial t} \Rightarrow \frac{dC_k}{dt} = \dot{C}_k \tag{2-48}$$

Substitution of equations (2-40) through (2-48) into the equations of the continuous dynamic distributed parameter tidal river model (2-35) and (2-36) yields:

$$\dot{L}_k = - B_k L_k + F_k L_{k+1} + E_k L_{k-1} + L_a \quad (2\text{-}49)$$

where:

$$B_k \equiv E_k + F_k + \frac{Q_k - Q_{k-1}}{A_k h_k} + K_r \quad (2\text{-}50)$$

$$E_k \equiv \frac{D}{h^2_{\;k}} \left(\frac{A_{k-1}}{A_k} + \frac{h_k}{h_{k+1}} - 1\right) + \frac{Q_k}{A_k h_k} \quad (2\text{-}51)$$

$$F_k \equiv \frac{D}{h^2_{\;k+1}} \quad (2\text{-}52)$$

and

$$\dot{C}_k = -G_k C_k + F_k C_{k+1} + E_k C_{k-1} - K_d L_k + K_s \quad (2\text{-}53)$$

where:

$$G_k \equiv B_k - K_r + K_a \quad (2\text{-}54)$$

$$K_s = K_a C_s + \bar{P} - \bar{R} - \bar{B} \quad (2\text{-}55)$$

The total number of spatial points resulting from subdivision of the reach into N increments is N+1, including the end points. If the upstream boundary conditions are given, K=2,4,---N+1, in equations (2-49) through (2-54).

The equations representing the dynamic BOD and DO balances of the discretized tidal river model may be regarded as state equations because the model may be expressed in state equation form as follows:

$$\begin{bmatrix} \dot{\underline{L}} \\ \dot{\underline{C}} \end{bmatrix} = \begin{bmatrix} B & 0 \\ K & G \end{bmatrix} \begin{bmatrix} \underline{L} \\ \underline{C} \end{bmatrix} + \text{constant matrix of dimension } 2N \qquad (2\text{-}56)$$

where:

$$B = \begin{bmatrix} B_2 & F_2 & & & & 0 & \\ E_3 & \ddots & \ddots & & & & \\ & \ddots & E_k & B_k & F_k & & \\ & & & \ddots & \ddots & \ddots & F_N \\ & 0 & & & & E_{N+1} & B_{N+1} \end{bmatrix} \qquad (2\text{-}57)$$

G is of the same form as the matrix B with

G_k in the place of B_k , $k=2,3,\ldots, N+1$

$$\underline{L} = (L_2, L_3, \ldots, L_{N+1})^T \qquad (2\text{-}58)$$

$$\underline{C} = (C_2, C_3, \ldots, C_{N+1})^T \qquad (2\text{-}59)$$

BOD and DO are the state variables for this formulation.

2.7.2 Spatial discretization of the tapered stream model. The spatially discretized form of the continuous dynamic distributed parameter model for concentrations in a tapered stream may be derived by applying the methods described in Section 2.6.1 to equations (2-26) and (2-27) or by setting the coefficient of dispersion, D, in equations (2-49) through (2-54) to zero. The spatially discretized model resulting from either approach is the following.

$$\dot{L}_k = -B_k L_k + E_k L_{k-1} + L_a \qquad (2\text{-}60)$$

where:

$$B_k = \frac{2Q_k - Q_{k-1}}{A_k h_k} + K_r \qquad (2\text{-}61)$$

$$E_k = \frac{Q_k}{A_k h_k} \qquad (2\text{-}62)$$

$$\dot{C}_k = -G_k C_k + E_k C_{k-1} - K_d L_k + K_s \qquad (2\text{-}63)$$

where G_k is defined in equation (2-54) and k=2,3...,N+1.

Equations (2-60) and (2-63) may be written as state equations in the same way as were the corresponding equations for the tidal river model, (2-49) and (2-53).

2.8 Multilevel Hierarchical Optimal Control of Discretized Dynamic Continuous Water Quality Models

Discretization of the partial differential equations of the original continuous distributed parameter water quality models frequently involves a trade off in the size of the increments used. The increments must be small enough so that the discretized model approximates the continuous model with sufficient accuracy, but decreasing the size of the increments increases the number of equations in the discretized model corresponding to each equation in the continuous model. The resulting relatively high dimension of the discretized model often severely limits the generality of practical problems that can be solved using discretization alone. The methods of multilevel hierarchical systems analysis have been shown to be especially effective in reducing equation sets of high dimension to a series of sets of equations of lower dimension.

In particular, the application of optimal control to the discretized water quality models derived earlier in this dissertation is facilitated by employing multilevel hierarchical techniques. The basic approach to multilevel hierarchical control of either lumped parameter or discretized continuous distributed parameter models is to first decompose the model into a series of models of lower dimension, apply standard optimal control techniques to each model of the decomposed system and later coordinate the solutions for the resulting series of control problems in a separate coordination problem. Specifically, combination of multilevel hierarchical systems analysis with Pontryagin's minimum principle[378,531] yields the following general procedure for application of multilevel hierarchical optimal control techniques to a model of high dimension.

1.) Apply decomposition to the system to be controlled to reduce it to a series of systems of lower dimension that are temporarily de-coupled from each other.

2.) Add control terms to the equations representing the balances to which the control is to be applied.

3.) Define a performance index functional dependent upon the relevant state variables and control terms that is to be minimized.

4.) Construct the corresponding Hamiltonian from the performance index, state equations and control equations.

5.) Employ Pontryagin's equations to determine the costate equations, constraint equations and control equations.

6.) Assemble the constraint equations of the previous two steps into an overall coordination subproblem, and assign the state equations, costate equations and control equations to their respective subproblems.

7.) Construct the subproblem hierarchy with the state, costate and control subproblems on the lower level and the coordination subproblem occupying the upper level.

8.) Determine appropriate boundary, initial and final conditions for the subproblems in the hierarchy.

9.) Solve the subproblems of the hierarchy iterating between the levels until the performance index is minimized.

2.8.1 Decomposition. Decomposition subdivides the set of equations constituting the original lumped parameter model or discretized continuous distributed parameter model into a series of submodels which also may be expressed in the form of state equations. These submodels generally are coupled with each other. A coordination variable is therefore introduced to each submodel to include all of the coupling terms and to temporarily suppress the coupling. An original model that has been subjected to this process is said to be decomposed.

The sum of the dimensions of the submodels of the decomposed model equals the dimension of the original model. The dimension of an individual submodel could be considerably smaller than that of the original model depending upon the number of subdivisions employed which is the dimension of the coordination subproblem to be solved later.

In general, the equations comprising the coordination subproblem are considerably more simple than those comprising the submodels. Thus, it is desirable for efficiency of solution of the associated hierarchy of subproblems to trade smaller dimensions of the submodels for larger dimension of the coordination subproblem. For many practical applications this trade off can be carried to the point where each submodel contains only a single equation. This latter condition is identified in this dissertation as <u>full decomposition</u>.

The subproblem hierarchical structure is a direct consequence of the initial application of decomposition. In particular, full decomposition leads to a subproblem hierarchy in which all lower level subproblems contain only a single equation thus obviating a vector-matrix approach in their solution. For this reason, full decomposition is applied to all of the models that are decomposed in the sequal.

2.8.1.1 Decomposition of the discretized tidal river model. Coupling in the discretized model of the BOD concentration rate balance for the tapered tidal river, equation (2-49), is represented by terms involving L_{k+1} and L_{k-1}. The coupling is suppressed by collecting all of these terms together and equating them to a coordination variable as follows,

$$S_k = F_k L_{k+1} + E_k L_{k-1} \qquad (2\text{-}64)$$

Coupling in the discretized model of the DO concentration rate balance of equation (2-53) is represented in addition to terms involving C_{k+1} and C_{k-1}, by a term due to coupling from the BOD equation, $K_d L_k$. Hence, the coordination variable for the DO equation is defined as:

$$R_k = F_k C_{k+1} + E_k C_{k-1} - K_d L_k \qquad (2\text{-}65)$$

Substitution of equation (2-64) into equation (2-49) reduces it to,

$$\dot{L}_k = - B_k L_k + S_k + L_a \qquad (2\text{-}66)$$

with B_k defined in equation (2-50).

Similarly, substitution of equation (2-65) in equation (2-53) reduces it to,

$$\dot{C}_k = -G_k C_k + R_k + K_s \qquad (2\text{-}67)$$

with G_k defined in equation (2-54).

Since k=2,3,...,N+1 for given upstream boundary conditions, inspection of equations (2-65) and (2-66) shows that the overall coordination problem involves the solution of 2N equations. A relatively large N can be tolerated because all of the equations are linear and algebraic.

2.8.1.2 Decomposition of the tapered stream model. The decomposed form of the discretized tapered stream model may be obtained by applying the methods presented in section 2.8.1 to equations (2-60) and (2-63) or by setting D=0 in equations (2-50) through (2-52), (2-54), (2-64) and (2-66). The resulting decomposed model is:

$$S_k = \frac{Q_k}{A_k h_k} L_{k-1} \qquad (2\text{-}68)$$

$$R_k = \frac{Q_k}{A_k h_k} C_{k-1} - K_d L_k \qquad (2\text{-}69)$$

$$\dot{L}_k = -B_k L_k + S_k + L_a \qquad (2\text{-}70)$$

$$\dot{C}_k = -G_k C_k + R_k + K_s \qquad (2\text{-}71)$$

where k=2,3,...,N+1 for given upstream boundary conditions,

B_k is defined by equation (2-61) and G_k is defined by equation (2-54).

2.8.2 Optimal aeration control of the spatially discretized tidal river model.

2.8.2.1 Addition of aeration control term. The aeration control term is added to the DO concentration rate balance of the decomposed discretized model, equation (2-67):

$$\dot{C}_k = -G_k C_k + R_k + K_s + (U_c)_k \qquad (2\text{-}72)$$

where $(U_c)_k$ represents a rate of addition of DO at spatial point k along the longitudinal axis.

2.8.2.2 Definition of performance index for optimal aeration control. Under the assumption that a specified level of DO concentration, C_{sp}, is to be attained with minimum energy expenditure, the spatially discretized performance index may be constructed as a weighted linear sum of quadratic functionals of the error in DO concentration and the magnitude of the aeration control terms integrated over time.

$$J = \sum_{k=1}^{N+1} \frac{J_k}{h_k} \qquad (2\text{-}73)$$

$$J_k = h_k \int_{t_o}^{t_f} \left[W_1 (C_{sp} - C_k)^2 + W_2 (U_c)_k^2 \right] dt \qquad (2\text{-}74)$$

where t_o = initial time and t_f = final time.

W_1 and W_2 are constant weighting coefficients for the error term and control energy, respectively. The relationships between the magnitudes of W_1 and W_2 reflect different tradeoffs as to whether accuracy of control or minimization of energy expenditure has higher priority.

Other performance index functionals could be defined to reflect different criteria of optimality. For example, if it is less important that the system be corrected for excess DO concentration, then equation (2-74) could be used for the performance index when $C_k < C_{sp}$ and a new performance index,

$$J_k \Big|_{C_k \geq C_{sp}} = h_k \int_{t_o}^{t_f} \left[W_5 (C_{sp} - C_k)^2 + W_2 (U_c)_k^2 \right] dt \tag{2-75}$$

where $W_5 << W_1$, could be defined for $C_k \geq C_{sp}$.

2.8.2.3 <u>Construction of Hamiltonian for optimal aeration control</u>. Combining the performance functional of equation (2-74) with the state equations of the decomposed discretized tidal river, equations (2-50) through (2-52) and (2-54), (2-66) and (2-72), coordinating equations (2-64)and (2-65) results in the following spatially discretized Hamiltonian.

$$H = \sum_{k=1}^{N+1} h_k H_k \tag{2-76}$$

where:

$$\begin{aligned} H_k = {} & W_1 \; (C_{sp} - C_k)^2 + W_2 \; (U_c)_k^2 \\ & + (CL)_k \; (-B_k L_k + S_k + L_a) \\ & + (CC)_k \; \left[-G_k C_k + R_k + K_s + (U_c)_k \right] \\ & + p_k \; (F_k \; L_{k+1} + E_k \; L_{k-1} - S_k) \\ & + q_k \; (F_k \; C_{k+1} + E_k \; C_{k-1} - K_d \; L_k - R_k) \end{aligned} \tag{2-77}$$

B_k, E_k, F_k and G_k are defined by equations (2-50), (2-51), (2-52) and (2-54), respectively, $(CL)_k$ and $(CC)_k$ are costate variables and p_k and q_k are Langrange coefficients at point k along the longitudinal axis.

2.8.2.4 <u>Costate equations for optimal aeration control</u>. In order to minimize the performance index for this problem a set of necessary conditions must be satisfied. Two of these necessary conditions yield the costate equations as follows,

$$\frac{d}{dt} (CL)_k = - \frac{\partial H}{\partial L_k}$$

$$= B_k \; (CL)_k - F_{k-1} \; p_{k-1} - E_{k+1} \; p_{k+1} + K_d \; q_k \tag{2-78}$$

where:

$$E_{k+1} = \frac{D}{h_{k+1}^2} \left(\frac{A_k}{A_{k+1}} + \frac{h_{k+1}}{h_{k+2}} - 1\right) + \frac{Q_{k+1}}{A_{k+1}h_{k+1}} \qquad (2\text{-}79)$$

$$F_{k-1} = \frac{D}{h^2_{\ k}} \qquad (2\text{-}80)$$

B_k is defined in equation (2-50)

$$\frac{d}{dt}(CC)_k = - \frac{\partial H}{\partial C_k}$$

$$= G_k\ (CC)_k - F_{k-1}\ q_{k-1} + 2W_1(C_{sp} - C_k) - E_{k+1}\ q_{k+1} \qquad (2\text{-}81)$$

where G_k is defined by equation (2-54). For equations (2-78) and (2-81) k=2,3,...,N-1 for given downstream boundary conditions.

2.8.2.5 <u>Additional coordination equations</u>. Additional necessary conditions for minimization of the performance index functional yield the following coordination equations for this control problem.

$$\frac{\partial H}{\partial S_k} = 0 \Rightarrow p_k = (CL)_k \qquad (2\text{-}82)$$

$$\frac{\partial H}{\partial R_k} = 0 \Rightarrow q_k = (CC)_k \qquad (2\text{-}83)$$

$$\frac{\partial H}{\partial p_k} = 0 \Rightarrow S_k = F_k L_{k+1} + E_k L_{k-1} \qquad (2\text{-}64)$$

$$\frac{\partial H}{\partial q_k} = 0 \Rightarrow R_k = F_k C_{k+1} + E_k C_{k-1} - K_d L_k \qquad (2\text{-}65)$$

2.8.2.6 <u>Temporal discretization of tidal river model with aeration control</u>. Temporal discretization of the spatially discretized model converts each of its ordinary linear differential equations to a set of simultaneous linear difference equations, one such equation for each point at the ends of the temporal increments. The expression of the model in the form of linear difference equations converts the associated control problem to a form amenable to digital computer solution.

It may be assumed that the temporal interval of interest for this work is divided into uniform increments with a total of I_m points at their ends. If the length of one of the temporal increments is given by h_t, zero-order terms may be expressed in terms of their temporal averages. For example, L_k becomes $(L_{k,i+1} + L_{k,i})/2$ under temporal discretization.

As stated earlier,[106], first derivatives with respect to time must be expressed as forward differences,

e.g., $$\frac{dL_k}{dt} \approx \frac{L_{k,i+1} - L_{k,i}}{h_t} \tag{2-84}$$

Applying these methods to the spatially discretized state equations for the tidal river with optimal aeration control then yields:

$$L_{k,i+1} = \frac{(2-h_t B_k)\ L_{k,i} + 2h_t\ S_{k,i} + 2h_t L_a}{2+h_t B_k} \qquad (2\text{-}85)$$

$$C_{k,i+1} = \frac{(2-h_t G_k)\ C_{k,i} + 2h_t R_{k,i} + 2h_t K_s + (U_C)_{k,i}}{2 + h_t G_k} \qquad (2\text{-}86)$$

where the spatial index is $k=2,3,...N+1$ and the temporal index is $i=1,2,...I_m-1$. Also, for the coordination equations,

$$S_{k,i} = F_k L_{k+1,i} + E_{k,i}\ L_{k-1,i} \qquad (2\text{-}87)$$

$$R_{k,i} = F_k\ C_{k+1,i} + E_{k,i}\ C_{k-1,i} - K_d\ L_{k,i} \qquad (2\text{-}88)$$

where $k=2,3...,N$; $i=1,2,...,I_m$

B_k, E_k, F_k, G_k, and K_s are defined in equations (2-50), (2-51), (2-52), (2-54) and (2-55), respectively. The longitudinal dispersion coefficient, D, is assumed both space and time invariant. The volume flow rate at the kth spatial point, Q_k, is assumed time invariant because time-varying flow rate would, in general, require a time-varying spatial increment according to equation (2-45). In a later chapter, a water quality model will be presented that obviates this limitation.

Similarly, the spatially and temporally discretized costate equations are obtained by applying the same methods to the spatially discretized costate equations and solving for the costate variable at the point (k,i) as a function of the costate variable at the point (k,i+1).

$$(CL)_{k,i} = \Big[(2-h_tB_k)\ (CL)_{k,i+1} + 2h_tF_{k-1}p_{k-1,i} + 2h_tE_{k+1}\ p_{k+1,i} - 2h_tK_dq_{k,i}\Big] / (2+h_tB_k) \qquad (2\text{-}89)$$

$$(CC)_{k,i} = \Big[(2-h_tG_k)\ (CC)_{k,i+1} + 2h_t\ F_{k-1}\ q_{k-1,i} + 2h_t\ E_{k+1}\ q_{k+1,i} - 2h_tW_1\ (C_{sp} - C_{k,i})\Big] / (2+h_tG_k) \qquad (2\text{-}90)$$

where the spatial index k=1,2,...,N for given downstream end boundary conditions and the temporal index $i=1,2,\ldots,I_m-1$ for given final conditions.

Under temporal discretization, the remaining spatially discretized coordination equations become

$$p_{k,i} = (CL)_{k,i} \qquad (2\text{-}91)$$

$$q_{k,i} = (CC)_{k,i} \qquad (2\text{-}92)$$

where k=1,2,...,N+1; $\quad i=1,2,\ldots,I_m$

2.8.2.7 <u>Construction of optimal control equations</u>. Using a gradient approach to optimization as in Pierre[371],

$$(U_C)^{(r+1)}_{k,i} = (U_C)^{(r)}_{k,i} - \epsilon_C\ (GRC)^{(r)}_{k,i} \qquad (2\text{-}93)$$

where the superscript denotes the number of the iteration and ϵ_C is a constant between 0 and +1.0 selected as a tradeoff between the rate of convergence and accuracy.

Under spatial and temporal discretization the Hamiltonian is:

$$H = \sum_{k=1}^{N+1} \sum_{i=1}^{I_m} h_t h_k H_{k,i} \tag{2-94}$$

where:

$$\begin{aligned} H_{k,i} = {} & W_1 (C_{sp} - \bar{C}_{k,i})^2 + W_2 (\bar{U}_C)^2_{k,i} \\ & + (\overline{CL})_{k,i} (-B_k \bar{L}_{k,i} + \bar{S}_{k,i} + L_a) \\ & + (\overline{CC})_{k,i} \left[- G_k \bar{C}_{k,i} + \bar{R}_{k,i} + K_s + (\bar{U}_C)_{k,i} \right] \\ & + \bar{p}_{k,i} (F_k \bar{L}_{k+1,i} + E_k \bar{L}_{k-1,i} - \bar{S}_{k,i}) \\ & + \bar{q}_{k,i} (F_k \bar{C}_{k+1,i} + E_k \bar{C}_{k-1} - K_d \bar{L}_{k,i} - \bar{R}_{k,i}) \end{aligned} \tag{2-95}$$

and the bar over a variable denotes its temporal average over the increment of length h_t, e.g.,

$$\bar{L}_{k,i} = (L_{k,i+1} + L_{k,i})/2 \tag{2-96}$$

The gradient for optimal aeration control, $(GRC)_{k,i}$, may be derived from the spatially and temporally discretized Hamiltonian as follows:

$$(GRC)_{k,i} = \frac{\partial H}{\partial (\bar{U}_C)_{k,i}} = 2W_2(\bar{U}_C)_{k,i} + (\overline{CC})_{k,i}$$

$$= W_2 \left[(U_C)_{k,i+1} + (U_C)_{k,i} \right] + \tfrac{1}{2} \left[(CC)_{k,i+1} + (U_C)_{k,i} \right] \quad (2\text{-}97)$$

Substitution of equation (2-97) in equation (2-93) yields:

$$(U_C)^{(r+1)}_{k,i} = (U_C)^{(r)}_{k,i} - 2W_2 \quad \epsilon_C \; (\bar{U}_C)^{(r)}_{k,i} \; - \epsilon_C (\overline{CC})^{(r)}_{k,i} \quad (2\text{-}98)$$

In many applications, the gradient control equation expressed by (2-98) may be approximated with reasonable accuracy by:

$$(U_C)^{(r+1)}_{k,i} = (U_C)^{(r)}_{k,i} - 2W_2 \quad \epsilon_C \; (U_C)^{(r)}_{k,i} - \; \epsilon_C \; (CC)^{(r)}_{k,i} \quad (2\text{-}99)$$

For either equation (2-98) or equation (2-99), $k=1,2,\ldots,N+1$ and $i=1,2,\ldots,I_m$.

Inspection of equation (2-74) for the discretized performance index and the corresponding state equations (2-66) and (2-72) reveals that the optimal aeration control problem for the tidal river actually is in the same form as the optimal tracking problem as presented in Kirk[222] with the BOD and DO concentrations as state variables and the specified level of DO concentration as the variable to be followed or tracked. Since in the problem considered here the plant is linear and the tracking variable actually is constant, it would seem that a standard linear regulator closed form solution would apply to this optimal control problem. However, neither the BOD nor the DO concentrations can be negative so that the constraints $L \geq 0$ and $C \geq 0$ are implicit in the optimal aeration control problem. Furthermore, in a practical problem there will be an upper bound on the magnitude of control due to physical limitations, $U_C \leq (U_C)_{max}$. The linear regulator solution of this problem would therefore hold only when neither the state variables nor the control variables are at their limiting values. When such a condition occurs, the system is said to be following a singular control trajectory or arc and the linear regulator solution is not valid. In order to accommodate this condition along with the solutions when neither the state nor control variables are at their bounds, the gradient approach was employed.

2.8.2.8 Construction of subproblem hierarchy.

The equations derived thus far for optimal aeration control of the spatially and temporally discretized tidal river concentrations may be assigned to four types of subproblems as follows:

Type of Subproblem	Number of Equations
State variable	$(2N)(I_m-1)$
Costate variable	$(2N)(I_m-1)$
Control	$(N)\ (I_m-1)$
Coordination	1

These subproblems to be solved may be assembled into a two level hierarchy with the single coordination subproblem occupying the supremal position and the state, costate and control equations in the infimal positions as shown in Figure 2-1.

If each infimal (state, costate or control) subproblem is subdivided into the equations pertaining to a particular spatial point , then the number of infimal subproblems interacting with the coordination subproblem would increase to 5N comprised of 2N state subproblems, 2N costate subproblems and N control subproblems.

It was stated earlier that due to temporal discretization each equation at a spatial point is represented by I_m-1 finite difference equations. If each infinimal subproblem is defined in such a way as to include only one such equation, then the hierarchy would contain $(2N)\ (I_m-1)$ state subproblems, $(2N)(I_m-1)$ costate subproblems and $N(I_m-1)$ control subproblems all interacting with a single coordination subproblem at the apex of the

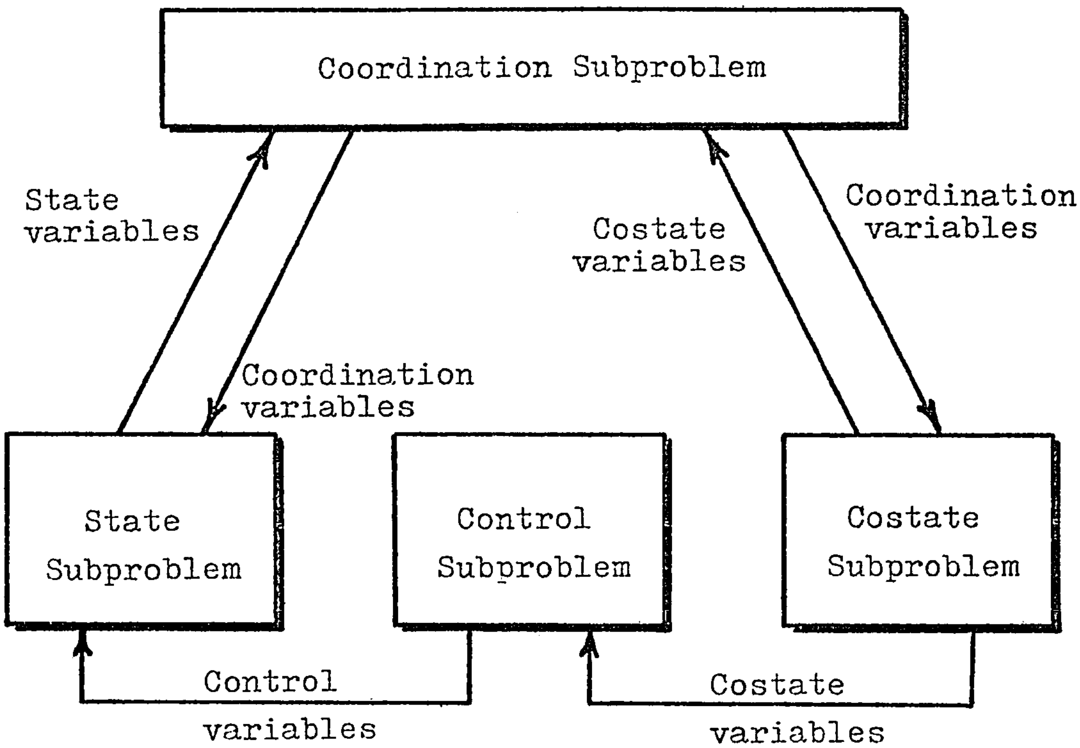


Figure 2-1: Subproblem hierarchy for concentrations model of tidal river reach

hierarchy.

All of the subproblem hierarchies listed share the overall structure depicted in Figure 2-1. They differ in the number of subproblems in the lower level and the corresponding dimension of each lower level (state, costate or control) subproblem. However, the total number of finite difference equations involved remains invariant at $5N(I_m-1)+1$.

2.8.2.9 Solution techniques for the subproblem hierarchy. Optimization of the overall control problem is accomplished by either assuming or generating an initial set of space-time profiles for the solutions of the infimal subproblems $L_{k,i}$, $C_{k,i}$, $(CL)_{k,i}$, $(CC)_{k,i}$ and $(U_C)_{k,i}$, substituting these profiles into the coordination equations and iterating between the levels of the hierarchy until the performance index of equations (2-73) and (2-74) is minimized.

Execution of this optimization procedure requires a priori information on the boundary, initial and final conditions for each equation in the subproblem hierarchy. At the outset, it is known that the final time condition and the downstream end condition for the costate variables is zero.[309] More specifically,

$$(CL)_{N+1,i} = (CC)_{N+1,i} = 0 \text{ for all } i \tag{2-100}$$

and

$$(CL)_{k,I_m} = (CC)_{k,I_m} = 0 \text{ for all } k \tag{2-101}$$

The upstream end boundary conditions for BOD and DO concentrations may be predetermined constants:

$$L_{1,i} = L_o \text{ for all } i \tag{2-102}$$

$$C_{1,i} = C_o \text{ for all } i \tag{2-103}$$

Many different spatial distributions of concentrations could be used to represent the initial conditions for the spatially and temporally discretized state equations. Some researchers have set all of the initial BOD concentrations equal to one constant value and all of the initial DO concentrations equal to another value. However, a distribution of initial concentrations generated from a suitable steady state model of the concentrations balances generally reduces the number of iterations required in order to attain the optimal space-time profiles of concentrations.

An estuary may be regarded as being at steady state when each concentration distribution does not change between temporal points within the tidal period. This implies that none of the terms in the spatially and temporally discretized model of the tidal river with aeration control, equations (2-86) and (2-87) is dependent upon the value of the temporal index, i. Hence, terms differing only with respect to the temporal index may be combined. If it is further assumed that no control is applied until after the initial time increment, the state equations reduce to the following:

$$L_{k+1,1} = \frac{B_k}{F_k} L_{k,1} - \frac{E_k}{F_k} L_{k-1,1} - \frac{1}{F_k} L_a \qquad (2\text{-}104)$$

$$C_{k+1,1} = \frac{G_k}{F_k} C_{k,1} - \frac{E_k}{F_k} C_{k-1,1} + \frac{K_d}{F_k} L_{k,1} - \frac{1}{F_k} K_s \qquad (2\text{-}105)$$

where B_k , E_k , F_k , G_k and K_s are defined by equations (2-50), (2-51), (2-52), (2-54) and (2-55), respectively.

For equations (2-104) and (2-105) k=2,3,...,N and

$$L_{1,1} = L_o \qquad (2\text{-}106)$$

$$C_{1,1} = C_o \qquad (2\text{-}107)$$

Equations (2-104) through (2-107) thus generate the initial steady state spatial distributions of BOD and DO concentrations.

Since control is not applied until after the first temporal increment,

$$(U_C)_{k,1} = 0 \text{ for all } k \qquad (2\text{-}108)$$

If it is also assumed that no control is applied until after the first spatial increment,

$$(U_C)_{1,i} = 0 \text{ for all } i \qquad (2\text{-}109)$$

Additional required boundary conditions, initial conditions and final conditions may be obtained by linear extrapolation from internal points of the space-time region of interest. Details on the method used appear in[340] and Chapter 4 of this dissertation.

An example of the application of the methods described for optimal aeration control of the dynamic tidal river concentrations model appears in Chapter 6.

2.8.3 Optimal aeration control of the discretized tapered stream model. The appropriate state, costate, control and coordination equations for optimal aeration control of the discretized dynamic tapered stream model may be derived by beginning with the equations of the decomposed spatially discretized model, equations (2-54), (2-61), (2-62) and (2-68) through (2-71) and applying the techniques of Section 2.8.2 to them. Alternatively, the required equations may be obtained by equating the dispersion coefficient of the corresponding tidal river equations to zero. The resulting equations for either approach are the following.

The state equations for the stream model with optimal aeration control are the same as equations (2-55), (2-85), and (2-86) except:

$$S_{k,i} = E_k L_{k-1,i} \quad (2\text{-}110)$$

$$R_{k,i} = E_k C_{k-1,i} - K_d L_{k,i} \quad (2\text{-}111)$$

B_k , E_k and G_k are defined in equations (2-61), (2-62), and (2-54), respectively.

The costate equations for the spatially and temporally discretized stream model under optimal aeration control are given by equations (2-89) and (2-90) with:

$$F_{k-1} = 0 \quad (2\text{-}112)$$

$$E_{k+1} = \frac{Q_{k+1}}{A_{k+1} h_{k+1}} \quad (2\text{-}113)$$

B_k as defined in equation (2-57). The remaining coordination equations are equations (2-91) and (2-92).

The optimal control equations for the stream model are the same as equations (2-101) and (2-102). The resulting subproblem hierarchy is thus of the same form as the one depicted in Figure 2-1 for the spatially and temporally discretized tidal river model under multilevel optimal aeration control.

The same boundary conditions, initial conditions and final conditions apply to the stream water quality model as to the tidal river model except that the equations for generating the initial distributions of BOD and DO concentrations are the following:

$$L_{k+1,1} = \frac{E_k}{B_k} L_{k,1} + \frac{1}{B_k} L_a \qquad (2\text{-}114)$$

$$C_{k+1,1} = \frac{E_k}{G_k} C_{k,1} - \frac{K_d}{G_k} + \frac{1}{G_k} K_s \qquad (2\text{-}115)$$

where B_k , E_k and G_k are defined by equations (2-57), (2-58) and (2-54) respectively. For equations (2-114) and (2-115) k=2,3,...,N and

$$L_{1,1} = L_o \qquad (2\text{-}116)$$

$$C_{1,1} = C_o \qquad (2\text{-}117)$$

An example of an application of the equations listed in this section appears in Chapter 6.

2.8.4 Optimal waste dumping control of the discretized tidal river model. The development of equations representing optimal waste dumping control of the discretized dynamic tapered tidal river water quality model parallels that for aeration control. The procedure is outlined in the sequel.

The waste dumping control term is added to the BOD concentration rate balance of the decomposed discretized model, equation (2-66):

$$\dot{L}_k = -B_k L_k + S_k + L_a + (U_L)_k \qquad (2\text{-}118)$$

with B_k defined in equation (2-50). $(U_L)_k$ represents the rate of addition of BOD at the kth spatial point.

If a specified level of DO concentration, C_{sp} , is to be attained with minimum expenditure of control energy, the spatially discretized performance index may be expressed as in equation (2-73) where:

$$J_k = h_k \int_{t_o}^{t_f} \left[W_1 (C_{sp} - C_k)^2 + W_4 (U_L)_k^2 \right] dt \quad (2\text{-}119)$$

Since the major role of the dumping control term is the use of points of excess DO concentration as opportunities for waste discharge, there is little practical advantage in allowing dumping at points where the DO concentration is less than C_{sp}. A switched performance index similar to that used for aeration control is advantageous in this situation. Accordingly, equation (2-119) may be used to represent the performance index for $C_k \geq C_{sp}$ and a new performance index,

$$J_k \Big|_{C_k < C_{sp}} = h_k \int_{t_o}^{t_f} \left[W_5 (C_{sp} - C_k)^2 + W_4 (U_L)_k^2 \right] dt \quad (2\text{-}120)$$

can be defined where $W_5 << W_1$.

The costate equations for dumping control are the same as those for aeration control, equations (2-78) through (2-81), (2-50) and (2-54). The coordination equations for dumping also are the same as the ones for aeration, equations (2-64), (2-65), (2-82) and (2-83).

Applying temporal discretization to the equations cited above yields the following set of spatially and temporally discretized equations for the application of optimal dumping control to the tidal river water quality model.

$$L_{k,i+1} =$$

$$\frac{(2-h_t B_k)L_{k,i} + 2h_t S_{k,i} + 2h_t L_a + 2h_t (U_L)_{k,i}}{2 + h_t B_k} \tag{2-121}$$

$$C_{k,i+1} =$$

$$\frac{(2-h_t G_k)C_{k,i} + 2h_t R_{k,i} + 2h_t K_s}{2 + h_t G_k} \tag{2-122}$$

where $S_{k,i}$, $R_{k,i}$, B_k , G_k and E_k are defined in equations (2-50), (2-51), (2-54), (2-87) and (2-88), F_k is defined in equation (2-52), and K_s is defined in equation (2-55).

The costate equations are given in (2-89) and (2-90) with $p_{k,i}$ and $q_{k,i}$ coordinated by equations (2-91) and (2-92), respectively.

The gradient approach to optimization of dumping control may be expressed as follows:

$$(U_L)^{(r+1)}_{k,i} = (U_L)^{(r)}_{k,i} - \epsilon_L \, (GRL)^{(r)}_{k,i} \qquad (2\text{-}123)$$

where the superscript denotes the number of the iteration and ϵ_L is a constant between zero and +1.0 representing a tradeoff between the rate of convergence and accuracy.

The spatially and temporally discretized Hamiltonian for optimal dumping control is:

$$H = \sum_{k=1}^{N+1} \sum_{i=1}^{I_m} h_t h_k \, H_{k,i} \qquad (2\text{-}94)$$

where:

$$\begin{aligned} H_{k,i} &= W_1 \, (C_{sp} - \bar{C}_{k,i})^2 + W_4 \, (\bar{U}_L)^2_{k,i} \\ &+ (\overline{CC})_{k,i} \, (-G_k \, \bar{C}_{k,i} + \bar{R}_{k,i} + K_s) \\ &+ (\overline{CL})_{k,i} \left[-B_k \, \bar{L}_{k,i} + \bar{S}_{k,i} + L_a + (U_L)_{k,i} \right] \\ &+ \bar{p}_{k,i} \, (F_k \, \bar{L}_{k+1,i} + E_k \, \bar{L}_{k-1,i} - \bar{S}_{k,i}) \\ &+ \bar{q}_{k,i} \, (F_k \, \bar{C}_{k+1,i} + E_k \, C_{k-1,i} - K_d \, \bar{L}_{k,i} - \bar{R}_{k,i}) \end{aligned} \qquad (2\text{-}124)$$

From $(GRL)_{k,i} = \dfrac{\partial H}{\partial (\bar{U}_L)_{k,i}}$ (2-125) applied to equation (2-124),

$$(GRL)_{k,i} = 2W_4 \, (\bar{U}_L)_{k,i} + (\overline{CL})_{k,i}$$

$$= W_4 \left[(U_L)_{k,i+1} + (U_L)_{k,i} \right]$$

$$+ \left[(CL)_{k,i+1} + (CL)_{k,i} \right] /2 \qquad (2\text{-}126)$$

Substitution of equation (2-126) in equation (2-124) yields:

$$(U_L)^{(r+1)}_{k,i} = (U_L)^{(r)}_{k,i} - 2W_4 \, \epsilon_L \, (\bar{U}_L)^{(r)}_{k,i} - \epsilon_L \, (\overline{CL})^{(r)}_{k,i}$$

(2-127)

The resulting subproblem hierarchy is of the form depicted in Figure 2-1. The boundary, initial and final conditions for optimal dumping control are given by equations (2-103) through (2-110).

Since dumping control is applied after the first temporal increment,

$$(U_L)_{k,1} = 0 \quad \text{for all } k \qquad (2\text{-}128)$$

Also, since the control is applied after the first spatial increment,

$$(U_L)_{1,i} = 0 \quad \text{for all } i \qquad (2\text{-}129)$$

2.8.5 Optimal waste dumping control of the discretized tapered stream model. The equations comprising the subproblems to be solved for optimal dumping control of the discretized dynamic tapered stream model may be derived by applying the techniques of Section 2.8.3 to the equations of the decomposed spatially discretized stream model represented by equations (2-61), (2-62) and (2-68) through (2-71). The same equations result from setting the longitudinal dispersion coefficient of the dumping control equations for the tidal river to zero. The resulting equations are listed in Table 2-3.

2.8.6 Optimal flow augmentation control of the discretized tidal river model.

2.8.6.1 Addition of flow augmentation control terms. Flow augmentation control is effective when the mean fresh water flow of the river is lower than normal. Its principal objective is the introduction of flows of water of lower BOD and higher DO concentrations than the river water to reduce BOD concentration and increase DO concentration in the river. With this means of control, the volume flow rate may be augmented at each of the N-1 internal points along the longitudinal axis. Due to physical limitations, volume flow rates of natural rivers and streams increase monotonically in the downstream direction. This also applies to the augmenting volume flow rate. Accordingly, flow augmentation at point k of the longitudinal axis may be represented as

$Q_k + (Q_c)_k$ where

$$(Q_c)_k = \sum_{m=2}^{k} (Q_a)_m \tag{2-130}$$

where: $(Q_c) = 0$ (2-131)

$(Q_c)_k$ is the cumulative augmenting volume flow rate at point k on the longitudinal axis under the assumption that no flow is added at the upstream end. $(Q_a)_m$ is the augmenting volume flow rate at spatial point m. Application of flow augmentation to the discretized and decomposed dynamic tidal river model represented by equations (2-70) and (2-71) results in equations of the same form as (2-85) and (2-122) with

$$B_k = E_k + F_k + \frac{Q_k - Q_{k-1} + (Q_a)_k}{A_k h_k} + K_r \tag{2-132}$$

$$E_k = \frac{D}{h^2_k}\left(\frac{A_{k-1}}{A_k} + \frac{h_k}{h_{k+1}} - 1\right) + \frac{Q_k + \sum\limits_{m=2}^{k} (Q_a)_m}{A_k h_k} \tag{2-133}$$

where it has been assumed that the BOD concentration in the augmenting flow is negligible and that its DO concentration is close to that of the river at the spatial point at which it enters.

2.8.6.2 Performance index for optimal flow augmentation control. To attain a specified level of DO concentration, C_{sp} , with minimum expenditure of control energy, the appropriate spatially discretized performance index is the following.

$$J = \sum_{k=1}^{N+1} \frac{J_k}{h_k} \tag{2-73}$$

$$J_k = h_k \int_{t_o}^{t_f} \left[W_1 (C_{sp} - C_k)^2 + W_3 \; (Q_a)_k^2 \right] dt \tag{2-134}$$

As with aeration control, if it is less important that the system be corrected for excess DO concentration, equation (2-134) could be assigned as the performance index for $C_k < C_{sp}$ and a new performance index could be defined for $C_k \geq C_{sp}$:

$$J_k \Big|_{C_k \geq C_{sp}} = h_k \int_{t_o}^{t_f} \left[W_5 (C_{sp} - C_k)^2 + W_3 (Q_a)_k^2 \right] dt \tag{2-135}$$

2.8.6.3 Spatially and temporally discretized model of tidal river with optimal flow augmentation control. Assuming that the mean advective flow of the river, Q_k , and the augmenting flow, $(Q_a)_k$, at spatial point k are time invariant leads via a development paralleling that for aeration control, Section 2.8.2, to the following set of spatially and temporally discretized equations.

The state equations are (2-85) and (2-122); $S_{k,i}$ and $R_{k,i}$ are defined by equations (2-87) and (2-88); B_k and G_k are defined by equations (2-132) and (2-54); E_k is defined by equation (2-133); F_k is defined by equation (2-52) and K_s is defined by equation (2-55).

The costate equations are presented as (2-89) and (2-90) with the remaining coordination equations (2-91) and (2-92).

The spatially and temporally discretized Hamiltonian for flow augmentation control may be expressed as follows.

$$H = \sum_{k=1}^{N+1} \sum_{i=1}^{I_m} h_t h_k H_{k,i} \qquad (2\text{-}94)$$

$$\begin{aligned} H_{k,i} = {} & W_1 (C_{sp} - \bar{C}_{k,i})^2 + W_3 (Q_a)_k^2 \\ & + (\overline{CL})_{k,i} (-B_k \bar{L}_{k,i} + \bar{S}_{k,i} + L_a) \\ & + (\overline{CC})_{k,i} (-G_k \bar{C}_{k,i} + \bar{R}_{k,i} + K_s) \qquad (2\text{-}136) \\ & + \bar{p}_{k,i} (F_k \bar{L}_{k+1,i} + E_k \bar{L}_{k-1,i} - \bar{S}_{k,i}) \\ & + \bar{q}_{k,i} (F_k \bar{C}_{k+1,i} + E_k \bar{C}_{k-1,i} - K_d \bar{L}_{k,i} - \bar{R}_{k,i}) \end{aligned}$$

Using a gradient approach to optimization,

$$(Q_a)_k^{(r+1)} = (Q_a)_k^{(r)} - \epsilon_Q \,(GRQ)_k^{(r)} \qquad (2\text{-}137)$$

$$(GRQ)_k = \frac{\sum_{i=1}^{I_m-1} (GRQ)_{k,i}}{I_m-1} \qquad (2\text{-}138)$$

$$(GRQ)_{k,i} = \frac{\partial H}{\partial (Q_a)_k} = 2W_3 \,(Q_a)_k - 2\,\frac{(\overline{CL})_{k,i}\,\bar{L}_{k,i} + (\overline{CC})_{k,i}\,\bar{C}_{k,i}}{A_k h_k} \qquad (2\text{-}139)$$

The spatially and temporally discretized equations for flow augmentation control may be organized into state, costate, control and coordinating subproblems to be solved. A hierarchy of these subproblems may be assembled as shown in Figure 2-2. The subproblem hierarchy for flow augmentation contains more control signal paths than depicted by Figure 2-1. This is to be expected because the flow augmentation control terms appear in both state equations, both costate equations and two of the coordination equations while the aeration and dumping control terms each appear only in one of the state equations.

The boundary, initial and final conditions are the same as those for the tidal river model under optimal

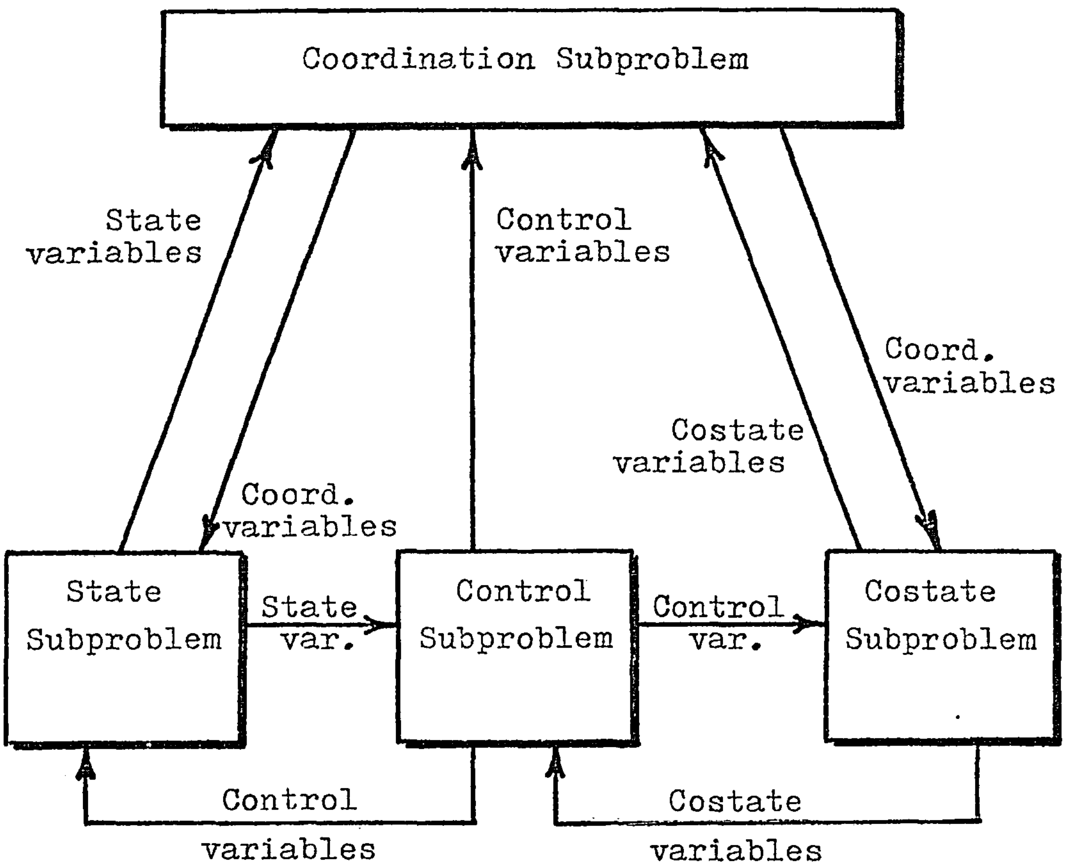


Figure 2-2: Subproblem hierarchy for concentrations model of tidal river reach with flow augmentation control

aeration control, (Table 2-2).

The initial distributions of BOD and DO concentrations are generated from the equations derived for aeration control (2-104) through (2-107) with B_k defined in equation (2-132) and E_k defined in equation (2-133).

For the flow augmentation control term, the upstream boundary condition is:

$$(Q_a)_1 = 0 \qquad (2\text{-}140)$$

2.8.7 Optimal flow augmentation control of the discretized tapered stream model. The spatially and temporally discretized equations for optimal flow augmentation control of the dynamic stream model may be derived by applying the techniques of Section 2.8.5 to the spatially discretized model, equations (2-61), (2-62) and (2-68) through (2-71). The same equations would result from setting the longitudinal dispersion coefficient to zero in the corresponding tidal river model equations.

The spatially and temporally discretized state equations for the tapered stream model with flow augmentation control are the same as equations (2-85) and (2-122) except that:

$$B_k = E_k + \frac{Q_k - Q_{k-1} + (Q_a)_k}{A_k h_k} + K_r \qquad (2\text{-}141)$$

$$E_k = \frac{Q_k + \sum_{m=2}^{k} (Q_a)_m}{A_k h_k} \qquad (2\text{-}142)$$

and $S_{k,i}$ and $R_{k,i}$ are defined by equations (2-113) and (2-114).

The costate equations for the stream model are the same as equations (2-89) and (2-90) for the tidal river model except B_k is defined by equation (2-145). The remaining coordination equations are presented as (2-91) and (2-92).

The equations for flow augmentation control of the tapered stream are the same as those for the tapered tidal river model. The subproblem hierarchy for flow augmentation control of the tapered stream model is the same as the one depicted in Figure 2-2 for flow augmentation control of the tidal river model.

The boundary, initial and final conditions for the tidal river model with flow augmentation control apply to the stream model with flow augmentation except that the equations for generating the initial distributions of BOD and DO concentrations are presented by equations (2-114) through (2-117), where B_k and E_k are defined in equations (2-141) and (2-142), respectively, and G_k is defined by equation (2-54).

An example of the application of the spatially and temporally discretized stream model with flow augmentation control appears in Chapter 6.

2.9 Aggregation of Single Reach Models Into Regional Multireach Models

All of the water quality models developed up to this point in this dissertation have represented concentration balances in a single reach of an estuary, river or stream. Physical or economic facters often require simultaneous representation of the concentration balances of more than one reach. For example, it may be necessary to model an entire region or river basin or a long portion of a river or stream within which tributaries enter the river or significant changes occur in one or more of the model's coefficients.

In general, multiple reach models may be assigned to three classes depending upon the physical relationships between their constituent reaches.

1.) Models of serially connected or contiguous reaches in which each reach interfaces with other reach(es) at one or both ends.

2.) Models of disjoint or separate reaches in which the component reaches are interrelated by some means other than direct contiguity, e.g., reaches on the same stream separated by intervening reaches.

3.) Hybrid multireach models comprised of both serially connected and disjoint reaches, e.g., reaches on tributaries in a single river basin.

Since the first class of multireach models occurs most frequently in the literature and is most sensitive to interface conditions, subsequent development in this dissertation will emphasize serially connected multiple reach models.

Aggregation of existing single reach models into a corresponding multi-reach model consists of three principal steps.

1.) Assignment of an additional subscript to each variable in the equations of each single reach model to identify it with respect to a particular reach.

2.) Formulation of interface equations to represent the physical and other interrelationships between the constituent reaches.

3.) Construction of the subproblem hierarchy for the multi-reach model.

This procedure represents aggregation as defined by Kulikowski[239].

2.9.1 <u>Regional tidal river model with optimal aeration control</u>. If it is assumed that the regional model consists of j_m contiguous reaches, the state equations for the concentrations balances at the kth spatial point of the jth reach may be derived from the corresponding equations of the single reach model, equations (2-85) through (2-88), (2-50) through (2-52), (2-54) and (2-55). The resulting state equations are:

$$L_{j,k,i+1} = \frac{(2-h_t B_{j,k})L_{j,k,i} + 2h_t S_{j,k,i} + 2h_t (L_a)_j}{2 + h_t B_{j,k}} \tag{2-143}$$

$$C_{j,k,i+1} = \Big[(2-h_t G_{j,k}) C_{j,k,i} + 2h_t R_{j,k,i} + 2h_t (K_s)_j + (U_C)_{j,k,i}\Big] / (2 + h_t G_{j,k}) \tag{2-144}$$

for $j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$; $i=1,2,\ldots,I_m-1$

where:

$$B_{j,k} = E_{j,k} + F_{j,k} + \frac{Q_{j,k} - Q_{j,k-1}}{A_{j,k}\, h_{j,k}} + (K_r)_j \tag{2-145}$$

$$E_{j,k} = \frac{D_j}{h_{j,k}^{2}} \left(\frac{A_{j,k-1}}{A_{j,k}} + \frac{h_{j,k}}{h_{j,k+1}} + 1 \right) + \frac{Q_{j,k}}{A_{j,k}\, h_{j,k}} \tag{2-146}$$

$$F_{j,k} = \frac{D_j}{h^2_{j,k+1}} \tag{2-147}$$

$$G_{j,k} = B_{j,k} - (K_r)_j + (K_a)_j \tag{2-148}$$

$$(K_s)_j = (K_a)_j\, (C_s)_j + \bar{P}_j - \bar{R}_j - \bar{B}_j \tag{2-149}$$

$$h_{j,k} = \frac{Q_{j,k} + Q_{j,k-1}}{A_{j,k} + A_{j,k-1}} \tag{2-150}$$

with the coordination equations:

$$S_{j,k,i} = F_{j,k}\, L_{j,k+1,i} + E_{j,k}\, L_{j,k-1,i} \tag{2-151}$$

$$R_{j,k,i} = F_{j,k}\, C_{j,k+1,i} + E_{j,k}\, C_{j,k-1,i} - (K_d)_j\, L_{j,k,i} \tag{2-152}$$

The upstream end boundary conditions for the concentrations are:

$$L_{1,1,i} = L_{1,0,i} = L_o \tag{2-153}$$

$$C_{1,1,i} = C_{1,0,i} = C_o \tag{2-154}$$

for $i = 1,2,\ldots,I_m$.

From equations (2-151) and (2-152) the upstream boundary conditions for two of the coordinating variables are:

$$S_{1,1,i} = F_{1,1}\ L_{1,2,i} + E_{1,1}\ L_o \tag{2-155}$$

$$R_{1,1,i} = F_{1,1}\ C_{1,2,i} + E_{1,1}\ C_o - (K_d)_1\ L_o \tag{2-156}$$

for $i=1,2,\ldots,I_m$.

From equations (2-104) and (2-105) the initial concentration distributions are given by:

$$L_{j,k+1,1} = \frac{B_{j,k}}{F_{j,k}}\ L_{j,k,1}\ \frac{E_{j,k}}{F_{j,k}}\ L_{j,k-1,1} - \frac{(L_a)_j}{F_{j,k}} \tag{2-157}$$

$$C_{j,k+1,1} = \frac{G_{j,k}}{F_{j,k}}\ C_{j,k,1} - \frac{E_{j,k}}{F_{j,k}}\ C_{j,k-1,1}\ \frac{(K_s)_j}{F_{j,k}} \tag{2-158}$$

for $j=1,2,\ldots,j_m$; $k=1,2,\ldots,N$.

Inspection of the equations of the regional (multi-reach) model of the tidal river reveals an important advantage of multi-reach modeling over single reach modeling of a given stretch of the river. The subscripts on the coefficients of the equations of the multi-reach model, such as D_j, provide for inter-reach, i.e. spatial, variation in their magnitudes. The boundaries between the constituent reaches of the regional model may be placed where significant changes in one or more coefficients occur. In this way, the multi-reach model can represent spatial changes of the coefficients without having them occur within any one reach.

Location of the boundaries between reaches also may be based upon placing them where major inputs to the river occur. General interface conditions may be defined to reflect the addition of a BOD concentration, $(L_{ad})_j$, and a DO concentration, $(C_{ad})_j$, associated with a volume flow rate, $(Q_{ad})_j$, at the upstream end of the jth reach of a regional model consisting of j_m reaches.

If the subscript, j, denoting the reach number, increases in the downstream direction and the upstream end point of every reach, except the first, coincides with the downstream end point of the reach immediately upstream, the general interface conditions for reaches in the model may be represented as follows:

$$Q_{j,1} = Q_{j-1,N+1} + (Q_{ad})_j \tag{2-159}$$

$$L_{j,1,i} = \frac{Q_{j-1,N+1} \, L_{j-1,N+1,i} + (Q_{ad})_j (L_{ad})_j}{Q_{j,1}} \tag{2-160}$$

$$C_{j,1,i} = \frac{Q_{j-1,N+1}\ C_{j-1,N+1,i} + (Q_{ad})_j (C_{ad})_j}{Q_{j,1}} \qquad (2\text{-}161)$$

$j=2,3,\ldots,j_m$; $i=1,2,\ldots,I_m$.

Also, from equations (2-155) and (2-156) the interface conditions for two of the coordinating variables are:

$$S_{j,1,i} = F_{j,1}\ L_{j,2,i} + E_{j,1}\ L_{j-1,N,i} \qquad (2\text{-}162)$$

$$R_{j,1,i} = F_{j,1}\ C_{j,2,i} + E_{j,1}\ C_{j-1,N,i} - (K_d)_j\ L_{j,1,i} \qquad (2\text{-}163)$$

where $j=2,3,\ldots,j_m$; $i=2,3,\ldots,I_m$.

From equations (2-89) and (2-90), the costate equations of the jth reach model are:

$$(CC)_{j,k,i} = \Big\{ (2-h_t\ G_{j,k})\ (CC)_{j,k,i+1} + 2h_t F_{j,k-1}\ q_{j,k-1,i} + 2h_t\ E_{j,k+1}\ q_{j,k+1,i} - 2h_t (W_1)_j \left[(C_{sp})_j - C_{j,k,i} \right]^2 \Big\} / (2 + h_t\ G_{j,k}) \qquad (2\text{-}164)$$

$$(CL)_{j,k,i} = \Big[(2-h_t\ B_{j,k})(CL)_{j,k,i+1} + 2h_t\ F_{j,k-1}\ p_{j,k-1,i} + 2h_t\ E_{j,k+1}\ p_{j,k+1,i} - 2h_t\ (K_d)_j\ q_{j,k,i} \Big] / (2 + h_t\ B_{j,k}) \qquad (2\text{-}165)$$

for $j=1,2,\ldots;j_m$; $k=1,2,\ldots,N$; $i=1,2,\ldots;I_m-1$.

The downstream boundary conditions are:

$$(CC)_{j_m,N+1,i} = 0 \quad \text{for all } i \qquad (2\text{-}166)$$

$$(CL)_{j_m,N+1,i} = 0 \quad \text{for all } i \qquad (2\text{-}167)$$

The final conditions on the costates are:

$$(CC)_{j,k,I_m} = 0 \qquad (2\text{-}168)$$

$$(CL)_{j,k,I_m} = 0 \qquad (2\text{-}169)$$

for $j=1,2,\ldots,j_m$; $k=1,2,\ldots,N+1$.

The remaining coordination equations for the jth reach from equations (2-91) and (2-92), are:

$$p_{j,k,i} = (CL)_{j,k,i} \qquad (2\text{-}170)$$

$$q_{j,k,i} = (CC)_{j,k,i} \qquad (2\text{-}171)$$

for $j=1,2,\ldots,j_m$; $k=1,2,\ldots,N$; $i=1,2,3,\ldots,I_m-1$.

From equations (2-166) through (2-171) the downstream boundary conditions are:

$$p_{j_m,N+1,i} = 0 \quad \text{for all } i \qquad (2\text{-}172)$$

$$q_{j_m,N+1,i} = 0 \quad \text{for all } i \qquad (2\text{-}173)$$

and the final conditions are:

$$p_{j,k,I_m} = 0 \quad \text{for all j and k} \tag{2-174}$$

$$q_{j,k,I_m} = 0 \quad \text{for all j and k} \tag{2-175}$$

From equation (2-99) the optimal aeration control equation for the jth reach is:

$$(U_C)^{(r+1)}_{j,k,i} = (U_C)^{(r)}_{j,k,i} - 2(W_2)_j \; (\epsilon_C)_j \; (\bar{U}_C)^{(r)}_{j,k,i}$$
$$-(\epsilon_C)_j \; (\overline{CC})^{(r)}_{j,k,i} \tag{2-176}$$

for $j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$; $i=2,3,\ldots,I_m$; with the initial condition from equation (2-111),

$$(U_C)_{j,k,1} = 0 \quad \text{for all j and k} \tag{2-177}$$

and upstream boundary condition from equation (2-112),

$$(U_C)_{1,1,i} = 0 \quad \text{for all i} \tag{2-178}$$

Since the downstream boundary conditions and the final conditions are given for the costate equations, they generally are solved in the reverse direction in space (from downstream to upstream) and time (from final time to initial time).

Accordingly, the costate interface conditions may be expressed in the following form.

$$(CC)_{j,N+1,i} = (CC)_{j+1,1,i} \tag{2-179}$$

$$(CL)_{j,N+1,i} = (CL)_{j+1,1,i} \tag{2-180}$$

and, from equations (2-170) and (2-171),

$$q_{j,N+1,i} = q_{j+1,1,i} \tag{2-181}$$

$$p_{j,N+1,i} = p_{j+1,1,i} \tag{2-182}$$

$j=1,2,\ldots,j_m-1$; $i=1,2,\ldots,I_{m-1}$

With upstream boundary and initial time conditions given, the appropriate interface conditions for the aeration control equations are:

$$(U_C)_{j,1,i} = (U_C)_{j-1,N+1,i} \tag{2-183}$$

$j=2,3,\ldots,j_m$; $i=1,2,\ldots,I_m$.

All of the interface equations may be collected into a regional (multi-reach) coordination subproblem. The remaining equations of this section may be assigned to state, costate, control and coordination subproblems for the jth reach, $j=1,2,\ldots,j_m$. These subproblems can then be assembled into a three-level hierarchy as shown in Figure 2-3. Comparison of this figure with Figure 2-1 reveals that the two-level hierarchy of Figure 1 appears once for each constituent reach in the multi-reach model.

2.9.2 Regional tapered stream model optimal aeration control. The state, costate, control and reach coordination equations can be obtained from the corresponding tidal river equations with the longitudinal dispersion coefficient, $D_j = 0$. The resulting state equations for the kth spatial point in the jth reach are the same as those for the spatially and temporally discretized tidal river model equations (2-143) and (2-144) with :

$$B_{j,k} = E_{j,k} + \frac{Q_{j,k} - Q_{j,k-1}}{A_{j,k}\, h_{j,k}} + (K_r)_j \qquad (2\text{-}184)$$

$$E_{j,k} = \frac{Q_{j,k}}{A_{j,k}\, h_{j,k}} \qquad (2\text{-}185)$$

$G_{j,k}$ is defined by equation (2-155)

$$S_{j,k,i} = E_{j,k}\, L_{j,k-1,i} \qquad (2\text{-}186)$$

$$R_{j,k,i} = E_{j,k}\, C_{j,k-1,i} - (K_d)_j\, L_{j,k,i} \qquad (2\text{-}187)$$

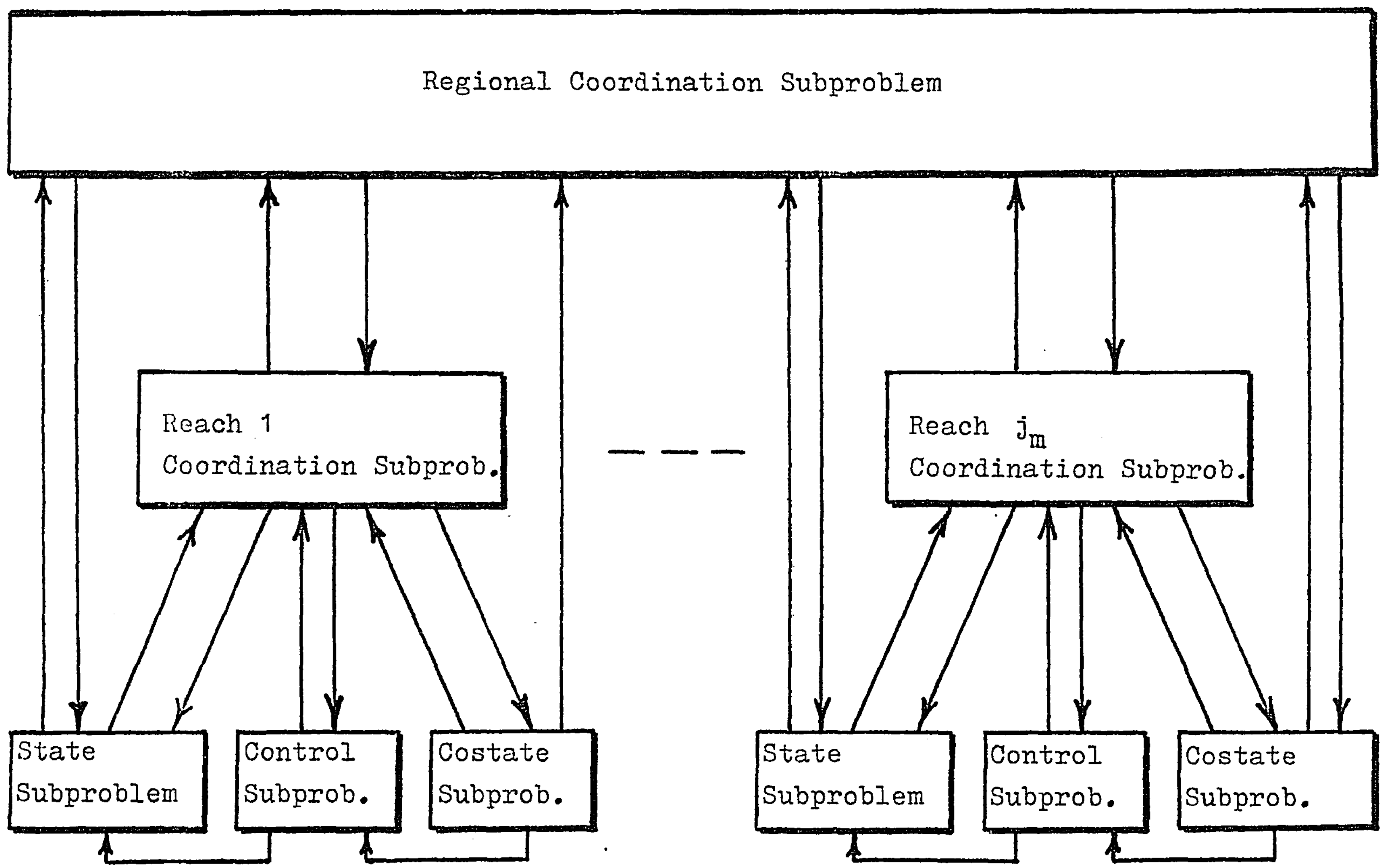


Figure 2-3: Regional multireach subproblem hierarchy

From equations (2-186) and (2-187) the corresponding upstream and boundary conditions for two of the coordinating variables are:

$$S_{1,1,i} = E_{1,1} L_o \tag{2-188}$$

$$R_{1,1,i} = E_{1,1} C_o - (K_d) L_o \tag{2-189}$$

for $i=1,2,\ldots,I_m$

The equations for generating the initial concentrations distributions are derived from equations (2-157) and (2-158).

$$L_{j,k+1,1} = \frac{E_{j,k}}{B_{j,k}} L_{j,k,1} + \frac{(L_a)_j}{B_{j,k}} \tag{2-190}$$

$$C_{j,k+1,1} = \frac{E_{j,k}}{G_{j,k}} C_{j,k,1} + \frac{(K_s)_j}{G_{j,k}} \tag{2-191}$$

for $j=1,2,\ldots,j_m$; $k=1,2,\ldots,N$.

The coordination variables interface equations derived from equations (2-162) and (2-163) of the tidal river model are:

$$S_{j,1,i} = E_{j,1} L_{j-1,N,i} \tag{2-192}$$

$$R_{j,1,i} = E_{j,1} C_{j-1,N,i} - (K_d)_j L_{j,1,i} \qquad (2\text{-}193)$$

for $j=2,3,\ldots,j_m$; $i=2,3,\ldots,I_m$.
The remaining equations for the regional stream model are the same as those of the regional tidal river model, (Tables 2-4 and 2-5).

The equations for the regional stream model with aeration control may be assigned to state, costate, control, reach coordination, and regional coordination subproblems. The resulting subproblem hierarchy is depicted by Figure 2-3.

2.9.3 <u>Regional tidal river model with optimal dumping control</u>. The state equations of the regional (multi-reach) discretized and decomposed tidal river model with dumping control are the same as the state equations for the coresponding model with aeration control except that the BOD control term, $(U_L)_{j,k,i}$ is applied to the BOD concentration rate balance. The resulting state equations are:

$$L_{j,k,i+1} = \Big[(2-h_t B_{j,k}) L_{j,k,i} + 2h_t S_{j,k,i}$$

$$+ 2 h_t (L_a)_j + (U_L)_{j,k,i}\Big] /(2 + B_{j,k}) \qquad (2\text{-}194)$$

$$C_{j,k,i+1} = \Big[(2-h_t\ G_{j,k})\ C_{j,k,i} - 2h_t\ R_{j,k,i} + 2h_t\ (K_s)_j\Big] / (2 + G_{j,k}) \qquad (2\text{-}195)$$

for $j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$; $i=1,2,\ldots,I_m-1$. $B_{j,k}$, $E_{j,k}$, $F_{j,k}$, $G_{j,k}$, $(K_s)_j$, $h_{j,k}$, $S_{j,k,i}$ and $R_{j,k,i}$ are defined in equations (2-145) through (2-152) and are the same for both aeration and dumping control.

The remaining equations for the regional tidal river model with dumping control are the same as for the corresponding model with aeration control except the control equations which follow from equation (2-127),

$$(U_L)^{(r+1)}_{j,k,i} = (U_L)^{(r)}_{j,k,i} - 2(W_4)_j\ (\epsilon_L)_j\ (\bar{U}_L)^{(r)}_{j,k,i} - (\epsilon_L)_j\ (\overline{CL})^{(r)}_{j,k,i} \qquad (2\text{-}196)$$

for $j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$; $i=2,3,\ldots,I_m$. The initial dumping control condition from equation (2-128) is:

$$(U_L)_{j,k,1} = 0 \quad \text{for all } j,k \qquad (2\text{-}197)$$

The upstream boundary condition, from equation (2-129), is:

$$(U_L)_{1,1,i} = 0 \quad \text{for all } i \tag{2-198}$$

The dumping control interface equation is:

$$(U_L)_{j,1,i} = (U_L)_{j-1,N+1,i} \tag{2-199}$$

for $j=2,3,\ldots,j_m$; $i=1,2,\ldots,I_m$.

The equations for the regional tidal river model with dumping control may be assembled into the subproblem hierarchy depicted by Figure 2-3.

The equations representing the water quality models derived in this chapter are tabulated on the following pages.

In this chapter dynamic continuous distributed parameter water quality models for six types of waterways were developed from a general three-dimensional water quality model. Presently available methods for evaluating the major variables and parameters of these models also were reviewed. The tapered tidal river and tapered stream continuous distributed parameter models each were reduced to a series of lumped models by spatial discretization. Three modes of optimal control were applied in sequence by a combination of multilevel hierarchical analysis and Pontryagin's minimum principle to the two discretized models to produce six combinations of model and multilevel optimal control for a waterway reach. Each resulting system consists of a hierarchy of subproblems to be solved. Finally, each of the six single reach models with optimal control was expanded into a regional multireach hierarchy of subproblems by aggregation.

In the next chapter a general two-dimensional discrete distributed parameter model will be derived directly from conservation of mass considerations, completely obviating the use of the continuous distributed parameter models developed in Sections 2.3 and 2.4 of the present chapter and requirements for discretization that they involve. Development of water quality models for specific types of waterways, application of multilevel optimal control to four of them and expansion of single reach models with optimal control into regional models all will parallel the treatment in the present chapter. A distinctive feature of the next chapter will be the application of Pontryagin's minimum principle for discrete systems in contrast with the application of Pontryagin's minimum principle for lumped systems optimal control in the present chapter.

Later chapters will treat consistency and convergence for the discretized models of the present chapter and boundary conditions, computational efficiency, sensitivity and stability for the subproblem hierarchies resulting from application of multilevel control to the models presented in this dissertation.

	Continuous	Spatially Discretized	Discretized and Decomposed
3-dimensional estuary	(2-18),(2-19)		
Non-stratified estuary	(2-20),(2-21)		
Stratified estuary	(2-22),(2-23)		
Tapered tidal river	(2-24),(2-25) (2-35),(2-36)	(2-49)-(2-59)	(2-64)-(2-67)
Tapered stream	(2-26),(2-27)	(2-60)-(2-63)	(2-68)-(2-71)
Steady state	(2-28),(2-29)		

Table 2-1. Equations of Water Quality Models Without Control

	CONTROL MODES		
	Aeration	Waste Dumping	Flow Augmentation
Coefficient equations	(2-45) (2-50)-(2-52) (2-54),(2-55)	Same as aeration	(2-45),(2-53) (2-130)- (2-133) (2-54),(2-55)
Decomposed state equations	(2-85),(2-86) (2-102)-(2-107)	(2-121), (2-122), (2-102)- (2-107)	(2-85),(2-122) (2-102)- (2-107)
Costate equations	(2-89),(2-90) (2-100),(2-101)	Same as aeration	Same as aeration
Control equations	(2-93),(2-98) (2-99), (2-108), (2-109)	(2-123), (2-127), (2-128), (2-129)	(2-130), (2-131), (2-137)- (2-140)
Coordination equations	(2-87),(2-88) (2-91),(2-92)	Same as aeration	Same as aeration
Performance indexes	(2-73)-(2-75)	(2-73), (2-119), (2-120)	(2-73), (2-134), (2-135)
Subproblem hierarchies	Figure 2-1	Fig. 2-1	Fig. 2-2

Table 2-2. Equations and Subproblem Hierarchies of Tidal River Reach Model With Multilevel Optimal Control

	CONTROL MODES		
	Aeration	Waste Dumping	Flow Augmentation
Coefficient equations	(2-45),(2-54) (2-55),(2-61) (2-62)	Same as aeration	(2-45),(2-54) (2-55),(2-141) (2-142)
Decomposed state equations	(2-85),(2-86) (2-102),(2-103) (2-106),(2-107) (2-114),(2-117)	(2-121), (2-122), (2-102), (2-103), (2-106), (2-107), (2-114)-(2-117)	(2-85),(2-122) (2-102), (2-103), (2-106), (2-107), (2-114)-(2-117)
Costate equations	(2-89),(2-90) (2-100),(2-101)	Same as aeration	Same as aeration
Control equations	(2-93),(2-98) (2-99),(2-108) (2-109)	(2-123), (2-127), (2-128), (2-129)	(2-130), (2-131), (2-137)-(2-140)
Coordination equations	(2-91),(2-92) (2-110),(2-111)	Same as aeration	Same as aeration
Subproblem hierarchies	Figure 2-1	Fig. 2-1	Fig. 2-2

Table 2-3. Equations and Subproblem Hierarchies of Tapered Stream Reach Model With Multilevel Optimal Control

	CONTROL MODES	
	Aeration	Waste Dumping
Coefficient equations	(2-145)-(2-150)	Same as aeration
Decomposed state equations	(2-143),(2-144),(2-153) (2-154),(2-157),(2-158)	(2-194),(2-195) (2-153),(2-154) (2-157),(2-158)
Costate equations	(2-164)-(2-169)	Same as aeration
Control equations	(2-176)-(2-178)	(2-196)-(2-199)
Coordination equations	(2-151),(2-152),(2-155) (2-156),(2-170)-(2-175)	Same as aeration
Interface	(2-159)-(2-163) (2-179)-(2-183)	Same as aeration
Subproblem hierarchies	Figure 2-3	Figure 2-3

Table 2-4. Equations and Subproblem Hierarchies of Regional Tidal River Model With Multilevel Optimal Control

	CONTROL MODES	
	Aeration	Waste Dumping
Coefficient equations	(2-184),(2-185), (2-148)-(2-150)	Same as aeration
Decomposed state equations	(2-143),(2-144),(2-153) (2-154),(2-190),(2-191)	(2-194),(2-195) (2-153),(2-154) (2-157),(2-158)
Costate equations	(2-164)-(2-169)	Same as aeration
Control equations	(2-176)-(2-178)	(2-196)-(2-199)
Coordination equations	(2-186)-(2-189) (2-170)-(2-175)	Same as aeration
Interface equations	(2-159)-(2-161),(2-192) (2-193),(2-179)-(2-183)	Same as aeration
Subproblem hierarchies	Figure 2-3	Figure 2-3

Table 2-5. Equations and Subproblem Hierarchies of Regional Tapered Stream Model With Multilevel Optimal Control

CHAPTER 3

TWO-STEP DISCRETE DYNAMIC DISTRIBUTED PARAMETER WATER QUALITY MODELS AND THEIR OPTIMAL CONTROL

In the previous chapter continuous dynamic distributed parameter water quality models for six types of waterways were developed from a general linear three-dimensional model. These continuous models were then approximated by discrete models which could be more readily solved numerically.

In the present chapter, no continuous distributed parameter models are utilized. Instead, a two-step discrete dynamic distributed parameter water quality model of a general two-dimensional waterway is derived by applying conservation of mass to a volume element in a reach of the waterway. The discrete model itself is thus the fundamental water quality model and not an approximation of the fundamental model as was the case in the previous chapter.

The class of water quality models developed in the present chapter results from an extension to two spatial dimensions of methods presented by Bella and Dobbins[27]. Although each two-step discrete model requires twice as many equations as the comparable discretized continuous model, the fact that it is the fundamental model obviates any need to demonstrate consistency between solutions of the discrete model and the continuous model that it approximates.

For the models of both this chapter and the previous one the critical variables for water quality evaluation are the dissolved oxygen (DO) and the biochemical oxygen demand (BOD) concentrations. The two-step discrete dynamic distributed parameter models of the current chapter utilized two additional concentrations: the convected dissolved oxygen concentration and the convected biochemical oxygen demand concentration. These two additional variables result from representing each dynamic concentration rate balance in the waterway in two steps:

1.) convection,

2.) all remaining processes[106].

These four variables and their associated equations constitute the state variables and state equations, respectively, of the two-step discrete water quality models derived in this chapter.

The chapter begins with the application of the principle of conservation of mass to a volume element in a waterway to derive, without the use of any continuous models, a discrete model of the dynamic concentrations balances in one of its reaches. This model is the general representation of a class of waterway water quality models from which four are then derived:

1.) two-dimensional stratified estuary,
2.) two-dimensional stratified estuary with negligible vertical velocity component,
3.) tapered tidal river,
4.) tapered stream.

All of these models may be assigned to a larger class of linear water quality models described by the general three-dimensional model presented at the beginning of Chapter 2.

Discrete volume flow rate distributions are developed for use with the two-dimensional waterway models and also for the one-dimensional tidal river and tapered stream models. These distributions are developed from continuous velocity distributions approximating measured values presented by Okunseinde[340]. They incorporate tidal and, in the two-dimensional case, salinity intrusion effects. Velocity profiles at selected points along the longitudinal axis of the time-averaged component of velocity with salinity intrusion are presented in Figure 3-2.

Accurate representation of the dynamic concentrations balances in these waterways necessitates the use of a relatively large number of increments along the spatial and temporal axes. This requirement, in conjunction with the doubling of the number of state equations cited earlier, leads to the presence of a large number of equations in most water quality models of practical utility.

Multilevel hierarchical systems analysis combined with Pontryagin's minimum principle was shown effective for the application of optimal control to mathematical models represented by large sets of equations in the previous chapter. The distinctive feature in following the same general approach in the present chapter is the utilization of Pontryagin's minimum principle for discrete systems[59].

A sequence of three modes of multilevel optimal control is applied to each of the four waterway models developed in this chapter:

1.) aeration,
2.) waste dumping,
3.) bimodal combination of aeration and waste dumping.

Although selected combinations of waterway and optimal control mode are presented in the text of the chapter, the equations developed are sufficiently general to be utilized in modelling all twelve possible combinations.

Since analyses of entire river basins, watersheds and other regions often require multireach water quality models, three of the more general single reach models developed in this chapter are extended to regional multireach models. More specifically, the stratified estuary, the stratified estuary with negligible velocity and the tidal river models, all with bimodal control, are aggregated into regional models in the final portion of this chapter. The regional stream model with multilevel bimodal control may be readily constructed from the equations developed in the balance of the dissertation. Regional models for the application of either aeration or dumping control alone may be obtained by proper combination of the equations of this chapter.

The contributions by the author in this chapter are the following.

1.) Extension of the Bella-Dobbins[27] one-dimensional discrete distributed parameter water quality model to a more general two-dimensional model;
2.) derivation of four tapered (variable cross section) single reach waterway models from the general two-dimensional model;
3.) development of discrete volume flow rate distributions for use with the four types of waterway models developed in this chapter;

4.) combined application of multilevel hierarchical systems analysis and Pontryagin's discrete minimum principle to each of the four single reach waterway models to effect a sequence of three modes of optimal control:

   a.) aeration,

   b.) waste dumping,

   c.) bimodal combination of aeration and dumping;

5.) aggregation of single reach models with multilevel optimal bimodal control into regional multireach models with general interface conditions between their contiguous reaches.

3.1 Two-dimensional Stratified Estuary Finite Difference Models

In a stratified estuary vertical mixing occurs at a rate comparable with the tidal velocity[340]. Hence, vertical distribution of velocity and concentration of constiuents must be specifically represented while lateral distributions may be averaged. The usual two-dimensional model of this type of waterway is based upon a plan view with the x-axis extending along the axis of principal flow and the z-axis extending vertically[185].

Both spatial axes and the temporal axis are discretized for direct derivation of the finite-difference distributed parameter model without any associated continuous model[27]. More specifically, the length of the reach being studied is divided into equal increments of length h_x, the laterally averaged depth into uniform increments of length h_z and the temporal axis into increments of length h_t. This subdivides the stratified estuary reach into M_m layers vertically and N segments longitudinally with the layers identified by the subscript $m=1,2,\ldots,M_m$ and the segments identified by the subscript $k=1,2,\ldots,N$. A volume element of length h_x , width $w_{k,m}$ and height h_z centered about the point at (k,m) is defined as in Figure 3-1.

3.1.1 <u>Two-dimensional convection model</u>. Let h_t represent the temporal increment between time i and time i+1. Then the mass balance associated with convection in and out of a volume element may be expressed in the following way[27].

Mass at time i+1	=	Mass at time i	+	Mass convected in during temporal increment h_t

- Mass convected out during temporal increment h_t (3-1)

For the volume element shown in Figure 3-1:

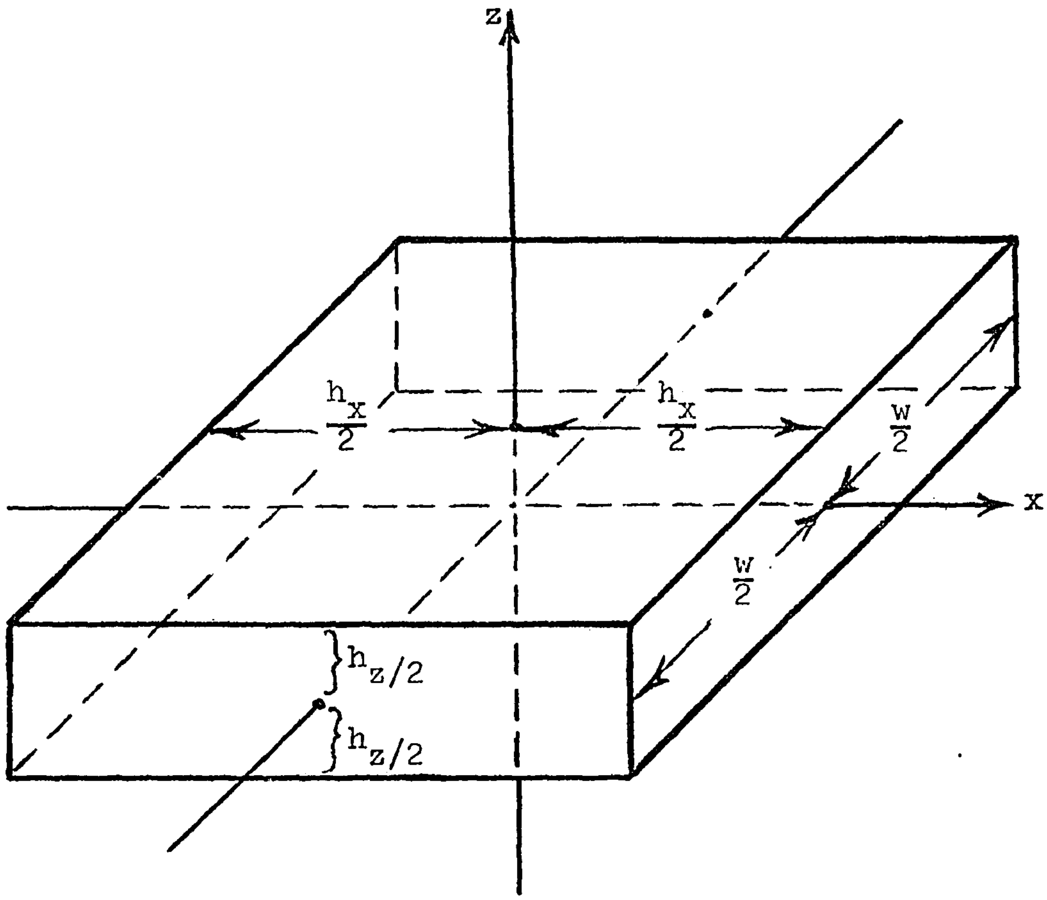


Figure 3-1: Segment k of layer m
(not to scale)

$$C_{k,m,i+1}A_{k,m}h_x = C_{k,m,i}A_{k,m}h_x$$
$$+ (Q_x)_{k-\frac{1}{2},m,i}C_{k-1,m,i}h_t - (Q_x)_{k+\frac{1}{2},m,i}C_{k,m,i}h_t$$
$$+ (V_z)_{k,m-\frac{1}{2},i}w_{k,m-\frac{1}{2}}C_{k,m-1,i}h_t h_x$$
$$- (V_z)_{k,m+\frac{1}{2},i}w_{k,m+\frac{1}{2}}C_{k,m,i}h_t h_x \qquad (3\text{-}2)$$

where:

$C_{k,m,i}$ = average concentration of dissolved constituent in segment k of layer m at time $i(h_t)$ after initial time.

$(Q_x)_{k,m,i}$ = average volume flow rate along horizontal (x) axis in segment k of layer m.

$(V_z)_{k,m,i}$ = average vertical velocity in segment k of layer m.

$w_{k,m}$ = average width of estuary in segment k of layer m (assumed time-invariant).

$A_{k,m}$ = average cross sectional area perpendicular to x-axis in segment k of layer $m=w_{k,m}h_z$.

With the definition

$$(V_zA_z)_{k,m,i} \equiv (V_z)_{k,m,i}w_{k,m}h_x \qquad (3\text{-}3)$$

and omission of the subscript from Q_x, equation (3-2) may be expressed in the following form for the BOD convection balance:

$$x_{1,k,m,i+1} = x_{5,k,m,i} = f_{1,k,m,i} \qquad (3\text{-}4)$$

where:

$$x_{5,k,m,i}\Big|_{\substack{Q_{k,m,i}\ \geq\ 0\\ (V_z)_{k,m,i}\ \geq\ 0}} = x_{2,k,m,i} + \frac{h_t}{h_x A_{k,m}} \Big[Q_{k-\frac{1}{2},m,i}x_{2,k-1,m,i} - Q_{k+\frac{1}{2},m,i}x_{2,k,m,i} + (V_zA_z)_{k,m-\frac{1}{2},i}x_{2,k,m-1,i} - (V_zA_z)_{k,m+\frac{1}{2},i}x_{2,k,m,i}\Big] \tag{3-5}$$

$$x_{5,k,m,i}\Big|_{\substack{Q_{k,m,i}\ <\ 0\\ (V_z)_{k,m,i}\ \geq\ 0}} = x_{2,k,m,i} + \frac{h_t}{h_x A_{k,m}} \Big[Q_{k+\frac{1}{2},m,i}x_{2,k+1,m,i} - Q_{k-\frac{1}{2},m,i}x_{2,k,m,i} + (V_zA_z)_{k,m-\frac{1}{2},i}x_{2,k,m-1,i} - (V_zA_z)_{k,m+\frac{1}{2},i}x_{2,k,m,i}\Big] \tag{3-6}$$

$$x_{5,k,m,i}\Big|_{\substack{Q_{k,m,i}\ <\ 0\\ (V_z)_{k,m,i}\ <\ 0}} = x_{2,k,m,i} + \frac{h_t}{h_x A_{k,m}} \Big[Q_{k+\frac{1}{2},m,i}x_{2,k+1,m,i} - Q_{k-\frac{1}{2},m,i}x_{2,k,m,i} + (V_zA_z)_{k,m+\frac{1}{2},i}x_{2,k,m+1,i} - (V_zA_z)_{k,m-\frac{1}{2},i}x_{2,k,m,i}\Big] \tag{3-7}$$

$$x_{5,k,m,i} \Bigg|_{\substack{Q_{k,m,i} \geq 0 \\ (V_z)_{k,m,i} < 0}} = x_{2,k,m,i}$$

$$+ \frac{h_t}{h_x A_{k,m}} \Big[Q_{k-\frac{1}{2},m,i} x_{2,k-1,m,i} - Q_{k+\frac{1}{2},m,i} x_{2,k,m,i}$$

$$+ (V_z A_z)_{k,m+\frac{1}{2},i} x_{2,k,m+1,i} - (V_z A_z)_{k,m-\frac{1}{2},i} x_{2,k,m,i} \Big]$$

(3-8)

$Q_{k,m,i}$ is positive downstream,

$(V_z)_{k,m,i}$ is positive upward,

$x_{1,k,m,i}$ is the convected BOD concentration in segment k of layer m at time i and, similarly, $x_{2,k,m,i}$ is the average BOD concentration. $x_{5,k,m,i}$ is a coordination variable.

The DO convection balance may be expressed:

$$x_{3,k,m,i+1} = x_{6,k,m,i} = f_{3,k,m,i} \qquad (3\text{-}9)$$

where $x_{6,k,m,i}$ is of the same form as $x_{5,k,m,i}$ except that $x_{2,k,m,i}$ is replaced by $x_{4,k,m,i}$. $x_{3,k,m,i}$ is the convected DO concentration, $x_{4,k,m,i}$ is the average DO concentration in segment k of layer m at time i and $x_{6,k,m,i}$ is a coordination variable.

3.1.2 Two-dimensional dispersion model. Following the same notation as for the mass balance of convection, the diffusion mass balance for the volume element of Figure 3-1 may be expressed as follows.

Mass at time i+1	=	Mass at time i	+	Net mass added due to dispersion during temporal increment, h_t

(3-10)

$$C_{k,m,i+1}A_{k,m}h_x = C_{k,m,i}A_{k,m}h_x$$

$$+ \frac{(D_xA)_{k+\frac{1}{2},m,i}h_t}{h_x}(C_{k+1,m,i} - C_{k,m,i})$$

$$+ \frac{(D_xA)_{k-\frac{1}{2},m,i}h_t}{h_x}(C_{k-1,m,i} - C_{k,m,i})$$

$$+ \frac{(D_zw)_{k,m+\frac{1}{2},i}h_xh_t}{h_z}(C_{k,m+1,i} - C_{k,m,i})$$

$$+ \frac{(D_zw)_{k,m-\frac{1}{2},i}h_xh_t}{h_z}(C_{k,m-1,i} - C_{k,m,i})$$

(3-11)

where:

$$(D_xA)_{k,m,i} = (D_x)_{k,m,i} \cdot A_{k,m} \qquad (3\text{-}12)$$

$$(D_zw)_{k,m,i} = (D_z)_{k,m,i} \cdot w_{k,m} \qquad (3\text{-}13)$$

$(D_x)_{k,m,i}$ = average coefficient of longitudinal dispersion in segment k of layer m at time i.

D_z = average coefficient of vertical diffusion.

$A_{k,m}$ = average cross sectional area perpendicular to longitudinal axis in segment k of layer m (assumed time-invariant).

$w_{k,m}$ = average width of estuary in segment k of layer m.

An alternate form for equation (3-13) is

$$
\begin{aligned}
C_{k,m,i+1} = C_{k,m,i} &+ \frac{h_t (D_x A)_{k+\frac{1}{2},m,i}}{A_{k,m} h_x^2} (C_{k+1,m,i} - C_{k,m,i}) \\
&+ \frac{h_t (D_x A)_{k-\frac{1}{2},m,i}}{A_{k,m} h_x^2} (C_{k-1,m,i} - C_{k,m,i}) \\
&+ \frac{h_t (D_z w)_{k,m+\frac{1}{2},i}}{A_{k,m} h_z} (C_{k,m+1,i} - C_{k,m,i}) \\
&+ \frac{h_t (D_z w)_{k,m+\frac{1}{2},i}}{A_{k,m} h_z} (C_{k,m-1,i} - C_{k,m,i})
\end{aligned}
\qquad (3\text{-}14)
$$

3.1.3 Two-dimensional first order decay reaction model. With the notation employed for the convection and dispersion mass balances for the volume element presented in Figure 3-1, the mass balance for a first order decay reaction may be expressed as follows.

Mass at time i+1	=	Mass at time i	+	Net mass removed due to first order reaction during time increment h_t

(3-15)

$$C_{k,m,i+1} A_{k,m} h_x = C_{k,m,i} A_{k,m} h_x - \frac{(K_r)_{k,m} h_t}{2} (C_{k,m,i} + C_{k,m,i+1}) A_{k,m} h_x \quad (3\text{-}16)$$

Dividing the volume terms out of the equation,

$$C_{k,m,i+1} = C_{k,m,i} - \frac{h_t (K_r)_{k,m}}{2} (C_{k,m,i} + C_{k,m,i+1}) \quad (3\text{-}17)$$

where:

$(K_r)_{k,m}$ = first order decay reaction coefficient for segment k of layer m.

3.1.4 General two-step two-dimensional model of convection and other processes. Each concentration's complete rate balance involves a combination of convection and the other processes described earlier in this chapter. Following the approach of Bella and Dobbins[27], and Dresnack and Dobbins[106], and extending it to two dimensions, each concentration rate balance is conducted in two steps:

1.) convection,

2.) all other processes.

Although this procedure doubles the number of equations involved compared with similar models, it eliminates false dispersive effects that can cause many models to converge to incorrect values.

The two-dimensional BOD concentration rate balance is accordingly represented by the following pair of equations.

Convection:

$$x_{1,k,m,i+1} = f_{1,k,m,i} = x_{5,k,m,i} \tag{3-4}$$

Remaining processes:

$$x_{2,k,m,i+1} = f_{2,k,m,i} = \Big\{ -B_{k,m,i}x_{1,k,m,i} + E_{k+\frac{1}{2},m,i}x_{1,k+1,m,i} + E_{k-\frac{1}{2},m,i}x_{1,k-1,m,i} + F_{k,m+\frac{1}{2},i}x_{1,k,m+1,i} + F_{k,m-\frac{1}{2},i}x_{1,k,m-1,i} + h_t\left[(L_a)_{k,m} + (U_L)_{k,m,i}\right]\Big\} \Big/ \left[1 + \frac{h_t(K_r)_{k,m}}{2}\right] \tag{3-18}$$

where: $k = 2,3,\ldots,N+1$; $m = 2,3,\ldots,M_m+1$

for given upstream and other boundary conditions and $i = 1,2,\ldots,I_m-1$.

$$B_{k,m,i} = \frac{h_t(K_r)_{k,m}}{2} + E_{k+\frac{1}{2}.m.i} + E_{k-\frac{1}{2},m,i}$$

$$+ F_{k,m+\frac{1}{2},i} + F_{k,m-\frac{1}{2},i} - 1 \qquad (3\text{-}19)$$

$$E_{k+\frac{1}{2},m,i} = \frac{h_t}{A_{k,m}h_x^2} (D_x)_{k+\frac{1}{2},m,i}A_{k+\frac{1}{2},m} \qquad (3\text{-}20a)$$

$$E_{k-\frac{1}{2},m,i} = \frac{h_t}{A_{k,m}h_x^2} (D_x)_{k-\frac{1}{2},m,i}A_{k-\frac{1}{2},m} \qquad (3\text{-}20b)$$

$$F_{k,m+\frac{1}{2},i} = \frac{h_t}{A_{k,m}h_z} (D_z)_{k,m+\frac{1}{2},i}w_{k,m+\frac{1}{2}} \qquad (3\text{-}21a)$$

$$F_{k,m-\frac{1}{2},i} = \frac{h_t}{A_{k,m}h_z} (D_z)_{k,m-\frac{1}{2},i}w_{k,m-\frac{1}{2}} \qquad (3\text{-}21b)$$

$(K_r)_{k,m}$ = BOD removal coefficient in segment k of layer m.

$$A_{k,m} = w_{k,m}h_z \qquad (3\text{-}22)$$

$(U_L)_{k,m,i}$ = controlled source of BOD in segment k of layer m.

The two-dimensional DO concentration rate balance is represented by the following equations.

Convection:

$$x_{3,k,m,i+1} = f_{3,k,m,i} = x_{6,k,m,i} \qquad (3\text{-}9)$$

Remaining Processes:

$$x_{4,k,m,i+1} = \Big\{ -G_{k,m,i}x_{3,k,m,i} + E_{k+\frac{1}{2},m,i}x_{3,k+1,m,i} + E_{k-\frac{1}{2},m,i}x_{3,k-1,m,i} + F_{k,m+\frac{1}{2},i}x_{3,k,m+1,i} + F_{k,m-\frac{1}{2},i}x_{3,k,m-1,i} + h_t\Big[(K_3)_{k,m} + (PS)_{k,m,i} + (K_d)_{k,m}x_{2,k,m,i} + (U_C)_{k,m,i}\Big]\Big\} \Big/ \left[1 + \frac{h_t(K_a)_{k,m}}{2}\right] = f_{4,k,m,i} \tag{3-23}$$

where: $k = 2,3,\ldots,N+1$; $m = 2,3,\ldots,M_m$;

$i = 1,2,\ldots,I_m-1$.

$$G_{k,m,i} = \frac{h_t(K_a)_{k,m}}{2} + E_{k+\frac{1}{2},m,i} + E_{k-\frac{1}{2},m,i} + F_{k,m+\frac{1}{2},i} + F_{k,m-\frac{1}{2},i} - 1 \tag{3-24}$$

$(K_a)_{k,m}$ = reaeration coefficient in segment k of layer m.

K_d = deoxygenation coefficient.

K_3 = $K_aC_s - \bar{B}$.

C_s = saturation level of DO.

$\bar{B}$ = average benthal deposit demand rate.

PS = $\bar{P} - \bar{B}$ = net rate of addition of DO due to combined effects of addition by photosynthesis and removal by benthal deposits demand.

$(U_C)_{k,m,i}$ = controlled source of DO in segment k of layer m.

$(D_xA)_{k,m,i} = (D_x)_{k,m,i} \cdot A_{k,m}$.

$(D_zw)_{k,m,i} = (D_z)_{k,m,i} \cdot w_{k,m}$.

$w_{k,m}$ = width of estuary in segment k of layer m.

Equations (3-4), (3-9), (3-18) and (3-23) constitute the state equations of the general two-step discrete dynamic distributed parameter model of the concentrations rate balances in a two-dimensional stratified estuary. Since they were derived directly from conservation of mass balances without use of any continuous distributed parameter model, these equations, along with equations (3-5) through (3-8) and the equations defining the coefficients, constitute the model itself. This fact obviates any need for showing consistency and convergence between the original model and an approximating discretized model.

The definitions of $x_{5,k,m,i}$ and $x_{6,k,m,i}$, equations (3-4) and (3-9), may be recast into discrete systems state variable form as follows.

$$x_{5,k,m,i+1} = f_{5,k,m,i} = f_{1,k,m,i} - x_{5,k,m,i} \quad (3\text{-}25)$$

$$x_{6,k,m,i+1} = f_{6,k,m,i} = f_{3,k,m,i} - x_{6,k,m,i} \quad (3\text{-}26)$$

Then the general two-dimensional estuary model with control terms in both the BOD and DO rate balances may be written in a generalized state variable form that includes the coordination equations, (3-25) and (3-26), as well as equations (3-4), (3-9), (3-18) and (3-23).

$$\underline{x}_{i+1} = \underline{f}_i(\underline{x}_i, \underline{u}_i) \tag{3-27}$$

$i = 1, 2, \ldots, I_m - 1$

with scalar components:

$$x_{n,k,m,i+1} = f_{n,k,m,i}(\underline{x}_i, \underline{u}_i) \tag{3-28}$$

$n = 1, 2, \ldots, 6$

where $\underline{x}_i = (\underline{x}_{1,i}, \ldots, \underline{x}_{n,i}, \ldots, \underline{x}_{6,i})^T$ (3-29)

$$\underline{x}_{n,i} = (\underline{x}_{n,2,i}, \ldots, \underline{x}_{n,k,i}, \ldots, \underline{x}_{n,N+1,i})^T \tag{3-30}$$

$$\underline{x}_{n,k,i} = (x_{n,k,2,i}, \ldots, x_{n,k,m,i}, \ldots, x_{n,k,M_m+1,i})^T \tag{3-31}$$

$$\underline{u}_i = \left[0,\ (\underline{U}_L)_i,\ 0,\ (\underline{U}_C)_i,\ 0,\ 0\right]^T \tag{3-32}$$

$(\underline{U}_L)_i$ and $(\underline{U}_C)_i$ may be expanded in terms of their scalar components in the same way as $\underline{x}_{n,i}$ and $\underline{f}_i$ may be expanded in terms of its scalar components in a manner completely analogous with $\underline{x}_i$'s expansion.

Equations (3-27) and (3-28), then, are compact representations of the general discrete dynamic distributed parameter model of the concentrations balances in the two-dimensional estuary with equation (3-27) as the vector-matrix form and equation (3-28) as the scalar form of this representation. The scalar component form is the one more suitable for direct application of Pontryagin's discrete minimum principle as it is presented by Butkovskii[59]. For aeration control alone $(U_L)_{k,m,i} = 0$ and for waste dumping control alone $(U_C)_{k,m,i} = 0$.

3.1.5 Two-step discrete estuary model with negligible vertical velocity. In some two-dimensional stratified estuary models, the vertical component of velocity may be neglected. An example of such an estuary model appears in Okunseinde[340], page 161. Application of the condition, $(V_z)_{k,m,i} = 0$ for all k,m and i reduces the equations defining $x_{5,k,m,i}$ and $x_{6,k,m,i}$. The remaining equations of the two-dimensional estuary model with negligible vertical velocity are identical with those for the general two-dimensional estuary. When the vertical component of velocity is negligible, the reduced equations are:

$$x_{5,k,m,i}\Big|_{Q_{k,m,i} \geq 0} = x_{2,k,m,i} + \frac{h_t}{h_x A_{k,m}} \left(Q_{k-\frac{1}{2},m,i} x_{2,k-1,m,i} - Q_{k+\frac{1}{2},m,i} x_{2,k,m,i}\right) \tag{3-33}$$

$$x_{5,k,m,i}\Big|_{Q_{k,m,i}<0} = x_{2,k,m,i} + \frac{h_t}{h_x A_{k,m}}\left(Q_{k+\frac{1}{2},m,i}x_{2,k+1,m,i} - Q_{k-\frac{1}{2},m,i}x_{2,k,m,i}\right) \tag{3-34}$$

$$x_{6,k,m,i}\Big|_{Q_{k,m,i}\geq 0} = x_{4,k,m,i} + \frac{h_t}{h_x A_{k,m}}\left(Q_{k-\frac{1}{2},m,i}x_{4,k-1,m,i} - Q_{k+\frac{1}{2},m,i}x_{4,k,m,i}\right) \tag{3-35}$$

$$x_{6,k,m,i}\Big|_{Q_{k,m,i}<0} = x_{4,k,m,i} + \frac{h_t}{h_x A_{k,m}}\left(Q_{k+\frac{1}{2},m,i}x_{4,k+1,m,i} - Q_{k-\frac{1}{2},m,i}x_{4,k,m,i}\right) \tag{3-36}$$

3.1.6 <u>Discretized volume flow rate distribution model</u>. Before the concentrations distributions, $L_{k,m,i}$ and $C_{k,m,i}$, can be obtained from the models described in this section, it is necessary to have available the discrete volume flow rate distribution, $Q_{k,m,i}$. The third subscript indicates that the volume flow rate may vary with time. For the finite-difference models discussed in this chapter, the volume flow rate may vary temporally without a concomitant variation in the spatial increment. This represents an important gain in flexibility over the discretized continuous distributed parameter models presented in the previous chapter.

The equation expressing the tidal velocity distribution in a two-dimensional stratified estuary with salinity intrusion presented by Okunseinde[340] may be used to obtain an expression for the corresponding volume flow rate distribution as follows.

The spatially and temporally discretized volume flow rate is related to the discretized velocity distribution by:

$$Q_{k,m,i} = A_{k,m} \cdot U_{k,m,i} \qquad (3\text{-}37)$$

$k=1,2,\ldots,N+1; \quad m=1,2,\ldots,M_m+1$

where:

$U_{k,m,i}$ = spatially and temporally discretized distribution of longitudinal velocity.

$A_{k,m}$ = average cross sectional area of estuary in segment k of layer m.

$Q_{k.m.i}$ = longitudinal volume flow rate.

The longitudinal velocity may be represented by the sum of a time-averaged portion and a time-varying portion.

$$U_{k,m,i} = (U_a)_{k,m} + (U_v)_{k,m,i} \tag{3-38}$$

$k = 1,2,\ldots,N+1; \quad m = 1,2,\ldots,M_m+1$

where:

$$(U_a)_{k,m} = U_F\left(1 - 2\,\frac{k-1}{N} \cdot \frac{m-1}{M_m}\right) \tag{3-39}$$

$$(U_v)_{k,m,i} = U_T\,\frac{k-1}{N}\,\sin\left[2\Pi(i-1)\,\omega_T h_t\right] \tag{3-40}$$

U_F = average magnitude of fresh water flow velocity.

U_T = magnitude of tidal velocity.

ω_T = tidal frequency.

Equations (3-38) through (3-40) are spatially and temporally discretized versions of equations appearing in Okunseinde's dissertation. The time-averaged component of the tidal velocity approximates the logarithmic vertical velocity profile resulting from salinity intrusion in an estuary(340). Figure 3-2 displays typical velocity profiles generated by the equation for the time-averaged component.

The time-varying component of the tidal velocity, $(U_v)_{k,m,i}$, represents a linear approximation of the results obtained in Segall and Gudland(418).

Combining equations (3-37) through (3-40) yields:

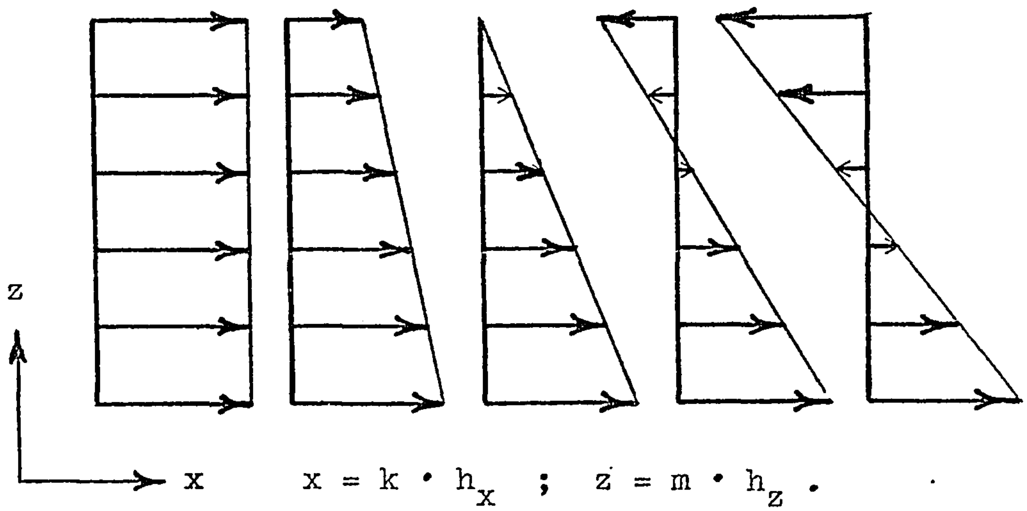


Figure 3-2: Typical velocity profiles for time-averaged component of tidal velocity based on equation from Okunseinde(340):

$$(U_a)_{k,m} = (U_F)\left(1 - 2\frac{k-1}{N} \cdot \frac{m-1}{M_m}\right)$$

$$Q_{k,m,i} = A_{k,m}U_F\left(1 - 2\frac{k-1}{N} \cdot \frac{m-1}{M_m}\right) + A_{k,m}U_T\frac{k-1}{N} \sin\left[2\Pi(i-1)\,\omega_T h_t\right] \qquad (3\text{-}41)$$

or

$$Q_{k,m,i} = Q_F\left(1 - 2\frac{k-1}{N} \cdot \frac{m-1}{M_m}\right) + Q_T\frac{k-1}{N} \sin\left[2\Pi(i-1)\,\omega_T h_t\right] \qquad (3\text{-}42)$$

where:

$$Q_F = A_{k,m}(U_F)_{k,m} \qquad (3\text{-}43)$$

$$Q_T = A_{k,m}(U_T)_{k,m} \qquad (3\text{-}44)$$

$k=1,2,\ldots,N+1;\quad m=1,2,\ldots,M_m+1;\quad i=1,2,\ldots,I_m+1.$

Depending upon availability of data, either equation (3-41) or equation (3-42) may be used to represent the volume flow rate distribution for two-dimensional finite-difference models. Equation (3-41) would be used where the velocities are constant and equation (3-42) would be used where the volume flow rates are constant.

3.2 One-dimensional Finite Difference Water Quality Models

One-dimensional models are most appropriate for those waterways that may be considered vertically and laterally homogeneous. An example of such a waterway is a tidal river where salinity intrusion is minimal.

3.2.1 Two-step finite-difference tidal river model. The concentration rate balance equations for the tidal river model may be derived from the general two-dimensional model's corresponding equations by reducing them to a one-dimensional form. The tidal river equations also may be derived directly from mass balances as in Bella and Dobbins[27]. Either approach yields the following equations.

BOD rate balances:

Convection:

$$x_{1,k,i+1} = f_{1,k,i} = x_{5,k,i} \tag{3-45}$$

where $x_{5,k,i}$ is defined by equations (3-33) and (3-34) with subscript, m, omitted.

Remaining processes:

$$x_{2,k,i+1} = f_{2,k,i} = \left\{ -B_{k,i}x_{1,k,i} + E_{k+\frac{1}{2},i}x_{1,k+1,i} + E_{k-\frac{1}{2}}x_{1,k-1,i} + h_t\left[(L_a)_k + (U_L)_{k,i}\right]\right\} \Big/ \left[1 + \frac{h_t(K_r)_k}{2}\right] \tag{3-46}$$

$k=2,3,\ldots,N+1; \quad i=1,2,\ldots,I_m-1$

where:

$$B_{k,i} = \frac{h_t(K_r)_k}{2} + E_{k+\frac{1}{2},i} + E_{k-\frac{1}{2},i} - 1 \tag{3-47}$$

$$E_{k+\frac{1}{2},i} = h_t D_{k+\frac{1}{2},i} A_{k+\frac{1}{2}} \Big/ A_k h_x^2 \tag{3-48a}$$

$$E_{k-\frac{1}{2},i} = h_t D_{k-\frac{1}{2},i} A_{k-\frac{1}{2}} \Big/ A_k h_x^{\,2} \qquad (3\text{-}48b)$$

DO rate balances:

Convection:

$$x_{3,k,i+1} = f_{3,k,i} = x_{6,k,i} \qquad (3\text{-}49)$$

where $x_{6,k,i}$ is defined by equations (3-35) and (3-36) with the subscript, m, omitted.

Remaining processes:

$$x_{4,k,i+1} = f_{4,k,i} = \Big\{ -G_{k,i} x_{3,k,i} + E_{k+\frac{1}{2},i} x_{3,k+1,i} + E_{k-\frac{1}{2},i} x_{3,k-1,i} + h_t \Big[(K_3)_k + (PS)_{k,i} - (K_d)_k x_{2,k,i} + (U_C)_{k,i} \Big] \Big\} \Big/ \left[1 + \frac{h_t (K_a)_k}{2} \right] \qquad (3\text{-}50)$$

$k=2,3,\ldots,N+1; \quad i=1,2,\ldots,I_m-1$

where:

$$G_{k,i} = \frac{h_t (K_a)_k}{2} + E_{k+\frac{1}{2},i} + E_{k-\frac{1}{2},i} - 1 \qquad (3\text{-}51)$$

The state equations of the tidal river model consist of equations (3-45), (3-46), (3-49) and (3-50). By a development paralleling that for the general two-dimensional estuary model, the definitions of the coordination variables, $x_{5,k,i}$ and $x_{6,k,i}$, may be written in the state variable form:

$$x_{5,k,i+1} = f_{5,k,i} = f_{1,k,i} - x_{5,k,i} \qquad (3\text{-}52)$$

$$x_{6,k,i+1} = f_{6,k,i} = f_{3,k,i} - x_{6,k,i} \qquad (3\text{-}53)$$

Then the generalized state equations of the tidal river model can be expressed in the form:

$$\underline{x}_{i+1} = \underline{f}_i(\underline{x}_i, \underline{u}_i) \qquad (3\text{-}27)$$

with scalar components

$$x_{n,k,i+1} = f_{n,k,i}(\underline{x}_i, \underline{u}_i) \qquad (3\text{-}54)$$

$n=1,2,\ldots,6$

where:

$$\underline{x}_i = (\underline{x}_{1,i},\ldots,\underline{x}_{n,i},\ldots,\underline{x}_{6,i})^T \qquad (3\text{-}29)$$

$$\underline{x}_{n,i} = (x_{n,2,i},\ldots,x_{n,k,i},\ldots,x_{n,N+1,i})^T \qquad (3\text{-}55)$$

$$\underline{u}_i = \left[0,\ (\underline{U}_L)_i,\ 0,\ (\underline{U}_C)_i,\ 0,\ 0\right]^T \qquad (3\text{-}56)$$

$\underline{U}_L$ and $\underline{U}_C$ may be expanded in terms of their scalar components in the same way as $\underline{x}_{n,i}$, and $\underline{f}_i$ may be expanded in terms of its components in the same way as $\underline{x}_i$.

3.2.2 Discretized volume flow rate model. The spatially and temporally discretized volume flow rate may be related to the discretized tidal velocity by:

$$Q_{k,i} = A_k \cdot U_{k,i} \qquad (3\text{-}57)$$

where:

$$U_{k,i} = U_F + U_T \sin\left[2\Pi(i-1)\,\omega_T h_t\right] \qquad (3\text{-}58)$$

U_F = average magnitude of fresh water flow velocity.

U_T = magnitude of tidal velocity.

ω_T = tidal frequency.

Equation (3-58) is a spatially and temporally discretized form of an equation appearing in Okunseinde's dissertation(340). Combination of equations (3-57) and (3-58) yields:

$$Q_{k,i} = A_k \cdot U_F + A_k \cdot U_T \sin\left[2\Pi(i-1)\,\omega_T h_t\right] \quad (3\text{-}59)$$

or,

$$Q_{k,i} = Q_F + Q_T \sin\left[2\Pi(i-1)\,\omega_T h_t\right] \quad (3\text{-}60)$$

where:

$$Q_F = A_k \cdot (U_F)_k \quad (3\text{-}61)$$

$$Q_T = A_k \cdot (U_T)_k \quad (3\text{-}62)$$

Equation (3-59) is used where the velocities are constant and equation (3-60) is used where the volume flow rates are constant.

3.2.3 Two-step discrete tapered stream model. Upstream from the tidal river reach, where the tidal effect can be neglected, the dispersion term also may be omitted from the model. The resulting equations are said to represent the concentration rate balances of the tapered stream model. The convection equations for the stream model are the same as those for the tidal river equations (3-45) and (3-49).

The equation for the concentration rate balance of the remaining BOD processes is:

$$x_{2,k,i+1} = f_{2,k,i} = \left(-B_k x_{1,k,i} + h_t \left[(L_a)_k + (U_L)_{k,i} \right] \right) \bigg/ \left[1 + \frac{h_t (K_r)_k}{2} \right] \qquad (3\text{-}63)$$

$k=2,3,\ldots,N+1$

where

$$B_k = \frac{h_t (K_r)_k}{2} - 1 \qquad (3\text{-}64)$$

The equation for the remaining processes of the DO concentrations rate balance is:

$$x_{4,k,i+1} = f_{4,k,i} = \left\{ -G_k x_{1,k,i} + h_t \left[(K_3)_k + (PS)_{k,i} - (K_d)_k x_{2,k,i} + (U_C)_{k,i} \right] \right\} \bigg/ \left[1 + \frac{h_t (K_a)_k}{2} \right] \qquad (3\text{-}65)$$

$k=2,3,\ldots,N+1$

$i=1,2,\ldots,I_m-1$

where

$$G_k = \frac{h_t (K_a)_k}{2} - 1 \qquad (3\text{-}66)$$

Since the tidal effect is negligible, the volume flow rate used with this model is uniform spatially and temporally and directed downstream.

$$Q_{k,i} = Q_o = \text{constant} > 0 \qquad (3\text{-}67)$$

3.3 Multilevel Hierarchical Optimal Control of Discrete Dynamic Distributed Parameter Water Quality Models

The BOD concentration, $x_{2,k,m,i}$, and the DO concentration, $x_{4,k,m,i}$, represent the average concentrations in the volume element centered at the spatial point (k,m) at time i. From Figure 3-1, it is evident that in order for $x_{2,k,m,i}$ and $x_{4,k,m,i}$ to approximate the corresponding actual concentrations, L(x,z,t) and C(x,z,t), with sufficient accuracy, the spatial increments, h_x and h_z , should be kept as small as possible. However, for a waterway reach of given length and depth, decreasing h_x increases the total number of segments of the longitudinal axis and decreasing h_z increases the number of layers along the vertical axis of the discrete model. Modelling of actual waterways in which large spatial changes in parameters may occur simultaneously with large reach lengths can all too easily lead to discrete models with equations of unwieldy dimensions. The problem of dimensionality can be so severe that attempts to apply optimal control to these models under realistic conditions by conventional methods can exceed available computer capacity. The one-dimensional finite-difference models are subject to the same problems.

The techniques of multilevel hierarchical systems analysis have been shown to be especially efficient for dealing with models consisting of coupled sets of equations of large dimension[248, 249, 309, 312]. Since the water quality models of this chapter are discrete systems, a combination of multilevel hierarchical techniques and Pontryagin's discrete minimum principle[59] is applied to them to effect optimal control.

The general procedure for this combined approach to optimal control of large-scale discrete systems is the following:

1.) Apply decomposition to the system to be controlled to reduce it to a series of systems of lower dimension that are temporarily de-coupled from each other.
2.) Express decomposed system in vector-matrix form.
3.) Define a performance index functional dependent upon the relevant state variables and control terms.
4.) Form set of augmented state equations by adding an equation corresponding to minimization of the performance index to the set of state equations.
5.) Employ Pontryagin's equations to determine the costate equations and constraint equations.

6.) Assemble constraint equations into an overall coordination subproblem and assign the state, costate and control equations to their respective subproblems.

7.) Employ gradient approach to derive control equations.

8.) Construct subproblem hierarchy with state, costate and control subproblems on the lower level and the overall coordination subproblem in the upper level.

9.) Determine appropriate boundary, initial and final conditions for the subproblems in the hierarchy.

10.) Obtain distributions of concentrations and control variables that minimize the performance index by iterating between the levels of the hierarchy.

3.3.1 Decomposition. For reasons discussed in detail in Chapter 2, full decomposition is employed throughout this dissertation. The basic approach of full decomposition is the subdivision of the original model into a series of models, each consisting of a single scalar equation, which are temporarily de-coupled from each other by substitution of a set of coordination variables to suppress the coupling.

3.3.1.1 <u>Decomposition of the general two-dimensional discrete distributed parameter water quality model</u>. Coupling in the BOD rate balance of the general two-dimensional estuary model is represented by all terms involving the convected BOD concentration, x_1, in equation (3-18). This coupling is suppressed by collecting all such terms and equating them to a co-ordination variable as follows.

$$x_{7,k,m,i} = - B_{k,m,i}x_{1,k,m,i} + E_{k+\frac{1}{2},m,i}x_{1,k+1,m,i}$$

$$+ E_{k-\frac{1}{2},m,i}x_{1,k-1,m,i} + F_{k,m+\frac{1}{2},i}x_{1,k,m+1,i}$$

where $B_{k.m.i}$, $E_{k.m.i}$, and F (3-68)

where $B_{k,m,i}$, $E_{k,m,i}$, and $F_{k,m,i}$ are defined in equations (3-19), (3-20) and (3-21).

Substitution of equation (3-68) in equation (3-18) yields:

$$x_{2,k,m,i+1} = \left[x_{7,k,m,i} + h_t(L_a)_{k,m} + h_t(U_L)_{k,m,i}\right] \Big/ \left[1 + \frac{h_t(K_r)_{k,m}}{2}\right] = f_{2,k,m,i} \qquad (3\text{-}69)$$

Equations (3-68) and (3-69) constitute the decomposed form of equation (3-18).

Coupling in the DO rate balance of the general two-dimensional estuary model is represented by all terms involving the convected DO concentration, x_3 , and also the BOD concentration, x_2 , in equation (3-23). Hence, the coordination variable for this equation is defined as follows.

$$x_{8,k,m,i} = -G_{k,m,i}x_{3,k,m,i} + E_{k+\frac{1}{2},m,i}x_{3,k+1,m,i}$$

$$+ E_{k-\frac{1}{2},m,i}x_{3,k-1,m,i} + F_{k,m+\frac{1}{2},i}x_{3,k,m+1,i}$$

$$+ F_{k,m-\frac{1}{2},i}x_{3,k,m-1,i} - h_t(K_d)_{k,m}x_{2,k,m,i} \qquad (3\text{-}70)$$

where $E_{k,m,i}$, $F_{k,m,i}$ and $G_{k,m,i}$ are defined in equations (3-20), (3-21) and (3-24), respectively.

Substitution of equation (3-70) in equation (3-23) yields:

$$x_{4,k,m,i+1} = \Big(x_{8,k,m,i}$$

$$+ h_t\left[(K_3)_{k,m} + (PS)_{k,m,i} + (U_C)_{k,m,i}\right]\Big)$$

$$\Big/ \left[1 + \frac{h_t(K_a)_{k,m}}{2}\right] = f_{4,k,m,i} \qquad (3\text{-}71)$$

Equations (3-4), (3-9), (3-69) and (3-71) constitute the state equations of the decomposed general two-dimensional estuary model. Coordination equations (3-68) and (3-70) may be written in state variable form as follows.

$$x_{7,k,m,i+1} = f_{7,k,m,i} = - B_{k,m,i}x_{1,k,m,i}$$

$$+ E_{k+\frac{1}{2},m,i}x_{1,k+1,m,i} + E_{k-\frac{1}{2},m,i}x_{1,k-1,m,i}$$

$$+ F_{k,m+\frac{1}{2},i}x_{1,k,m+1,i} + F_{k,m-\frac{1}{2},i}x_{1,k,m-1,i} - x_{7,k,m,i}$$

$$(3\text{-}72)$$

$$x_{8,k,m,i+1} = f_{8,k,m,i} = -G_{k,m,i}x_{3,k,m,i}$$

$$+ E_{k-\frac{1}{2},m,i}x_{3,k-1,m,i} + E_{k+\frac{1}{2},m,i}x_{3,k+1,m,i}$$

$$+ F_{k,m-\frac{1}{2},i}x_{3,k,m-1,i} + F_{k,m+\frac{1}{2},i}x_{3,k,m+1,i}$$

$$- x_{8,k,m,i} \qquad (3\text{-}73)$$

If the coordination equations (3-25), (3-26), (3-72) and (3-73) are appended to the state equations, (3-4), (3-9), (3-69) and (3-71), they constitute a set of scalar component equations of the form,

$$x_{n,k,m,i+1} = f_{n,k,m,i}(\underline{x}_i \, , \, \underline{u}_i) \qquad (3\text{-}28)$$

$n=1,2,...,8$

of the generalized vector-matrix state equation.

$$\underline{x}_{i+1} = \underline{f}_i(\underline{x}_i \, , \, \underline{u}_i) \qquad (3\text{-}27)$$

$i=1,2,...,I_m-1$

where:

$$\underline{x}_i = (\underline{x}_{1,i},...,\underline{x}_{n,i},...,\underline{x}_{8,i})^T \qquad (3\text{-}74)$$

$$\underline{u}_i = \left[0,(\underline{U}_L)_i,0,(\underline{U}_C)_i,0,0,0,0 \right]^T \qquad (3\text{-}75)$$

3.3.1.2 Decomposition of the discrete two-dimensional model with negligible vertical velocity. The equations representing this decomposed model are identical with those representing the general two-dimensional model except that $x_{5,k,m,i}$ and $x_{6,k,m,i}$ are defined by equations

(3-33) through (3-36).

3.3.1.3 Decomposition of the discrete dynamic tidal river model. The coordination variable for the remaining processes BOD rate balance of this model, equation (3-46), is:

$$x_{7,k,i} = -B_{k,i}x_{1,k,i} + E_{k+\frac{1}{2},i}x_{1,k+1,i} + E_{k-\frac{1}{2},i}x_{1,k-1,i} \qquad (3\text{-}76)$$

which reduces equation (3-46) to:

$$x_{2,k,i+1} = f_{2,k,i} = \left(x_{7,k,i} + h_t\left[(L_a)_k + (U_L)_{k,i}\right] \right) \Big/ \left[1 + \frac{h_t(K_r)_k}{2}\right] \qquad (3\text{-}77)$$

where $B_{k,i}$ and $E_{k,i}$ are defined in equations (3-47) and (3-48), respectively.

The coordination variable for the remaining processes portion of the DO concentration rate balance equations, (3-50), is:

$$x_{8,k,i} = - G_{k,i}x_{3,k,i} + E_{k+\frac{1}{2},i}x_{3,k+1,i} + E_{k-\frac{1}{2},i}x_{3,k-1,i} - h_t(K_d)_k x_{2,k,i} \qquad (3\text{-}78)$$

This reduces equation (3-50) to:

$$x_{4,k,i+1} = f_{4,k,i} = \left(x_{8,k,i} + h_t\left[(K_3)_k + (PS)_{k,i} + (U_C)_{k,i}\right] \right) \Big/ \left[1 + \frac{h_t(K_a)_k}{2}\right] \qquad (3\text{-}79)$$

where $G_{k,i}$ is defined in equation (3-51).

The state equations of the decomposed tidal river model consist of (3-45), (3-49), (3-77) and (3-79). If the coordination equations (3-76) and (3-78), are written in the state variable forms,

$$x_{7,k,i+1} = f_{7,k,i} = -B_{k,i}x_{1,k,i} + E_{k+\frac{1}{2},i}x_{1,k+1,i} + E_{k-\frac{1}{2},i}x_{1,k-1,i} - x_{7,k,i} \quad (3\text{-}80)$$

$$x_{8,k,i+1} = f_{8,k,i} = -G_{k,i}x_{3,k,i} + E_{k+\frac{1}{2},i}x_{3,k+1,i} + E_{k-\frac{1}{2},i}x_{3,k-1,i} - h_t(K_d)_k x_{2,k,i} - x_{8,k,i} \quad (3\text{-}81)$$

the coordination equations, (3-80) and (3-81), (3-52) and (3-53) may be appended to the state equations (3-45), (3-49), (3-77) and (3-79)to form the following set of scalar equations

$$x_{n,k,i+1} = f_{n,k,i}(\underline{x}_i \ , \ \underline{u}_i) \quad (3\text{-}54)$$

$n=1,2,...,8$

which are the scalar components of the generalized vector-matrix state equation

$$\underline{x}_i = \underline{f}_i(\underline{x}_i \ , \ \underline{u}_i) \quad (3\text{-}27)$$

$i=1,2,...,I_m-1$

where $\underline{x}_i$ and $\underline{u}_i$ may be expanded as in equations (3-74) and (3-75), respectively.

3.3.1.4 Decomposition of the discrete distributed parameter tapered stream model. The equations representing the decomposed stream model are the same as those for the decomposed tidal river model except that the coordination variables, $x_{7,k,i}$ and $x_{8,k,i}$ are defined as follows.

$$x_{7,k,i} = -B_k x_{1,k,i} \quad (3\text{-}82)$$

$$x_{8,k,i} = -G_k x_{3,k,i} - h_t (K_d)_k x_{2,k,i} \quad (3\text{-}83)$$

which, in state variable form, become

$$x_{7,k,i+1} = f_{7,k,i} = -B_k x_{1,k,i} - x_{7,k,i} \quad (3\text{-}84)$$

$$x_{8,k,i+1} = f_{8,k,i} = -G_k x_{3,k,i} - h_t (K_d)_k x_{2,k,i} - x_{8,k,i} \quad (3\text{-}85)$$

where B_k and G_k are defined in equations (3-64) and (3-66), respectively. Substitution of equation (3-82) in equation (3-63) yields equation (3-77) and substitution of equation (3-83) in equation (3-65) yields equation (3-79).

3.3.2 Optimal aeration control of the decomposed discrete dynamic distributed parameter general two-dimensional water quality model.

3.3.2.1 Construction of performance index. If a specified level of DO concentration is to be attained with a minimum expenditure of control energy, the spatially and temporally discrete performance index can be written as a weighted linear sum of quadratics in terms of the error in DO concentration and the magnitude of the aeration control terms summed over the spatial and temporal region of interest.

$$J = \sum_{i=2}^{I_m} \sum_{k=2}^{N} \sum_{m=2}^{M_m} \frac{J_{k,m,i}}{h_x h_z h_t} \tag{3-86}$$

where, for $(U_L)_{k,m,i} = 0$,

$$J_{k,m,i} = h_x h_z h_t \left\{ W_1 \left[(C_{sp})_{k,m} - x_{4,k,m,i} \right]^2 + W_2 (U_C)^2_{k,m,i} \right\} \tag{3-87}$$

W_1 and W_2 are constant weighting coefficients for the error term and control term, respectively. Different ratios between the magnitudes of W_1 and W_2 represent different tradeoffs as to whether accuracy of control or minimization of energy expenditure has higher priority.

If it is deemed less important that the system be corrected for excess DO concentration, then equation (3-87) could be used for the performance index when $x_{4,k,m,i} = C_{k,m,i} \quad (C_{sp})_{k,m}$ and a new performance index:

$$J_{k,m,i}\Big|_{C_{k,m,i} \geq (C_{sp})_{k,m}}$$

$$= h_x h_z h_t \left\{ W_5 \left[(C_{sp})_{k,m} - x_{4,k,m,i} \right]^2 + W_2 (U_C)^2_{k,m,i} \right\} \tag{3-88}$$

could be defined for $x_{4,k,m,i} = C_{k,m,i} \geq (C_{sp})_{k,m}$.

3.3.2.2 Augmented vector-matrix equations. The performance index equation of (3-87) may be expressed in the form of a scalar component of the vector-matrix equation, equation (3-27), as follows.

$$x_{9,k,m,i+1} = f_{9,k,m,i}(\underline{x}_i\ ,\ \underline{u}_i)$$

$$= h_x h_z h_t \left\{ W_1 \left[(C_{sp})_{k,m} - x_{4,k,m,i} \right]^2 + W_2 (U_C)^2_{k,m,i} \right\} \tag{3-89}$$

Equation (3-89) may be appended to equations (3-28) and (3-74) to form the scalar components of the augmented vector-matrix equations for the model with aeration control as follows.

$$x_{n,k,m,i+1} = f_{n,k,m,i}(\underline{x}_i\ ,\ \underline{u}_i) \tag{3-90}$$

$n=1,2,\ldots,9$; $k=1,2,\ldots,N$

$m=1,2,\ldots,M_m$; $i=1,2,\ldots,I_m$

The corresponding augmented vector-matrix equation is in the form of equation (3-27).

3.3.2.3 Application of Pontryagin's discrete minimum principle. Since the mathematical model of the concentrations balances with aeration control is in vector-matrix finite-difference form, equation (3-27), it is appropriate to determine the optimal space-time distributions of the concentrations and the control variable by applying Pontryagin's discrete minimum principle to it. According to this principle[59], a discrete system to be controlled of the form of equation (3-27) and with scalar component equations of the form of (3-90) with performance index given by equations (3-87) and (3-89) attains a minimum of the performance index where the following necessary conditions are satisfied.

$$\sum_{n=1}^{9} \sum_{k=1}^{N+1} \sum_{m=1}^{M_m+1} (cx)_{n,k,m,i} \frac{\partial f_{n,k,m,i_1}}{\partial x_{n_1,k_1,m_1,i_1}} = 0 \qquad (3\text{-}91)$$

$n_1=5,6,7,8$; n_1, k_1, m_1, i_1 are fixed integers.

The corresponding costate equations to be satisfied when the performance index is minimized are given by:

$$(cx)_{n_1,k_1,m_1,i_1-1} = \sum_{n=1}^{9} \sum_{k=2}^{N} \sum_{m=2}^{M_m} (cx)_{n,k,m,i_1} \frac{\partial f_{n,k,m,i_1}}{\partial x_{n_1,k_1,m_1,i_1}} \qquad (3\text{-}92)$$

where n_1, k_1, m_1, and i_1 are fixed integers; $n_1=1,2,3,4$.
The $f_{n,k,m,i}$ are defined by the scalar components of the vector-matrix equation (3-27) as expressed by equation (3-90) and the variables, $(cx)_{n,k,m,i}$, correspond to the variables $x_{n,k,m,i}$ as depicted by Table 3-1.

Using the correspondences across the rows of Table 3-1 in conjunction with equation (3-92) yields the costate equations listed in Appendix 3. The necessary conditions of equation (3-91) yield the remaining coordination equations which also are listed in Appendix 3.

3.3.2.4 Construction of coordination subproblem. The coordination subproblem for the general two-dimensional estuary model with optimal multilevel control consists of the following equations:

1.) equations (3-4) and (3-9) with $x_{5,k,m,i}$ and $x_{6,k,m,i}$ defined by equations (3-5) through (3-8);
2.) equations (3-68) and (3-70);
3.) equations (A3-8) through (A3-11).

3.3.2.5 Construction of optimal control equations. Using a gradient approach to optimization as in Pierre[371],

Costate variables	State variables
$(cx)_1$	x_1
$(cx)_2$	x_2
$(cx)_3$	x_3
$(cx)_4$	x_4
Coordination variables	
$(cx)_5$	x_5
$(cx)_6$	x_6
$(cx)_7$	x_7
$(cx)_8$	x_8
Performance index	
$(cx)_9$	x_9

Table 3-1: Correspondences between $(cx)_n$ and x_n

$$(U_C)^{(r+1)}_{k,m,i} = (U_C)^{(r)}_{k,m,i} - \epsilon_C (GRC)^{(r)}_{k,m,i} \qquad (3\text{-}93)$$

where the superscript denotes the number of the iteration and ϵ_C is a constant between zero and +1.0 chosen as a tradeoff between speed of convergence and accuracy.

$$(GRC)_{k_1,m_1,i_1} =$$

$$\sum_{n=1}^{9} \sum_{k=2}^{N} \sum_{m=2}^{M_m} (cx)_{n,k,m,i_1} \frac{\partial f_{n,k,m,i_1}}{\partial (U_C)_{k_1,m_1,i_1}} \qquad (3\text{-}94)$$

k_1, m_1 and i_1 are constants.

From equations (3-71), (3-89) and (3-90),

$$(GRC)_{k,m,i} = (cx)_{4,k,m,i} \Big/ \left[1 + \frac{h_t (K_a)_{k,m}}{2}\right]$$

$$+ 2h_x h_z h_t W_2 (U_C)_{k,m,i} \qquad (3\text{-}95)$$

Equations (3-93) and (3-95) may be combined into a single control equation.

3.3.2.6 Subproblem hierarchy. Equation (3-90) with n=1,2,3,4 and equations (3-4), (3-9), (3-69), (3-71) comprise the state subproblem equations; Equations (A3-1) through (A3-7) comprise the costate subproblem equations and equations (3-93) and (3-95) constitute the control subproblem. The equations of the overall coordination subproblem were listed in Section 3.3.2.5. All of these subproblems may be assembled into the hierarchical structure depicted in Figure 2-1. Boundary, initial and final conditions for the solution of the subproblems are presented in Appendix 4. Optimization of the overall control problem is accomplished by either assuming or generating an initial set of space-time profiles for the solution of the state, costate and control subproblems, substituting these profiles into the coordination equations and iterating between the levels of the subproblem hierarchy until the performance index of equations (3-86) and (3-87) is minimized.

3.3.3 <u>Optimal aeration control of the two-dimensional model with negligible vertical velocity</u>. The state equations for this model are the same as those for the general two-dimensional estuary model, equations (3-90) (with n=1,2,3,4) (3-4), (3-9), (3-69) and (3-71). When the vertical velocity component, $(V_z)_{k,m,i}$ is set to zero, the equations defining $x_{5,k,m,i}$ and $x_{6,k,m,i}$ for coordination equations (3-4) and (3-9) reduce to equations (3-33) through (3-36). The costate equations for the model with negligible vertical velocity are the same as those for the general two-dimensional model, equations (A3-1) through (A3-7) except that the equations of

Appendix 5 are substituted for equations (A3-2) through (A3-5) and (A3-7).

The remaining equations of the two-dimensional model with negligible vertical velocity are identical with those for the general two-dimensional model.

3.3.4 Optimal aeration control of the discrete dynamic distributed parameter tidal river model. The scalar components of the augmented vector-matrix state equations of the tidal river model with aeration control may be expressed as follows.

$$x_{n,k,i+1} = f_{n,k,i}(\underline{x}_i \ , \ \underline{u}_i) \qquad (3\text{-}96)$$

$n=1,2,\ldots,9$; $k=2,3,\ldots,N+1$; $i=1,2,3,\ldots,I_m-1$
where the first four components are given by equations (3-45), (3-49), (3-77), (3-79), the state equations, the next four are given by equations (3-52), (3-53), (3-80) and (3-81), the coordination equations, and the ninth component is given by equation (3-89) with the subscript, m, omitted and $h_z = 1$.

The costate equations are obtained by applying equation (3-92), with subscripts, m and m_1, omitted, to the set of scalar equations represented by equation (3-96). The resulting equations are listed in Appendix 6 along with the remaining coordination equations.

The optimal aeration control equations for the tidal river model may be obtained from those for the two-dimensional models by omitting the subscript, m, and setting $h_z=1$ in equations (3-93) and (3-95). The initial and upstream boundary conditions for the control variables are given by equations (A4-14) and (A4-15) with the subscript, m, omitted.

The costate final time and downstream boundary conditions for the tidal river model are:

$$(cx)_{n,k,I_m} = 0 \qquad (3\text{-}97)$$

$n=1,2,3,4$; $k=1,2,\ldots,N+1$.

$$(cx)_{n,N+1,i} = 0 \qquad (3\text{-}98)$$

$n=1,2,3,4$; $i=1,2,\ldots,I_m$.

The upstream end boundary conditions of the BOD and DO concentrations are:

$$x_{n,1,i} = L_o \qquad (3\text{-}99)$$

$n=1,2$; $i=1,2,\ldots,I_m$

$$x_{n,1,i} = C_o \qquad (3\text{-}100)$$

$n=3,4$; $i=1,2,\ldots,I_m$

The initial BOD and DO concentration distributions may be obtained from equations (2-104) and (2-105).

The subproblems of the tidal river model with multilevel optimal aeration control may be assembled into the hierarchy depicted by Figure 2-1.

3.3.5 Optimal aeration control of the discrete dynamic distributed parameter tapered stream model. The equations comprising the tapered stream model with multilevel optimal aeration control are identical with those for the tidal river model except for the following modifications.

1.) Equations (3-82) and (3-83) are substituted for equations (3-76) and (3-78), respectively.
2.) Equations (2-114) and (2-115) are substituted for equations (2-104) and (2-105).
3.) The following equations are substituted for equations (A6-1) and (A6-4).

$$(cx)_{1,k,i-1} = - B_k(cx)_{7,k,i} \qquad (3\text{-}101)$$

$$(cx)_{3,k,i-1} = - G_k(cx)_{8,k,i} \qquad (3\text{-}102)$$

where B_k is defined by equation (3-64) and G_k is defined by equation (3-66).

3.3.6 Optimal waste dumping control of the discrete dynamic distributed parameter general two-dimensional water quality model. The performance index corresponding to attainment of a specified level of DO with a minimum expenditure of dumping control energy may be expressed in the form of equation (3-86) with $J_{k,m,i}$ given by the following.

For $(U_C)_{k,m,i} = 0$,

$$J_{k,m,i} = h_x h_z h_t \left\{ W_1 \left[(C_{sp})_{k,m} - C_{k,m,i} \right]^2 + W_4 (U_L)^2_{k,m,i} \right\} \tag{3-103}$$

where W_1 and W_4 are constant weighting coefficients for the error term and control term, respectively. This performance index may be expressed in the form of a generalized state equation as follows.

$$x_{9,k,m,i+1} = f_{9,k,m,i}(\underline{x}_i \, , \, \underline{u}_i)$$
$$= h_x h_z h_t \left\{ W_1 \left[(C_{sp})_{k,m} - x_{4,k,m,i} \right]^2 + W_4 (U_L)^2_{k,m,i} \right\} \tag{3-104}$$

Equation (3-104) may be appended to the state equations of the general two-dimensional model, (3-4), (3-9), (3-69) and (3-71) and the coordination equations (3-25), (3-26), (3-72) and (3-73), to form the scalar components,

$$x_{n,k,m,i+1} = f_{n,k,m,i}(\underline{x}_i \, , \, \underline{u}_i) \tag{3-90}$$

$n=1,2,\ldots,9$; $k-1,2,\ldots,N+1$; $m=1,2,\ldots,M_m+1$; $i=1,2,\ldots,I_m-1$.

of the augmented vector-matrix state equation of the form of equation (3-27) for dumping control.

All of the remaining equations for the general two-dimensional model under waste dumping control are the same as those for aeration control except for the optimal control equations which follow.

$$(U_L)^{(r+1)}_{k,m,i} = (U_L)^{(r)}_{k,m,i} - \epsilon_L (GRL)^{(r)}_{k,m,i} \qquad (3\text{-}105)$$

where the superscript denotes the number of the iteration and ϵ_L is a constant between zero and +1.0 chosen as a tradeoff between speed of convergence and accuracy. Equations (3-69) and (3-104) combined with:

$$(GRL)_{k_1,m_1,i_1} =$$

$$\sum_{n=1}^{9} \sum_{k=2}^{N} \sum_{m=2}^{M_m} (cx)_{n,k,m,i_1} \frac{f_{n,k,m,i_1}}{(U_L)_{k_1,m_1,i_1}} \qquad (3\text{-}106)$$

yield:

$$(GRL)_{k,m,i} = (cx)_{2,k,m,i} \Big/ \left[1 + \frac{h_t (K_r)_{k,m}}{2}\right]$$

$$+ 2h_x h_z h_t W_4 (U_L)_{k,m,i} \qquad (3\text{-}107)$$

with the boundary and initial conditions,

$$(U_L)_{k,m,1} = 0 \qquad (3\text{-}108)$$

$k=2,3,\ldots,N+1$; $m=2,3,\ldots,M_m+1$.

$$(U_L)_{1,m,i} = 0 \qquad (3\text{-}109)$$

$m=1,2,\ldots,M_m+1$; $i=1,2,\ldots,I_m$.

$$(U_L)_{k,1,i} = 0 \qquad (3\text{-}110)$$

$k=1,2,\ldots,N+1$; $i=1,2,\ldots,Im$.

The equations for the general two-dimensional model with multilevel optimal waste dumping control presented in this section may be assembled into the subproblem hierarchy shown in Figure 2-1.

3.3.7 Optimal dumping control of the discrete distributed parameter tidal river model. The scalar components of the augmented vector-matrix state equations of the tidal river model with dumping control are:

$$x_{n,k,i+1} = f_{n,k,i}(\underline{x}_i \ , \ \underline{u}_i) \qquad (3\text{-}96)$$

where the state equations (3-45), (3-49), (3-77) and (3-79), are the first four components, the coordination equations (3-52), (3-53), (3-80) and (3-81), are the next four components and the ninth component is given by equation (3-104) with the subscript, m, omitted and h_z=1.

The optimal dumping control equations for the tidal river model are the same as those for the two-dimensional models with the subscript, m, omitted and h_z=1. The remaining equations for the tidal river model optimal dumping control are identical with those for the same model with optimal aeration control. The equations listed in this section may be collected into subproblems arranged in the hierarchy shown in Figure 2-1.

3.3.8 Optimal bimodal control of the discrete stratified estuary model. Since optimal aeration control increases the DO concentration rate at points where observed DO is below the specified level and optimal dumping control increases the BOD concentration rate at points where observed DO is above the specified level, C_{sp}, the two modes of control have complementary effects upon the water quality of the model. With the appropriate switching criterion, better optimization can be attained by sequential application of the two modes of control than could be attained by applying either one of them individually.

If optimal control is begun in one of the two modes cited above, an especially appropriate criterion for mode switching is an increase beyond a predetermind threshhold value of the composite performance index, stated by equation (3-86) and the following:

$$J_{k,m,i} = h_x h_z h_t \left(W_1 \left[(C_{sp})_{k,m} - C_{k,m,i} \right]^2 + W_2 (U_C)^2_{k,m,i} + W_4 (U_L)^2_{k,m,i} \right) \qquad (3\text{-}111)$$

associated with successive iterations of the optimal control subproblem hierarchy. Inspection of the composite performance index reveals that it is a weighted linear sum of a quadratic error term and quadratics proportional to the control energy expanded for each of the control modes applied to the system where W_1 ,W_2 and W_4 are constant weighting coefficients.

The overall procedure for bimodal optimization is thus as follows;

1.) commence generation of optimal concentrations and control variable distributions by successive iterations between the levels of the subproblem hierarchy using one of the optimal control modes,

2.) when the performance index increases sufficiently between successive iterations switch to the other control mode while retaining the most recently generated control variable distribution for the mode just prior to the switching,

3.) generate optimal concentrations and control variable distributions by successive iterations between the levels of the subproblem keeping the control variables of the mode applied before the switching fixed,

4.) iterate between steps 3) and 4) until the increases in the performance index become negligibly small.

For example, if the optimization were begun with waste dumping control, after the first switching <u>both</u> aeration and dumping control would be applied to the model with the dumping control variables fixed at the values attained just prior to the switching. The dumping control variables would remain fixed throughout the iterations associated with the aeration control mode until the next switching occurred at which point the system would return to the dumping control mode and the aeration control variables would then be held constant. This performance index-dependent switching would continue with one control mode being optimized while the other is held constant until the increases between successive values of the performance index would become sufficiently small.

The specific set of optimal control equations employed by the bimodal system depends upon the mode in which it is operating. For aeration control, the appropriate equations are (3-93) and (3-95) with initial and boundary conditions given by equations (A4-14) through (A4-16). For waste dumping control, they are (3-105) and (3-107) through (3-110).

The remaining equations for the general two-dimensional model with bimodal optimal control are identical with the corresponding equations for either optimal aeration control or optimal dumping control of the same model.

The subproblems resulting from bimodal multilevel control of the general two-dimensional model may be assembled into the hierarchical structure depicted by Figure 2-1, if the mode switching is regarded as occurring within the control subproblem block.

3.3.9 Optimal bimodal control of the discrete dynamic distributed parameter tidal river model. When the system is operating in the aeration control mode, the optimal control equations are expressed by the equations for aeration control of the two-dimensional models (3-93), (3-95), (A4-14) through (A4-16), with subscript, m, omitted and $h_z=1$. For dumping control of the tidal river model, the appropriate equations are (3-105) and (3-107) through (3-110) with the corresponding modifications. The remaining equations for the tidal river model with bimodal optimal control are the same as those for either optimal aeration or dumping control of the same model.

3.4 Aggregation of Single Reach Models Into Regional Multireach Models

The models developed up to this point in the chapter represent the application of various modes of optimal multilevel control to a single reach of four different waterway models. As stated in the previous chapter, various practical factors may lead to a requirement for representing a set of contiguous reaches, with a regional multireach model. The general procedure for aggregating single reach models, in the sense of Kulikowski[(239)], into regional models of Section 2.9 also applies to the discrete distributed parameter models with optimal multilevel control developed in the present chapter. This procedure may be summarized as follows.

1.) Assign an additional reach-identifying subscript to each variable in the equations of the corresponding single reach model.
2.) Formulate inter-reach interface equations.
3.) Construct the subproblem hierarchy for the multireach model.

3.4.1 Regional multireach two-dimensional general water quality model with optimal bimodal control. If it is assumed that the regional model consists of j_m contiguous reaches, the scalar components of the generalized state equation of reach $j(j=1,2,\ldots,j_m)$ may be written by adding the reach-identifying subscript, j, to the corresponding equations of the single reach model. These equations for reach j of the general two-dimensional regional model with bimodal aeration and dumping control are presented in Appendix 7. All of these equations may be represented in the form,

$$x_{n,j,k,m,i+1} = f_{n,j,k,m,i}(\underline{x}_i \ , \ \underline{u}_i) \qquad (3\text{-}112)$$

$n=1,2,\ldots,8$; $j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$

$m=2,3,\ldots,M_m+1$; $i=1,2,\ldots,I_m-1$

which constitute the scalar components of:

$$\underline{x}_{i+1} = \underline{f}_i(\underline{x}_i \ , \ \underline{u}_i) \qquad (3\text{-}27)$$

For operation in the aeration control mode equations (3-93) and (3-95), with addition of the subscript, j, represent the optimal control equations for reach j, with initial and upstream boundary conditions given by equations (A4-14) through (A4-16) with the same modification. The corresponding equations for operation in the waste dumping mode may similarly be obtained from equations (3-105) and (3-107) through (3-110). Additional boundary conditions for this regional model may be obtained by adding the subscript, j, to equations (A4-1) through (A4-13), boundary conditions for the single reach corresponding model.

General interface conditions between the contiguous reaches of the regional model may be defined to reflect the addition at the upstream end of reach j of the following:

1.) a BOD concentration rate, $(L_{ad})_{j,m}$

2.) a DO concentration rate $(C_{ad})_{j,m}$

3.) a volume flow rate, $(Q_{ad})_{j,m}$

If the subscript, j, increases in the downstream direction and the upstream end points of every reach, except the first, coincide with the downstream end points of the reach immediately upstream, the general interface conditions for reaches in the regional model may be represented as follows for $j=2,3,\ldots,j_m$.

$$Q_{j,1,m,i} = Q_{j-1,N+1,m,i} + (Q_{ad})_{j,m} \qquad (3\text{-}113)$$

$$x_{2,j,1,m,i} = \left[Q_{j-1,N+1,m,i}x_{2,j-1,N+1,m,i} + (Q_{ad})_{j,m}(L_{ad})_{j,m} \right] \Big/ Q_{j,1,m,i} \qquad (3\text{-}114)$$

$$x_{4,j,1,m,i} = \left[Q_{j-1,N+1,m,i}x_{4,j-1,N+1,m,i} + (Q_{ad})_{j,m}(C_{ad})_{j,m} \right] \Big/ Q_{j,1,m,i} \qquad (3\text{-}115)$$

where $j=2,3,\ldots,j_m$; $m=1,2,\ldots,M_m+1$; $i=1,2,\ldots,I_m$.

The costate equations for layer m of segment k of reach j are given by the corresponding single reach equations (3-25), (3-26), (3-72), (3-73), (A3-1) through (A3-7), with addition of the subscript, j, where $j=1,2,\ldots,j_m$.

Since the downstream boundary conditions and the final conditions are given for the costate equations, (see Appendix 3), they generally are solved in the reverse order in the space-time region of interest. Accordingly, the costate interface conditions may be expressed in the following form.

$$(cx)_{n,j,N+1,m,i} = (cx)_{n,j+1,1,m,i} \tag{3-116}$$

for $j=1,2,\ldots,j_m-1$; $m=1,2,\ldots,M_m+1$; $i=1,2,\ldots,I_m$; $n=1,2,3,4$.

From equations (3-93) and (3-95) the optimal aeration control equation for layer m, segment k of reach j is the following.

$$\begin{aligned}(U_C)^{(r+1)}_{j,k,m,i} &= (U_C)^{(r)}_{j,k,m,i} \\ &- 2(h_x)_j(h_z)_j h_t(\epsilon_C)_j(W_2)_j(U_C)^{(r)}_{j,k,m,i} \\ &- (\epsilon_C)_j(cx)^{(r)}_{4,j,k,m,i} \Big/ \left[1 + \frac{h_t(K_a)_{j,k,m}}{2}\right]\end{aligned} \tag{3-117}$$

where $j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$

$m=2,3,\ldots,M_m+1$; $i=2,3,\ldots,Im$.

From equations (3-105) and (3-107) the optimal dumping control equation for layer m, segment k of reach j is:

$$(U_L)^{(r+1)}_{j,k,m,i} = (U_L)^{(r)}_{j,k,m,i} - 2(h_x)_j(h_z)_j h_t(\epsilon_L)_j(W_4)_j(U_L)^{(r)}_{j,k,m,i} - (\epsilon_L)_j(cx)^{(r)}_{2,j,k,m,i} \Big/ \left[1 + \frac{h_t(K_r)_{j,k,m}}{2}\right] \qquad (3\text{-}118)$$

The initial and upstream boundary conditions are obtained for dumping control in the regional model by adding the subscript, j, to equations (3-108) through (3-110) for the single reach model. The initial and upstream boundary conditions for aeration control are obtained in a similar fashion from equations (A4-14) through (A4-16).

Since the initial and upstream boundary conditions are given for the optimal control equations, their solution proceeds in the forward direction in space and time. The appropriate interface conditions are:

$$(U_C)_{j,1,m,i} = (U_C)_{j-1,N+1,m,i} \qquad (3\text{-}119)$$

$$(U_L)_{j,1,m,i} = (U_L)_{j-1,N+1,m,i} \qquad (3\text{-}120)$$

$j=2,3,\ldots,j_m$; $m=1,2,\ldots,M_m+1$; $i=1,2,\ldots,I_m$.

Four of the coordination variables are expressed as functions of the state variables by equations (3-5) through (3-8) and equations (3-68) and (3-70), all with subscript, j, added. Since initial and upstream boundary conditions are known for each of the state variables, these equations may be used to obtain corresponding conditions for these four coordination variables, x_n, (n=5,6,7,8). Further, the availability of these conditions implies that the set of coordination equations corresponding to these variables should be solved in the forward direction in the space-time region of interest and the interface conditions for these second level variables should be expressed in the forward direction as was the case for the state variable interface conditions expressed by equations (3-114) and (3-115). The resulting interface conditions are presented in equations (A8-1) through (A8-6) in Appendix 8.

The four remaining coordination equations are functions of the costate variables as expressed by equations (A3-8) through (A3-11) of Appendix 3 with subscript, j, added to each equation. Since downstream boundary and final conditions are known for the costate variables, these equations can be used to determine downstream boundary and final time conditions for these four coordination variables. Further, the availability of these conditions implies solution of the associated coordination equations in the reverse direction in space and time. Hence, the interface conditions also should be expressed in the reverse direction. This means, for example, that conditions at the downstream end of a given reach should be expressed as a function of conditions at the upstream end of the reach which is contiguous to the given reach at its downstream end. The corresponding reverse direction interface conditions are expressed in equations (A8-7) through (A8-10) of Appendix 8.

All of the interface equations may be collected into a regional (multireach) coordination subproblem. The remaining equations of the regional model may be assigned to state, costate, control and coordination subproblems for reach j, $j=1,2,\ldots,j_m$. These subproblems can then be assembled into the three-level hierarchy shown in Figure 2-3. Additional boundary conditions for the subproblems of this hierarchy are presented in Chapter 4.

3.4.2 Regional two-dimensional model with negligible vertical velocity and optimal bimodal control. The equations for the regional two-dimensional model with negligible vertical velocity are the same as those for the general two-dimensional stratified estuary model with bimodal control except for the following distinctions.

1.) The equations defining the coordination variables, $x_{5,j,k,m,i}$ and $x_{6,j,k,m,i}$, are given by equations (3-33) through (3-36) with subscript, j, added.

2.) The equations associated with the costate variables, $(cx)_{2,j,k,m,i}$ and $(cx)_{4,j,k,m,i}$, are reduced to the form of equations (A5-1) through (A5-4) in Appendix 5 with subscript j added in each case.

The equations for this model also may be assembled into the subproblem hierarchy depicted by Figure 2-3.

3.4.3 Regional discrete dynamic tidal river model with optimal bimodal control. The equations representing concentration rate balances in the jth reach of the regional tidal river model may be obtained from the corresponding equations for the single reach model by adding the reach-identifying subscript, j, to them. The scalar components of the vector-matrix generalized state equation for reach j are presented in equations (A9-1) through (A9-8) of Appendix 9.

The upstream end boundary conditions for the state variables are given by equations (A4-4) and (A4-5) with subscript, m, omitted and the initial distributions of the state variables are given by equations (2-157) and (2-158). Accordingly, the interface conditions for the state variables are in the forward direction. More specifically, the state variable interface conditions for the regional tidal river may be obtained from the interface conditions for the two-dimensional models, equations (3-113) through (3-115), by omitting the subscript, m.

The costate equations for the discrete tidal river regional model are given by the corresponding single reach equations, (A6-1) through (A6-6), with the addition of the reach-identifying subscript, j. The downstream end boundary conditions are represented by equation (A4-2) with subscript, m, omitted. The final conditions on the costate variables are given by equation (A4-1) with the subscript, m, omitted. Accordingly, equations (3-116), with subscript,m, omitted, represent the costate interface equations for the tidal river model.

For operation in the aeration control mode equation (3-117) yields the following regional control equation for the tidal river model.

$$(U_C)^{(r+1)}_{j,k,i} = (U_C)^{(r)}_{j,k,i}$$

$$- 2(h_x)_j h_t(\epsilon_C)_j (W_2)_j (U_C)^{(r)}_{j,k,i} - (\epsilon_C)_j (cx)^{(r)}_{4,j,k,i}$$

$$\Big/ \left[1 + \frac{h_t (K_a)_{j,k}}{2}\right] \tag{3-121}$$

$j=1,2,\ldots,j_m$; $k=2,3,\ldots,N+1$; $i=2,3,\ldots,I_m$.

For operation in the waste dumping control mode, the corresponding control equation, derived from equation (3-118) is:

$$(U_L)^{(r+1)}_{j,k,i} = (U_L)^{(r)}_{j,k,i}$$

$$- 2(h_x)_j h_t(\epsilon_L)_j (W_4)_j (U_L)^{(r)}_{j,k,i} - (\epsilon_L)_j (cx)^{(r)}_{2,j,k,i}$$

$$\Big/ \left[1 + \frac{h_t (K_r)_{j,k}}{2}\right] \tag{3-122}$$

The initial conditions and upstream boundary conditions for these equations are given in Chapter 2. The corresponding interface equations are given in equations (2-183) and (2-199).

Four of the coordination variables, $x_{n,j,k,i}$ (n=5,6,7,8), are expressed as functions of the state variables by equations (3-45), (3-49), (3-76) and (3-78) with subscript, j, added. Since initial and upstream end boundary conditions are known for the state variables, the same conditions can be determined for these coordination variables via the cited equations. Hence, the interface conditions involving these variables should be in the forward direction. These conditions are expressed by equations (A10-1) through (A10-6) in Appendix 10.

The remaining coordination equations for the regional tidal river model may be obtained from equations (A3-8) through (A3-11) of Appendix 3 by omitting the subscript, j. Since the coordination variables defined by these equations are expressed as functions of the costate variables, their final and downstream boundary conditions can be determined from those of the costate variables. Accordingly, their interface conditions should be defined in the reverse direction. The resulting interface equations are presented in Appendix 10 as equations (A10-7) through (A10-10).

This chapter began with the use of mass-balance techniques to derive a two-step discrete dynamic distributed parameter model of a general two-dimensional waterway exemplified by a stratified estuary. Three additional two-step discrete water quality models were derived from this general model:

1.) two-dimensional estuary model with negligible vertical velocity,
2.) tidal river model,
3.) tapered stream model.

resulting in discrete dynamic models for a total of four types of waterways.

A combination of multilevel hierarchical systems analysis and Pontryagin's discrete minimum principle was employed to apply optimal aeration control, waste dumping control and both modes of control to each of the four waterway models. This resulted, for each of the twelve combinations of waterway model and optimal control mode, in a hierarchy of subproblems to be solved. Three of the single reach models with both aeration and dumping (bimodal) control were expanded into regional multireach hierarchies of subproblems by aggregation.

In the next chapter, additional boundary conditions required for the solution of the subproblems of the hierarchies developed in both the present chapter and Chapter 2 will be discussed. Consistency, convergence stability and computational efficiency also will be treated in the next chapter.

Later chapters will present sensitivity analyses of models under multilevel optimal control, numerical examples of the application of multilevel control to the models developed in the present and prior chapter and an application of one of the models to a regional economic water quality problem.

CHAPTER 4

BOUNDARY CONDITIONS, CONSISTENCY AND CONVERGENCE, STABILITY AND COMPUTATIONAL EFFICIENCY

In the application of the water quality models presented in Chapters 2 and 3 the following topics are of practical significance. Due to their diversity, separate introductions are provided for each of them within this chapter.

Sufficient boundary conditions are required to generate specific solutions of the subproblems comprising the multilevel hierarchical models presented in Chapters 2 and 3. Some of these conditions have been presented in the cited chapters; the remaining conditions are presented in the first section of the present chapter.

The second major topic of practical significance is the consistency and convergence of the semidiscretized approximations of the continuous distributed parameter water quality models. Satisfaction of the consistency conditions ensures that the set of ordinary differential equations of the semidiscretized model corresponding to each partial differential equation of the original model properly represents that equation. Satisfaction of the convergence conditions ensures that the solutions of the set of discretized equations approaches the solution of the corresponding equation of the original distributed parameter model as the number of sample points along the axis being discretized is increased. Proofs of the satisfaction of these conditions are presented for a representative continuous distributed parameter water quality model in the second section of this chapter.

A third topic of practical importance is the stability of the water quality models presented in Chapters 2 and 3. Stability analyses of representative models of classes of discretized continuous distributed parameter and discrete distributed parameter water quality models are conducted in the third and fourth sections, respectively, of this chapter.

A fourth topic of practical significance is the relationship between the structure of a subproblem hierarchy and the efficiency with which its overall solution may be obtained. This topic is treated in the fifth section of this chapter.

4.1 Boundary Conditions

As stated earlier in this dissertation, boundary, initial and final conditions are required for the generation of specific solutions of the subproblems comprising the hierarchies resulting from the application of multilevel optimal control to various water quality models. Boundary, initial and final condition equations presented for the semidiscretized continuous distributed parameter models in Chapter 2 and the discrete distributed parameter models in Chapter 3 are associated with their respective subproblems in Table 4-1. These conditions are sufficient for determining specific solutions of the subproblems comprising the tapered stream model under unidirectional flow conditions. The principal objective of this section is the generation of additional boundary values to facilitate specific solution of the subproblems of all of the water quality models presented in Chapters 2 and 3. Since the boundary conditions required for the solution of the discrete models of Chapter 3 differ from those of the continuous models of Chapter 2, the sequel is divided accordingly.

4.1.1 Boundary conditions for semidiscretized continuous distributed parameter models. The boundary conditions presented in Table 4-1 are sufficient for the solution of the subproblems of the tapered stream model because each state equation at spatial point, k, includes coupling only from the adjacent upstream point, k-1, and each costate equation at point k involves coupling only from the adjacent downstream point, k+1. Addition of dispersion terms to the stream model in the formation of

	Subproblems		
	State	Costate	Control
Initial Conditions	x	--	x
Upstream Boundary Conditions	x	--	x
Downstream Boundary Conditions	--	x	--
Final Conditions	--	x	--

Table 4-1: Boundary, initial and final condition equations presented for water quality subproblems of Chapters 2 and 3.

the tidal river model introduces bi-directional coupling along the spatial axis, i.e., coupling of the equation at point k with both points k-1 and k+1. This restricts the state equations to determination of concentrations only at internal points with a requirement for a priori evaluation of the concentrations at the upstream end and a means for extrapolating the concentrations at the internal points to obtain the concentrations at the downstream end of the reach of the waterway under study.

An approach to this extrapolation adapted from Okunseinde's dissertation(340) is to assume that the concentration at the point one spatial increment upstream from the downstream end of the reach is the average of the concentration two increments upstream from the downstream end and the concentration at the downstream end. For the BOD concentrations in the one-dimensional semidiscretized water quality models represented by the tidal river and the tapered stream this relationship may be expressed by:

$$L_N = \frac{L_{N-1} + L_{N+1}}{2} \qquad (4-1)$$

where, as before, the reach is divided into N spatial increments yielding a total of N+1 points including both end points. Solving equation (4-1) for L_{N+1} yields:

$$L_{N+1} = 2L_N - L_{N-1} \tag{4-2}$$

The corresponding extrapolation for the DO concentration at the downstream end of the reach is:

$$C_{N+1} = 2C_N - C_{N-1} \tag{4-3}$$

Addition of dispersion terms also introduces bi-directional coupling to the costate equations of the model leading to a requirement for upstream boundary values in addition to the downstream boundary conditions already available. In this instance, each costate variable one spatial increment downstream from the up-stream end of the reach is regarded as the average of its value at the upstream end and its value two spatial increments downstream from the upstream end. The resulting extrapolation equations for the costate variables of the one-dimensional semi-discretized water quality models are:

$$(CL)_1 = 2(CL)_2 - (CL)_3 \tag{4-4}$$

$$(CC)_1 = 2(CC)_2 - (CC)_3 \tag{4-5}$$

The conditions listed in Table 4-1 in conjunction with equations (4-2) through (4-5) are sufficient for determining specific solutions of the subproblem hierarchy of a water quality model in which dispersive effects are included. This follows from the fact that if only internal values of the state, costate and control variables are calculated, only internal values of the coordination variables need be evaluated. Extrapolation schemes involving more internal points could have been applied to this class of models, but the simpler scheme presented here was deemed sufficiently accurate for the present study.

For the fully (spatially and temporally) discretized form of the model the corresponding extrapolation equations are of the same form as those for the semidiscretized model, equations (4-2) through (4-5), except that the temporal subscript, i, is added to each variable in the equations. The extrapolation equations for the regional models are identical with those for the corresponding single reach models except that the reach-identifying subscript, j, is added to each variable and upstream conditions apply only to the upstream end of the reach furthest upstream and downstream conditions apply only to the downstream end of the reach furthest downstream.

4.1.2 Boundary conditions for two-step discrete distributed parameter models. Boundary conditions for the one-dimensional two-step finite-difference tidal river and tapered stream water quality models parallel those for the corresponding semidiscretized continuous distributed parameter models listed in Table 4-1 and equations (4-2) through (4-5). The forms of the boundary conditions differ from those for the semidiscretized models because the two-step discrete models involve twice as many equations and because they are written in the form of scalar components of a vector-matrix state equation.

For the two-step finite-difference models the conditions listed in Table 4-1 and stated specifically in Appendix 4 are sufficient only for determining specific solutions of the subproblems of the tapered stream model. Addition of dispersive effects necessitates utilization of extrapolation equations for evaluating downstream boundary values of the state variables and upstream values of the costate variables. Following are extrapolation equations which can be used in conjunction with the boundary conditions of Appendix 4 to determine specific solutions of subproblems of models with dispersive effects included.

Downstream values of state variables:

$$x_{n,N+1,i} = 2x_{n,N,i} - x_{n,N-1,i} \tag{4-6}$$

for $n=1,2,3,4$; $i=1,2,\ldots,I_m$.

Upstream values of costate variables:

$$(cx)_{n,1,i} = 2(cx)_{n,2,i} - (cx)_{n,3,i} \tag{4-7}$$

for $n=1,2,3,4$; $i=1,2,\ldots,I_m$.

The addition of extrapolation equations (4-6) and (4-7) to the equations of Appendix 4 obviates direct calculation of the values of the state and costate variables at the upstream and downstream boundaries of the reach. Since only values of the coordination variables at points internal to the space-time region of interest are utilized in the evaluation of state and costate variables at internal points, equations (4-6) and (4-7), in conjunction with the boundary, initial and final condition equations of Appendix 4, with subscript, m, omitted, are sufficient for determining specific solutions of the subproblems of models that include dispersive effects.

Upstream and downstream boundary conditions for the two-dimensional two-step discrete stratified estuary and stratified estuary with negligible vertical velocity component water quality models are the same as equations (4-6) and (4-7) with subscript, m, added combined with equations (A4-2), (A4-4) and (A4-5) of Appendix 4. The initial and final conditions are presented in equations (A4-1), (A4-6), (A4-11) and (A4-14). (The initial condition for U_L is the same as that expressed for U_C in equation (A4-14).)

The assumption that no transfer of pollutants occurs across the surface or bottom boundary of the two-dimensional estuary models leads to the following vertical boundary conditions.

1.) The vertical component of velocity is zero at both the surface and the bottom of the estuary.

$$(V_z)_{k,1,i} = (V_z)_{k,M_m+1,i} = 0 \qquad (4\text{-}8)$$

2.) The coefficient of vertical diffusion is zero at both the surface and the bottom.

$$(D_z)_{k,1,i} = (D_z)_{k,M_m+1,i} = 0 \qquad (4\text{-}9)$$

Application of the boundary condition equations of equation (4-8) to the equations defining $x_{5,k,m,i}$ and $x_{6,k,m,i}$ reduces them to the form of equations (3-33) through (3-36) with m=1 for the bottom conditions and $m=M_m+1$ for the surface conditions. Applications of the boundary conditions of equation (4-9) to the equations defining $x_{7,k,m,i}$ and $x_{8,k,m,i}$ reduces them to the following forms.

Bottom boundary conditions:

$$x_{7,k,1,i} = B_{k,1,i}x_{1,k,1,i} + E_{k+\frac{1}{2},1,i}x_{1,k+1,1,i} + E_{k-\frac{1}{2},1,i}x_{1,k-1,1,i} \qquad (4\text{-}10)$$

$$x_{8,k,1,i} = -G_{k,1,i}x_{3,k,1,i} + E_{k+\frac{1}{2},1,i}x_{3,k+1,1,i} + E_{k-\frac{1}{2},1,i}x_{3,k-1,1,i} - h_t(K_d)_{k,1}x_{2,k,1,i} \qquad (4\text{-}11)$$

Surface boundary conditions:

$$x_{7,k,M_m+1,i} = -B_{k,M_m+1,i}x_{1,k,M_m+1,i}$$

$$+ E_{k+\frac{1}{2},M_m+1,i}x_{1,k+1,M_m+1,i}$$

$$+ E_{k-\frac{1}{2},M_m+1,i}x_{1,k-1,M_m+1,i} \qquad (4\text{-}12)$$

$$x_{8,k,M_m+1,i} = -G_{k,M_m+1,i}x_{3,k,M_m+1,i}$$

$$+ E_{k+\frac{1}{2},M_m+1,i}x_{3,k+1,M_m+1,i}$$

$$+ E_{k-\frac{1}{2},M_m+1,i}x_{3,k-1,M_m+1,i}$$

$$- h_t(K_d)_{k,M_m+1}x_{2,k,M_m+1,i} \qquad (4\text{-}13)$$

The surface boundary conditions given by equations (A4-3) for the costate variables of the two-dimensional discrete distributed parameter models may be supplemented by the following extrapolation equations for determining the bottom boundary values of the costate variables.

$$(cx)_{n,k,1,i} - 2(cx)_{n,k,2,i} - (cx)_{n,k,3,i} \qquad (4\text{-}14)$$

The equations of Appendix 4 in conjunction with suitably modified equations (3-33) through (3-36), equations (4-6) and (4-7) with subscript, m, added and equations (4-10) through (4-14) provide sufficient boundary, initial and final conditions for the determination of specific solutions for the subproblems of the two-dimensional discrete distributed parameter water quality models presented in Chapter 3. The boundary, initial and final condition equations for regional models may be developed from the corresponding single reach equations by adding the reach-identifying subscript, j, to each variable and applying upstream boundary conditions to the upstream end of the upstream reach and downstream conditions to the downstream end of the downstream reach.

4.2 Consistency and Convergence of Semidiscretized Approximations of Continuous Distributed Parameter Water Quality Models

When a partial differential equation is approximated by a corresponding set of discretized equations, two important questions arise.

1.) What conditions ensure that the set of discretized equations actually represents the original partial differential equation? This is known as the question of consistency.

2.) What conditions ensure that the solutions of the discretized equations approach the solution of the original equation as discretization increments are reduced, i.e., the number of sample points in the interval being discretized is increased? This is known as the question of convergence.

Since the literature on these considerations with respect to distributed parameter systems appears to be rather sparse, the sequel follows the treatment presented in Wismer[531,532] with adaptations for the types of equations representing BOD and DO rate balances in a stream reach.

For simplicity of presentation, the specific equations treated are those for a modification of O'Conner's model[336] derived from the more general model of Bella and Dobbins[27], for a stream reach model with a single spatial dimension in which both the volume flow rate, Q, and the cross sectional area, A, may vary with spatial location. The methods utilized may be applied to a fairly broad class of partial differential equations including many of those representing BOD and DO concentration rate balances in various waterways.

The principal contributions of this section are the extensions of the methods of Wismer to a class of partial differential equations in which partial differentiation of a product of variables occurs in the right hand side and the spatial increment varies spatially. The need for the first extension is a direct consequence of treating the BOD and DO equations for which the volume flow rate and the cross sectional area may vary spatially. The need for the second extension arises indirectly because the resulting condition on the spatial increment presented by Bella and Dobbins[27] requires that the increment vary spatially.

4.2.1 <u>Original state equations in operator form</u>.

BOD balance:

$$O\left[L(x,t)\right] = \frac{\partial L}{\partial t} + K_r L + \frac{Q}{A}\frac{\partial L}{\partial x} + \frac{L}{A}\frac{dQ}{dx} = u_L \quad (4\text{-}15)$$

DO balance:

$$O'\left[C(x,t),\ L(x,t)\right] = \frac{\partial C}{\partial t} + K_a C + K_d L + \frac{Q}{A}\frac{\partial C}{\partial x}$$

$$+ \frac{C}{A}\frac{dQ}{dx} = u_C + K_s \quad (4\text{-}16)$$

where:

$$K_s = K_r C_s + \overline{P - R} - \bar{B} \quad (4\text{-}17)$$

$$L\big|_{x=0} = L_o \quad (4\text{-}18)$$

$$C\big|_{x=0} = C_o \quad (4\text{-}19)$$

$$L(0,t) = f_1(t) \quad (4\text{-}20)$$

$$C(0,t) = f_2(t) \quad (4\text{-}21)$$

$$C \leq C_s \quad (4\text{-}22)$$

4.2.2 <u>Spatial discretization</u>. Let N = the number of spatial increments into which the axis of the stream reach is divided. Then the number of spatial points, including both endpoints, is N+1 and the spatially discretized variables may be represented as follows.

$$L_k = L(x_k,t) \tag{4-23}$$

$$C_k = C(x_k,t) \tag{4-24}$$

$$Q_k = Q(x_k) \tag{4-25}$$

$$A_k = A(x_k) \tag{4-26}$$

$$(U_L)_k = u_L(x_k,t) \tag{4-27}$$

$$(U_C)_k = u_C(x_k,t) \tag{4-28}$$

The spatial increment terminating at x_k is given by:

$$h_k = x_k - x_{k-1} \tag{4-29}$$

Then the various derivative terms may be discretized as follows.

$$\left.\frac{\partial L}{\partial t}\right|_{x=x_k} = \frac{dL_k}{dt} = \frac{dv_k}{dt} \tag{4-30}$$

$$\left.\frac{\partial C}{\partial t}\right|_{x=x_k} = \frac{dC_k}{dt} = \frac{dw_k}{dt} \tag{4-31}$$

$$\left.\frac{dQ}{dx}\right|_{x=x_k} \approx \frac{1}{h_k}(Q_k - Q_{k-1}) \tag{4-32}$$

$$\left.\frac{\partial L}{\partial x}\right|_{x=x_k} \approx \frac{1}{h_k}(v_k - v_{k-1}) \tag{4-33}$$

$$\left.\frac{\partial C}{\partial x}\right|_{x=x_k} \approx \frac{1}{h_k}(w_k - w_{k-1}) \tag{4-34}$$

The symbol, v_k, represents the solution of the spatially discretized BOD equation at x_k:

$$O_k \left| v(x_k, t) \right| = \frac{dv_k}{dt} + K_r v_k + \frac{Q_k}{A_k h_k}(v_k - v_{k-1}) + \frac{v_k}{A_k h_k}(Q_k - Q_{k-1}) = (U_L)_k \tag{4-35}$$

while w_k represents the solution of the spatially discretized DO equation at x_k:

$$O_k' \left| w(x_k, t),\ v(x_k, t) \right| = \frac{dw_k}{dt} + K_a w_k + K_d v_k + \frac{Q_k}{A_k h_k}(w_k - w_{k-1}) + \frac{w_k}{A_k h_k}(Q_k - Q_{k-1}) = (U_C)_k + K_s \tag{4-36}$$

where:

$$v_k(0) = L_o \tag{4-37}$$

$$w_k(0) = C_o \tag{4-38}$$

$$v_1(t) = f_1(t) \tag{4-39}$$

$$w_1(t) = f_2(t) \tag{4-40}$$

4.2.3 Proof of consistency. The spatially discretized BOD equation is said to be consistent with the original BOD equation if:

$$\lim_{h_k \Rightarrow 0} \left\{ O\left[L(x_k, t)\right] - O_k\left[L(x_k, t)\right] \right\} = 0 \tag{4-41}$$

and the corresponding consistency condition for the DO equation is:

$$\lim_{h_k \Rightarrow 0} \left\{ O' \left[C(x_k,t) \right] - O_k' \left[C(x_k,t) \right] \right\} = 0 \qquad (4\text{-}42)$$

where O, O_k, O' and O_k' are linear operators.

More specifically,

$$O\left[L(x_k,t)\right] = \frac{\partial L}{\partial t}\bigg|_{x=x_k} + K_r L(x_k,t) + \frac{Q(x_k)}{A(x_k)} \frac{\partial L}{\partial x}\bigg|_{x=x_k} + \frac{L(x_k,t)}{A(x_k)} \frac{dQ}{dx}\bigg|_{x=x_k} \qquad (4\text{-}43)$$

$$O_k\left[L(x_k,t)\right] = \frac{dL_k}{dt} + K_r L_k + \frac{Q_k}{A_k h_k}(L_k - L_{k-1}) + \frac{L_k}{A_k h_k}(Q_k - Q_{k-1}) \qquad (4\text{-}44)$$

$$O'\left[C(x_k,t),\ L(x_k,t)\right] = \frac{\partial C}{\partial t}\bigg|_{x=x_k} + K_a C(x_k,t) + K_d L(x_k,t) + \frac{Q(x_k)}{A(x_k)} \frac{\partial C}{\partial x}\bigg|_{x=x_k} + \frac{C(x_k,t)}{A(x_k)} \frac{dQ}{dx}\bigg|_{x=x_k} \qquad (4\text{-}45)$$

$$O_k'\left[C(x_k,t),\ L(x_k,t)\right] = \frac{dC_k}{dt} + K_a C_k + K_d L_k + \frac{Q_k}{A_k h_k}(C_k - C_{k-1}) + \frac{C_k}{A_k h_k}(Q_k - Q_{k-1}) \qquad (4\text{-}46)$$

Employing a Taylor series expansion about $x=x_k$,

$$L_{k-1} = L_k - h_k \left.\frac{\partial L}{\partial x}\right|_{x=x_k} + \frac{h_k^2}{2} \left.\frac{\partial^2 L}{\partial x^2}\right|_{x=x_k} - \frac{h_k^3}{3!} \left.\frac{\partial^3 L}{\partial x^3}\right|_{x=x_k} + \cdots \tag{4-47}$$

$$\left.\frac{\partial L}{\partial x}\right|_{x=x_k} - \frac{1}{h_k}(L_k - L_{k-1}) = \frac{h_k}{2} \left.\frac{\partial^2 L}{\partial x^2}\right|_{x=x^{(1)}} = \tau_k^{(1)} \tag{4-48}$$

where $x^{(1)}$ is a suitable value between x_{k-1} and x_k. (remainder for Taylor's series after two terms).

Similarly,

$$\left.\frac{\partial C}{\partial x}\right|_{x=x_k} - \frac{1}{h_k}(C_k - C_{k-1}) = \frac{h_k}{2} \left.\frac{\partial^2 C}{\partial x^2}\right|_{x=x^{(2)}} = \tau_k^{(2)} \tag{4-49}$$

where $x^{(2)}$ is a suitable value between x_{k-1} and x_k, and:

$$\left.\frac{dQ}{dx}\right|_{x=x_k} - \frac{1}{h_k}(Q_k - Q_{k-1}) = \frac{h_k}{2} \left.\frac{d^2 Q}{dx^2}\right|_{x=x^{(3)}} = \tau_k^{(3)} \tag{4-50}$$

From (4-30),

$$\left.\frac{\partial L}{\partial t}\right|_{x=x_k} - \frac{dL_k}{dt} = 0$$

From (4-31),

$$\left.\frac{\partial C}{\partial t}\right|_{x=x_k} - \frac{dC_k}{dt} = 0$$

Subtracting (4-44) from (4-43) to form the difference between the original BOD equation and the discretized BOD equation yields:

$$O\left[L(x_k,t)\right] - O_k\left[L(x_k,t)\right] = \frac{\partial L}{\partial t}\Big|_{x=x_k} - \frac{dL_k}{dt}$$

$$+ K_r\left[L(x_k,t) - L_k\right] + \frac{Q_k}{A_k}\left[\frac{\partial L}{\partial x}\Big|_{x=x_k} - \frac{1}{h_k}(L_k - L_{k-1})\right]$$

$$+ \frac{L_k}{A_k}\left[\frac{dQ}{dx}\Big|_{x=x_k} - \frac{1}{h_k}(Q_k - Q_{k-1})\right] \qquad (4\text{-}51)$$

Applying (4-30), (4-23), (4-48) and (4-50) to (4-51) yields:

$$O\left[L(x_k,t)\right] - O_k\left[L(x_k,t)\right] = \frac{Q_k}{A_k}\tau_k^{(1)} + \frac{L_k}{A_k}\tau_k^{(3)} \qquad (4\text{-}52)$$

But from (4-48):

$$\tau_k^{(1)} \propto h_k \qquad (4\text{-}53)$$

and from (4-50):

$$\tau_k^{(3)} \propto h_k \qquad (4\text{-}54)$$

With:

$$Q = \max_k\left[Q_k\right] \qquad (4\text{-}55)$$

$$a = \min_k\left[A_k\right] \neq 0 \qquad (4\text{-}56)$$

$$L = \max_k\left[L_k\right] \qquad (4\text{-}57)$$

an upper bound on the difference of (4-52) is:

$$O\left[L(x_k,t)\right] - O_k\left[L(x_k,t)\right] \leq \frac{Q}{a}\tau_k^{(1)} + \frac{L}{a}\tau_k^{(3)} \qquad (4\text{-}58)$$

Now $$\lim_{h_k \Rightarrow 0}\left[\frac{Q}{a}\tau_k^{(1)} + \frac{L}{a}\tau_k^{(3)}\right] = 0 \qquad (4\text{-}59)$$

Therefore (4-41) is proved and thus the spatially discretized BOD equation is consistent with the original BOD equation. The proof of (4-42) is of the same form. Thus, by similar reasoning, the spatially discretized DO equation is consistent with the original DO equation.

4.2.4 Proof of convergence of the solutions of the spatially discretized state equations to the corresponding solutions of the original state equations. The difference between the solution of the spatially discretized BOD equation, v_k, and the solution of the original BOD equation at the kth spatial point, $L(x_k,t)$, is expressed as:

$$(e_1)_k(t) = v_k(t) - L(x_k,t) \tag{4-60}$$

Correspondingly, for the DO state equation,

$$(e_2)_k(t) = w_k(t) - C(x_k,t) \tag{4-61}$$

The objective of this proof is to show that, under the proper conditions,

$$\lim_{h_k \Rightarrow 0} \left|(e_1)_k\right| = 0 \tag{4-62}$$

$$\lim_{h_k \Rightarrow 0} \left|(e_2)_k\right| = 0 \tag{4-63}$$

The proof itself is presented in Appendix 11.

4.3 Stability Analysis of a Class of Discretized Water Quality Models

The main purpose of this section is the presentation of a stability analysis of a set of simultaneous ordinary linear differential equations representing the spatially discretized model of a water quality control problem. In Chapter 2, multilevel hierarchical control techniques were applied to this spatially discretized model.

The contributions of the present section may be enumerated as follows.

1.) The first formulation of a water quality control problem as an optimal tracking control problem appears herein.

2.) This section presents the first application of stability analysis to an optimal water quality control problem in which the performance index is used as the Liapunov function.

3.) The first illustration of the relationship between the Kalman regulator solution and the gradient solution of the optimal water quality control problem appears in this section.

The first step in the overall analysis is the recasting of the equations of the semidiscretized (spatially discretized) model into vector-matrix form. The state equations used and the performance index for the associated optimal control problem appear in Chapter 2.

The use of the performance index functional as a Liapunov function was suggested by the work of Kuo[241] and publications in adaptive control. The recasting of the original problem posed into an optimal tracking control form is a necessary preliminary to using the performance index as a Liapunov function and this approach follows Kirk[222]. This Liapunov function is developed and the proper sign relationship of its first time derivative is demonstrated. This developement is then illustrated with an example of the case in which the stream reach is subdivided into three spatial increments producing two internal points.

Next, the effects of decomposition upon the stability of the system are evaluated. This is accomplished by dividing the coefficient matrix of the vector-matrix model into its diagonal and off-diagonal portions.

The stability analysis up to this point has assumed a Kalman regulator solution to the optimal water quality control problem. In the sequel, the stability analysis is extended to systems involving a gradient controller.

The fully discretized, (both spatially and temporally), water quality model is introduced to facilitate later analysis of the effect on stability of distinct transport lags due to decomposition. To this end the finite-difference equations of the fully discretized model are written in vector-matrix form, and, following the approach of Freeman[145], transformed into the z-domain. Stability of the fully discretized model is first evaluated without lags in the z-domain. Then the lags due to decomposition are introduced and the stability analysis is repeated in the z-domain.

4.3.1 Spatially discretized tapered stream model state equations in vector-matrix form. The state equations of the spatially discretized continuous distributed parameter tapered stream model, equations (2-54) and (2-56) through (2-59), with an aeration control term added to the DO rate balance, can be written in the following vector-matrix form.

$$\begin{bmatrix} \dot{\underline{L}} \\ \dot{\underline{C}} \end{bmatrix} = \begin{bmatrix} A_L & 0 \\ -F & A_C \end{bmatrix} \begin{bmatrix} \underline{L} \\ \underline{C} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{I} \end{bmatrix} \begin{bmatrix} 0 \\ \underline{U}_C \end{bmatrix} + \underline{K} \tag{4-64}$$

where:

$$\underline{L} = (L_2, L_3, \ldots, L_{N+1})^T \tag{4-65}$$

$$\underline{C} = (C_2, C_3, \ldots, C_{N+1})^T \tag{4-66}$$

$$\mathbf{I} = \begin{bmatrix} 1 & & & 0 \\ & & 1 & \\ & 0 & & \\ & & & 1 \end{bmatrix} \tag{4-67}$$

$$F = K_d \mathbf{I} \tag{4-68}$$

$$A_L = \begin{bmatrix} -B_2 & & & 0 \\ E_3 & -B_3 & & \\ & 0 & & \\ & & E_{N+1} & -B_{N+1} \end{bmatrix} \tag{4-69}$$

$$A_C = \begin{bmatrix} -G_2 & & & 0 \\ E_3 & -G_3 & & \\ & 0 & & \\ & & E_{N+1} & -G_{N+1} \end{bmatrix} \tag{4-70}$$

$$\underline{U}_C = \left[(U_C)_2, (U_C)_3, \ldots, (U_C)_{N+1}\right]^T \tag{4-71}$$

$$\underline{K} = (\underbrace{L_a, L_a, \ldots, L_a}_{N \text{ terms}}, \underbrace{K_s, K_s, \ldots, K_s}_{N \text{ terms}})^T \tag{4-72}$$

Equation (4-64) may be written more compactly as:

$$\dot{\underline{x}} = A\underline{x} + B\underline{u} \tag{4-73}$$

where the scalar components of $\underline{x}$ are expressed in terms of the scalar components of $\underline{L}$ and $\underline{C}$ as presented in Appendix 12 and:

$$A = \begin{bmatrix} A_L & 0 \\ -F & A_C \end{bmatrix} \tag{4-74}$$

$$B = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{I} \end{bmatrix} \tag{4-75}$$

$$\underline{u} = \Big[\underbrace{0,0,\ldots,0}_{N},(U_C)_2,(U_C)_3,\ldots,(U_C)_{N+1}\Big]^T \tag{4-76}$$

4.3.2 Linear tracking problem formulation. The spatially discretized optimal control problem for a tapered stream model is in the form of a linear tracking problem as described in Kirk(222). In the notation of the linear tracking problem, the spatially discretized performance index of equations (2-73) and (2-74) may be written as follows.

$$J = \tfrac{1}{2}\int_{t_o}^{t_f} \left\{ \left[\underline{x}_e, Q\underline{x}_e\right] + \left[\underline{U}_C, R\underline{U}_C\right] \right\} dt \tag{4-77}$$

where:

$$Q = 2\begin{bmatrix} 0 & 0 \\ 0 & \mathbf{I} \end{bmatrix} \tag{4-78}$$

$$R = 2W_2\mathbf{I} \quad (4\text{-}79)$$

$$\underline{x}_e = \underline{x} - \underline{x}_{sp} \quad (4\text{-}80)$$

$$\underline{x}_{sp} = \Big[\underbrace{0,0,\ldots,0}_{N},(x_{sp})_{N+2},(x_{sp})_{N+3},\ldots,(x_{sp})_{2N+2}\Big]^T \quad (4\text{-}81)$$

The vector of specified concentrations of DO may be written as,

$$\underline{C}_{sp} = \Big[(C_{sp})_1,(C_{sp})_2,\ldots,(C_{sp})_{N+1}\Big]^T \quad (4\text{-}82)$$

where the scalar components of $\underline{x}_{sp}$ are related to the scalar components of $\underline{C}_{sp}$ as the scalar components of $\underline{x}$ are related to the scalar components of $\underline{C}$ in Appendix 12.

Costate equations

$$\dot{\underline{p}}^* = -Q\underline{x}^* - A^T\underline{p}^* + Q\underline{x}_{sp} \quad (4\text{-}83)$$

where:

$$-A^T = \begin{bmatrix} -A_L^T & F \\ 0 & -A_C^T \end{bmatrix} \quad (4\text{-}84)$$

and the asterisk superscript denotes the optimal value of the variable

From Kirk(222), the optimal control vector for this linear tracking problem may be expressed as:

$$\underline{U}_C^* = -R^{-1}B^T\underline{p}^* \quad (4\text{-}85)$$

where:

$$\underline{p}^* = K\underline{x}^* + \underline{s} \tag{4-86}$$

Hence,

$$\underline{U}_C^* = - R^{-1}B^T(K\underline{x}^* + \underline{s}) \tag{4-87}$$

where the symmetric matrix, K, may be determined from the following Riccati equation:

$$\dot{K} = -KA - A^TK - Q - \frac{KBB^TK}{2W_2} \tag{4-88}$$

and $\underline{s}$, a vector of dimension 2N, may be obtained from:

$$\dot{\underline{s}} = - (A^T - \frac{KBB^T}{2W_2})\underline{s} + Q\underline{x}_{sp} \tag{4-89}$$

The optimal value of the performance index, J, is therefore given by:

$$J^o = \frac{1}{2}\int_{t_o}^{t_f} \left\{ \left[\underline{x}_e, Q\underline{x}_e\right] + \left[R^{-1}B^T(K\underline{x} + \underline{s}), B^T(K\underline{x} + \underline{s})\right] \right\} dt \tag{4-90}$$

But

$$\left[\underline{x}, A\underline{x}\right] = \left[A^T\underline{x}, \underline{x}\right] \tag{4-91}$$

Therefore,

$$\left[R^{-1}B^T(K\underline{x} + \underline{s}), B^T(K\underline{x} + \underline{s})\right] = \left[(K\underline{x} + \underline{s}), B(R^{-1})^TB^T(K\underline{x} + \underline{s})\right] \tag{4-92}$$

Substitution of (4-92) in (4-90) yields:

$$J^o = \frac{1}{2}\int_{t_o}^{t_f} \Big\{ \big[\underline{x}_e, Q\underline{x}_e \big]$$

$$+ \big[(K\underline{x} + \underline{s}), B(R^{-1})^T B^T (K\underline{x} + \underline{s}) \big] \Big\} \, dt \qquad (4\text{-}93)$$

which is positive definite in terms of $\underline{x}_e$ and $(K\underline{x} + \underline{s}) = \underline{p}^*$.

4.3.3 Use of performance index as Liapunov function. This last result suggests the use of J^o as a Liapunov function for the stated linear tracking problem. Accordingly, following Kuo(241), one may write:

$$V = \frac{1}{2}\int_{t}^{T} \Big\{ \big[\underline{x}_e, Q\underline{x}_e \big]$$

$$+ \big[(K\underline{x} + \underline{s}), B(R^{-1})^T B^T (K\underline{x} + \underline{s}) \big] \Big\} \, dt \qquad (4\text{-}94)$$

as the Liapunov function for this problem.

Then

$$\dot{V} = \frac{1}{2}\frac{d}{dt}\int_{t}^{T} \Big\{ \big[\underline{x}_e, Q\underline{x}_e \big]$$

$$+ \big[(K\underline{x} + \underline{s}), B(R^{-1})^T B^T (K\underline{x} + \underline{s}) \big] \Big\} \, dt \qquad (4\text{-}95)$$

By the Fundamental Theorem of integral calculus,

$$\frac{d}{dt}\int_{t}^{T} f(\cdot)dt = -\frac{d}{dt}\int_{t}^{T} f(\cdot)dt = -f(\cdot) \qquad (4\text{-}96)$$

Application of (4-96) to (4-95) yields:

$$\dot{V} = -\tfrac{1}{2}\left\{\left[\underline{x}_e, Q\underline{x}_e\right] + \left[(K\underline{x} + \underline{s}), B(R^{-1})^T B^T (K\underline{x} + \underline{s})\right]\right\} \qquad (4\text{-}97)$$

which is clearly negative definite.

Since a Liapunov function with a negative definite first derivative with respect to time has been found for the linear tracking control problem, the system,

$$\dot{\underline{x}} = A\underline{x} + B\underline{u} \qquad (4\text{-}73)$$

optimized with respect to performance index,

$$J = \tfrac{1}{2}\int_{t_o}^{t_f} \left\{\left[\underline{x}_e, Q\underline{x}_e\right] + \left[\underline{U}_C, R\underline{U}_C\right]\right\} dt \qquad (4\text{-}77)$$

is asymptotically stable in the large provided R^{-1} exists and is positive definite which implies, from (4-79), $W_2 > 0$. From Appendix 12 it is evident that each scalar component of $\underline{L}$ and of $\underline{C}$ differs from the corresponding scalar component of $\underline{x}$ by an additive term. Hence, the asymptotic stability in the large of the system described by equation (4-73) implies the asymptotic stability of the system described by equation (4-64) provided $B_k \neq 0$ for $k=2,3,\ldots,N+1$.

4.3.4 Stability analysis of decomposed system. Under decomposition the spatially discretized system of equation

(4-72) may be expressed as follows.

$$\dot{\underline{x}} = \bar{A}\underline{x} + B\underline{u} + \tilde{A}\underline{x} \tag{4-98}$$

where the scalar components of $\underline{x}$ are defined in terms of the scalar components of $\underline{L}$ and $\underline{C}$ in Appendix 12 and $\underline{u}$ is defined by equation (4-76). Also,

$$\bar{A} = \begin{bmatrix} \bar{A}_L & 0 \\ 0 & \bar{A}_C \end{bmatrix} \tag{4-99}$$

$$\tilde{A} = \begin{bmatrix} \tilde{A}_L & 0 \\ 0 & \tilde{A}_C \end{bmatrix} \tag{4-100}$$

$$\bar{A}_L = \text{diag}\ (-B_2, -B_3, \ldots, -B_{N+1}) \tag{4-101}$$

$$\bar{A}_C = \text{diag}\ (-G_2, -G_3, \ldots, -G_{N+1}) \tag{4-102}$$

$$F = K_d \mathbf{I} \tag{4-68}$$

$$B = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{I} \end{bmatrix} \tag{4-103}$$

$$\tilde{A}_L = \begin{bmatrix} 0 & & & & 0 \\ E_3 & 0 & & & \\ & \ddots & \ddots & & \\ & 0 & & \ddots & \\ & & & E_{N+1} & 0 \end{bmatrix} = \tilde{A}_C \tag{4-104}$$

The performance index for this control problem under decomposition is of the same form as it is without decomposition. Accordingly, the optimal control vector can be determined by employing equations (4-85) through (4-89) with $\underline{x}_{sp}$ defined by equation (4-81) and

$$A = \bar{A} + \tilde{A} \tag{4-105}$$

Further, the development and application of the Liapunov function for this decomposed system parallels that for the corresponding system without decomposition in equations (4-94) through (4-97). Thus, the decomposed system expressed by equation (4-98) optimized with respect to the performance index given by equation (4-77) is asymptotically stable in the large provided $W_2 > 0$.

4.3.5 Extension to gradient control. The above derived results may be extended to gradient control as follows. For gradient control:

$$\underline{U}_C^{(n+1)} = \underline{U}_C^{(n)} - \epsilon_C \underline{GRC}^{(n)} \tag{4-106}$$

where:

$$\underline{GRC}^{(n)} = 2W_2(\underline{U}_C)^{(n)} + \underline{p}_2^{(n)} \tag{4-107}$$

$$\underline{p} = (\underline{p}_1, \underline{p}_2)^T \tag{4-108}$$

$$\underline{p}_1 = (p_1, p_2, \ldots, p_N)^T$$

$$\underline{p}_2 = (p_{N+2}, p_{N+3}, \ldots, p_{2N+1})^T \tag{4-109}$$

$\epsilon > 0$

and the superscripts denote the number of the iteration.

Now for

$$= \frac{1}{2W_2}\ , \quad \underline{U}_C^{(n+1)} = -\frac{1}{2W_2}\,\underline{p}_2^{(n)} = \underline{U}_C^* \qquad (4\text{-}110)$$

Hence, all of the stability results obtained for the linear tracking problem apply for gradient control when

$\epsilon = \frac{1}{2W_2}$.

If, for values of $\epsilon \neq \frac{1}{2W_2}$, one can show that $\underline{p}^*$ may be expressed in the form,

$$\underline{p}^* = K\underline{x}^* + \underline{s} \qquad (4\text{-}86)$$

where K is a 2N x 2N symmetric matrix that may be obtained from a Riccati equation and $\underline{s}$ may be obtained from another such equation, then the above stability analysis holds for those values of ϵ for which this condition is satisfied.

4.3.6 Fully discretized tapered stream model. Temporal discretization yields the following set of state equations for the tapered stream model described at the beginning of Section 4.3.1.

BOD

$$L_{k,i+1} = \hat{B}_k L_{k,i} + \hat{E}_k L_{k-1,i} + L_a \qquad (4\text{-}111)$$

where:

$$\hat{B}_k = \left[1 - h_t\left(\frac{K_r}{2} + \frac{2Q_k}{A_k h_k} - \frac{Q_{k-1}}{A_k h_k}\right)\right] \Big/ \left(1 + \frac{h_t K_r}{2}\right) \tag{4-112}$$

$$\hat{E}_k = \frac{h_t Q_k}{A_k h_k\left(1 + \frac{h_t K_r}{2}\right)} \tag{4-113}$$

$k=2,3,\ldots,N+1$; $i=1,2,\ldots,I_m$.

DO

$$C_{k,i+1} = \hat{G}_k C_{k,i} + \hat{F}_k C_{k-1,i} + M_k I_{k,i} + \frac{h_t K_s}{\left(1 + \frac{h_t K_a}{2}\right)} + \frac{h_t (U_C)_{k,i}}{\left(1 + \frac{h_t K_a}{2}\right)} \tag{4-114}$$

where:

$$\hat{G}_k = \left[1 - h_t\left(\frac{K_a}{2} + \frac{2Q_k}{A_k h_k} - \frac{Q_{k-1}}{A_k h_k}\right)\right] \Big/ \left(1 + \frac{h_t K_a}{2}\right) \tag{4-115}$$

$$\hat{F}_k = \frac{h_t Q_k}{A_k h_k\left(1 + \frac{h_t K_a}{2}\right)} \tag{4-116}$$

$$M_k = \frac{h_t K_d}{\left(1 + \frac{h_t K_a}{2}\right)} \tag{4-117}$$

Performance Index

$$J = \sum_{k=2}^{N} \sum_{i=1}^{i_m-1} \left[(C_{k,i} - C_{sp})^2 + W_2 (U_C)^2_{k,i}\right] h_t h_k \tag{4-118}$$

The state equations of the fully discretized tapered stream model may be written in vector-matrix form as follows.

$$\begin{bmatrix} \underline{L}_{i+1} \\ \underline{C}_{i+1} \end{bmatrix} = \begin{bmatrix} E & 0 \\ M & G \end{bmatrix} \begin{bmatrix} \underline{L}_i \\ \underline{C}_i \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & B_C \end{bmatrix} \begin{bmatrix} 0 \\ (\underline{U}_C)_i \end{bmatrix} + \underline{\hat{K}} \tag{4-119}$$

where:

$$\underline{L} = (L_2, L_3, \ldots, L_{N+1})^T \tag{4-65}$$

$$\underline{C} = (C_2, C_3, \ldots, C_{N+1})^T \tag{4-66}$$

$$\underline{U}_C = \left[(U_C)_2, (U_C)_3, \ldots, (U_C)_{N+1}\right]^T \tag{4-71}$$

$$\underline{\hat{K}} = (\hat{L}_a, \hat{L}_a, \ldots, \hat{L}_a, \hat{K}_s, \hat{K}_s, \ldots, \hat{K}_s)^T \tag{4-120}$$

$$\hat{L}_a = \frac{h_t L_a}{1 + \frac{h_t K_r}{2}} \tag{4-121}$$

$$\hat{K}_s = \frac{h_t K_s}{1 + \frac{h_t K_a}{2}} \tag{4-122}$$

$$E = \frac{h_t}{1 + \frac{h_t K_r}{2}} A_L \tag{4-123}$$

$$G = \frac{h_t}{1 + \frac{h_t K_a}{2}} A_C \tag{4-124}$$

$$M = \frac{-h_t K_d}{1 + \frac{h_t K_a}{2}} \mathbf{I} \tag{4-125}$$

$$B_C = \frac{h_t}{1 + \frac{h_t K_a}{2}} \mathbf{I} \qquad (4\text{-}126)$$

These state equations may be written more compactly in the form,

$$\underline{x}_{i+1} = A\underline{x}_i + B\underline{u}_i \qquad (4\text{-}127)$$

by using an approach similar to the one presented in Appendix 12 for expressing the scalar compents of $\underline{x}$ in terms of the scalar components of $\underline{L}$ and $\underline{C}$, equation (4-75) and the following relationships

$$A = \begin{bmatrix} E & O \\ M & G \end{bmatrix} \qquad (4\text{-}128)$$

$$B = \begin{bmatrix} O & O \\ O & B_C \end{bmatrix} \qquad (4\text{-}129)$$

4.3.7 <u>Application of z-transform</u>. Since the above equations represent a stationary system, many standard methods of stability analysis may be applied to them. The z-transform approach is chosen here in order to facilitate later analysis involving transport lags.

Taking the z-transform of the state equations without control yields:

$$z\underline{X}(z) - \underline{x}(o) \quad - A\underline{X}(z) = 0 \tag{4-130}$$

The characteristic equation in the z-domain is given by:

$$\left| z\mathbf{I} - A \right| = \begin{vmatrix} z\mathbf{I} - E & 0 \\ -M & z\mathbf{I} - G \end{vmatrix} = \left| z\mathbf{I} - E \right| \left| z\mathbf{I} - G \right|$$

$$= \begin{vmatrix} z-B_2 & & & 0 & \\ -E_3 & z-B_3 & & & \\ & \ddots & \ddots & & \\ & 0 & & \ddots & \\ & & & -E_{N+1} & z-B_{N+1} \end{vmatrix} \begin{vmatrix} z-G_2 & & & 0 & \\ -F_3 & z-G_3 & & & \\ & \ddots & \ddots & & \\ & 0 & & \ddots & \\ & & & -F_{N+1} & z-G_{N+1} \end{vmatrix}$$

$$= \prod_{k=2}^{N+1} (z - B_k)(z - G_k) = 0 \tag{4-131}$$

If $\left|B_k\right| < 1$ and $\left|G_k\right| < 1$ K, all of the roots of the characteristic equation in the z-domain have magnitudes < 1 and the system described by equation (4-127) is stable for bounded control terms, $\underline{u}_i$, according to the modified Schur-Cohn criterion presented in Freeman[145].

Since from (4-112)

$$B_k < \frac{1 - \frac{h_t K_r}{2}}{1 + \frac{h_t K_r}{2}} \qquad (4\text{-}132)$$

$|B_k| < 1$ for:

$$h_t K_r > 0 \qquad (4\text{-}133)$$

$$h_t\left(\frac{K_r}{2} + \frac{Q}{Ah}\right) < 1 \qquad (4\text{-}134)$$

where:

$$\frac{Q}{Ah} = \max_k \left(\frac{2Q_k - Q_{k-1}}{A_k h_k}\right) \qquad (4\text{-}135)$$

$$0 < h_t < \frac{1}{\frac{K_r}{2} + \frac{Q}{Ah}} \qquad (4\text{-}136)$$

Similarly, $|G_k| < 1$ (4-137)

for

$$0 < h_t < \frac{1}{\frac{K_a}{2} + \frac{Q}{Ah}} \qquad (4\text{-}138)$$

where $\frac{Q}{Ah}$ is defined above.

Since decomposition suppresses the off-diagonal terms in the system's coefficient matrix,

$$A = \begin{bmatrix} E & O \\ M & G \end{bmatrix},$$

it could associate distinct transport lags with each element of A except those on the principal diagonal of A. However, from the expansion of $|z\mathbf{I} - A|$ that leads to the characteristic z-domain equation in (4-130) it is evident that only the elements of the principal diagonal appear in the characteristic equation. Hence, the stability of the system is not affected by transport lags due to decomposition. The stability of the system described by equation (4-127) implies the stability of the system described by equations (4-119) through (4-126).

4.4 Stability Analysis of a Finite-difference Water Quality Model

The overall objective of this section is the presentation of a stability analysis of two-step discrete distributed parameter water quality models to which multilevel hierarchical control techniques were applied in Chapter 3.

The contributions of this section include the following.

1.) This section presents the first application of stability analysis to a finite-difference distributed parameter water quality model for which no continuous time analog exists.

2.) Included in this section is the first application to a nonstationary environmental model of stability analysis by transformation to the equivalent stationary system.

3.) Also in this presentation is the first application of the z-transform to a vector-matrix form of a set of simultaneous finite-difference equations in which each state variable is subjected to a distinct transport lag.

The first step in the overall analysis is the expression of the finite-difference equations of the water quality model in vector-matrix form. Matrix partitioning is introduced to facilitate later analysis. The nonstationarity of the model motivates the transformation to an equivalent stationary model. The z-transformation is applied to the stationary system to facilitate stability analysis.

4.4.1 Two-step discrete tidal river model in vector-matrix form. The state equations of the discrete distributed parameter tidal river model presented in Chapter 3 can be written in the following vector-matrix form for net flow positive downstream. Applying the approach of Appendix 12 to equations (3-33), (3-35) and

(3-45) through (3-51) yields:

$$\begin{bmatrix} \hat{\underline{x}}_{1,i+1} \\ \hat{\underline{x}}_{2,i+1} \\ \hat{\underline{x}}_{3,i+1} \\ \hat{\underline{x}}_{4,i+1} \end{bmatrix} = \begin{bmatrix} 0 & K_1 & 0 & 0 \\ K_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & K_1 \\ 0 & K_4 & K_3 & 0 \end{bmatrix} \begin{bmatrix} \hat{\underline{x}}_{1,i} \\ \hat{\underline{x}}_{2,i} \\ \hat{\underline{x}}_{3,i} \\ \hat{\underline{x}}_{4,i} \end{bmatrix} \tag{4-139}$$

where:

$$\hat{\underline{x}}_{n,i} = (\hat{x}_{n,2,i}, \hat{x}_{n,3,i}, \ldots, \hat{x}_{n,N+1,i})^T \tag{4-140}$$

$n=1,2,3,4;\quad i=1,2,\ldots,I_m-1.$

$$K_1 = \begin{bmatrix} 1 - \frac{h_t Q_{2\frac{1}{2},i}}{A_2 h_x} & & & 0 \\ \frac{h_t Q_{2\frac{1}{2},i}}{A_3 h_x} & 1 - \frac{h_t Q_{3\frac{1}{2},i}}{A_3 h_x} & & \\ & \ddots & \ddots & \\ 0 & & \frac{h_t Q_{N+\frac{1}{2},i}}{A_{N+1} h_x} & 1 - \frac{h_t Q_{N+1\frac{1}{2},i}}{A_{N+1} h_x} \end{bmatrix} \tag{4-141}$$

$$K_2 = \frac{1}{1 + \frac{h_t K_r}{2}} \begin{bmatrix} -B_{2,i} & \frac{h_t (DA)_{2\frac{1}{2},i}}{A_2 h_x^2} & & & 0 \\ \frac{h_t (DA)_{2\frac{1}{2},i}}{A_3 h_x^2} & -B_{3,i} & \ddots & & \\ & \ddots & \ddots & & \frac{h_t (DA)_{N+\frac{1}{2},i}}{A_N h_x^2} \\ 0 & & & \frac{h_t (DA)_{N+\frac{1}{2},i}}{A_{N+1} h_x^2} & -B_{N+1,i} \end{bmatrix} \qquad (4\text{-}142)$$

where:

$$B_{k,i} = \frac{h_t (K_r)}{2} + \frac{h_t}{A_k h_x^2} \quad (DA)_{k+\frac{1}{2},i} + (DA)_{k-\frac{1}{2},i} \quad - 1 \qquad (4\text{-}143)$$

for $k=2,3,\ldots,N+1$ and $(K_r)_2 = (K_r)_3 = \ldots = (K_r)_{N+1}$

$$K_3 = \frac{1}{1 + \frac{h_t K_a}{2}} \begin{bmatrix} -G_{2,i} & \frac{h_t (DA)_{2\frac{1}{2},i}}{A_2 h_x^2} & & & 0 \\ \frac{h_t (DA)_{2\frac{1}{2},i}}{A_3 h_x^2} & -G_{3,i} & \ddots & & \\ & \ddots & \ddots & & \frac{h_t (DA)_{N+\frac{1}{2},i}}{A_N h_x^2} \\ 0 & & & \frac{h_t (DA)_{N+\frac{1}{2},i}}{A_{N+1} h_x^2} & -G_{N+1,i} \end{bmatrix} \qquad (4\text{-}144)$$

for $(K_a)_2 = (K_a)_3 = \ldots = (K_a)_{N+1}$

$$K_4 = \frac{-(K_d)}{1 + \frac{h_t(K_a)}{2}} \mathbf{I} \tag{4-145}$$

for $(K_d)_2 = (K_d)_3 = \ldots = (K_d)_{N+1}$

$$G_{k,i} = \frac{h_t K_a}{2} + \frac{h_t}{A_k h_x^2} \left[(DA)_{k+\frac{1}{2},i} + (DA)_{k-\frac{1}{2},i}\right] - 1 \tag{4-146}$$

for $k=2,3,\ldots,N+1$ and $(K_a)_2 = (K_a)_3 = \ldots = (K_a)_{N+1}$

For net flow positive upstream the discrete tidal river model state equations are equations (3-34), (3-36) and (3-45) through (3-51). These may be expressed in the vector-matrix form of equation (4-139) with corresponding changes in the submatrices K_1, K_2 and K_3 to account for the upstream direction of the net flow. Due to the parallelism in structure of matrices K_1, K_2 and K_3 for the downstream flow and upstream flow cases, the balance of this section will treat only the downstream flow case. The same approach also would apply for net flow upstream. For

$$\underline{\hat{x}} = (\underline{\hat{x}}_1, \underline{\hat{x}}_2, \underline{\hat{x}}_3, \underline{\hat{x}}_4)^T \tag{4-147}$$

and

$$A(i) = \begin{bmatrix} 0 & K_1 & 0 & 0 \\ K_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & K_1 \\ 0 & K_4 & K_3 & 0 \end{bmatrix} \qquad (4-148)$$

the state equations of (4-136) may be represented more compactly as follows.

$$\hat{\underline{x}}_{i+1} = A(i)\hat{\underline{x}}_i \qquad (4-149)$$

4.4.2 Discrete vector-matrix tidal river model with optimal control. Addition of control terms to the vector-matrix form of the tidal river state equations of (4-149) yields the following equation.

$$\hat{\underline{x}}_{i+1} = A(i)\hat{\underline{x}}_i + B\underline{u}_i \qquad (4-150)$$

where $\hat{\underline{x}}_i$ and $A(i)$ are defined above and

$$\underline{u}_i = \left[(U_L)_i, (U_C)_i\right]^T \qquad (4-151)$$

$$\underline{U}_L = \left[(U_L)_2,\ (U_L)_3, \ldots, (U_L)_{N+1}\right]^T \qquad (4-152)$$

$$\underline{U}_C = \left[(U_C)_2,\ (U_C)_3, \ldots, (U_C)_{N+1}\right]^T \qquad (4-153)$$

$$B = \begin{bmatrix} B_L & 0 \\ 0 & B_C \end{bmatrix} \qquad (4-154)$$

$$B_L = \frac{h_t}{1 + \frac{h_t(K_r)}{2}} \mathbf{I} \qquad (4-155)$$

$$B_C = \frac{h_t}{1 + \frac{h_t(K_a)}{2}} \mathbf{I} \tag{4-156}$$

4.4.3 <u>Transformation to stationary system</u>. Both the finite-difference model without control, (4-148), and the finite-difference model with control, (4-149), contain time-varying coefficient matrices. To facilitate stability analysis of these TVP systems a matrix transformation of the form,

$$\tilde{A} = S_{i+1} A(i) S_i^{-1} \tag{4-157}$$

is sought such that $\tilde{A}$ is time-independent using methods presented in Freeman[145].

Based upon the form of the partitioned coefficient matrix of (4-148) the following partitioned matrix is proposed for S_i.

$$S_i = \begin{bmatrix} 0 & s_{1,i} & 0 & 0 \\ s_{3,i} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{2,i} \\ 0 & s_{5,i} & s_{4,i} & 0 \end{bmatrix} \tag{4-158}$$

where:

$$s_{j,i} = \begin{bmatrix} s_{j,2,2,i} & s_{j,2,3,i} & \cdots & s_{j,2,N+1,i} \\ s_{j,3,2,i} & & & \vdots \\ \vdots & & & \vdots \\ s_{j,N+1,2,i} & \cdots & \cdots & s_{j,N+1,N+1,i} \end{bmatrix} \quad (4\text{-}159)$$

j=1,2,3,4,5

By using standard inversion techniques for partitioned matrices, one can show that:

$$S_i^{-1} = \begin{bmatrix} 0 & s_{3,i}^{-1} & 0 & 0 \\ s_{1,i}^{-1} & 0 & 0 & 0 \\ -s_{4,i}^{-1}\, s_{5,i}\, s_{1,i}^{-1} & 0 & 0 & s_{4,i}^{-1} \\ 0 & 0 & s_{2,i}^{-1} & 0 \end{bmatrix}$$

Further, (4-160)

$$A(i)S_i^{-1} = \begin{bmatrix} K_1 s_{1,i}^{-1} & 0 & 0 & 0 \\ 0 & K_2 s_{3,i}^{-1} & 0 & 0 \\ 0 & 0 & K_1 s_{2,i}^{-1} & 0 \\ (K_4 - K_3 s_{4,i}^{-1} s_{5,i}) s_{1,i}^{-1} & 0 & 0 & K_3 s_{4,i}^{-1} \end{bmatrix}$$

(4-161)

and $S_{i+1}A(i)S_i^{-1}$ =

$$\begin{bmatrix} 0 & s_{1,i+1}K_2 s_{3,i}^{-1} & 0 & 0 \\ s_{3,i+1}K_1 s_{1,i}^{-1} & 0 & 0 & 0 \\ s_{2,i+1}(K_4 - K_3 s_{4,i}^{-1} s_{5,i}) s_{1,i}^{-1} & 0 & 0 & s_{2,i+1}K_3 s_{4,i}^{-1} \\ 0 & s_{5,i+1}K_2 s_{3,i}^{-1} & s_{4,i+1}K_1 s_{2,i}^{-1} & 0 \end{bmatrix} \tag{4-162}$$

If it is now assumed that $\tilde{A}$ is a constant matrix of the form,

$$\tilde{A} = \begin{bmatrix} 0 & \rho_1 & 0 & 0 \\ \rho_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_2 \\ 0 & \rho_5 & \rho_4 & 0 \end{bmatrix} \tag{4-163}$$

where ρ_1, ρ_2, ρ_3, ρ_4 and ρ_5 are time-invariant sub-matrices of appropriate dimension, the following matrix equations result from:

$$\tilde{A} = S_{i+1}A(i)S_i^{-1} \tag{4-164}$$

$$s_{1,i+1}K_2 s_{3,i}^{-1} = \rho_1 \quad \Rightarrow \quad s_{1,i+1} = \rho_1 s_{3,i} K_2^{-1} \tag{4-165}$$

$$s_{2,i+1}K_3 s_{4,i}^{-1} = \rho_2 \quad \Rightarrow \quad s_{2,i+1} = \rho_2 s_{4,i} K_3^{-1} \tag{4-166}$$

$$s_{3,i+1}K_1 s_{1,i}^{-1} = \rho_3 \Rightarrow s_{3,i+1} = \rho_3 s_{1,i}K_1^{-1} \quad (4\text{-}167)$$

$$s_{4,i+1}K_1 s_{2,i}^{-1} = \rho_4 \Rightarrow s_{4,i+1} = \rho_4 s_{2,i}K_1^{-1} \quad (4\text{-}168)$$

$$s_{5,i+1}K_2 s_{3,i}^{-1} = \rho_5 \Rightarrow s_{5,i+1} = \rho_5 s_{3,i}K_2^{-1} \quad (4\text{-}169)$$

$$s_{2,i+1}(K_4 - K_3 s_{4,i}^{-1} s_{5,i})s_{1,i}^{-1} = 0 \Rightarrow K_3 s_{4,i}^{-1} s_{5,i} = K_4$$

$$\Rightarrow s_{5,i} = s_{4,i}K_3^{-1}K_4 \quad (4\text{-}170)$$

4.4.4 Submatrix nonsingularity conditions. Inspection of equations (4-164) through (4-170) reveals that their utility depends upon the nonsingularity of matrices K_1, K_2 and K_3, i.e., Det $K_j \neq 0$ for j=1,2,3. From equation (4-141),

$$\text{Det } K_1 = \prod_{k=2}^{N+1} \left(1 - \frac{h_t Q_{k+\frac{1}{2},i}}{A_k h_x}\right) \quad (4\text{-}171)$$

But this requires $A_k h_x > h_t Q_{k+1,i}$

$$h_x > \frac{Q}{A} h_t \quad (4\text{-}172)$$

where:

$$Q = \max_{k,i}(Q_{k,i}) \quad (4\text{-}173)$$

$$A = \min_{k}(A_k) \quad (4\text{-}174)$$

Equation (4-172) states a sufficient condition for nonsingularity of the matrix, K_1.

In order to satisfy numerical stability criteria for the tridiagonal matrices K_2 and K_3, all of the elements in both of these matrices must be positive. A sufficient condition to assure this, based on a method presented by Okunseinde[340], is stated as follows.

$$\frac{1}{\frac{2(DA)}{Ah_x^2} + \frac{M}{2}} > h_t \qquad (4\text{-}175)$$

where:

$$(DA) = \max_{k,i} (D_{k,i} \cdot A_k) \qquad (4\text{-}176)$$

$$A = \max_{k} (A_k) \qquad (4\text{-}177)$$

$$M = \max(K_r, K_a) \qquad (4\text{-}178)$$

Now, for a tridiagonal matrix of the form,

$$\begin{bmatrix} \alpha & 1 & & & 0 \\ 1 & \alpha & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ 0 & & & 1 & \alpha \end{bmatrix}$$

the determinant is positive if $\alpha \geq 2$. Hence, a tridiagonal matrix in which all elements are positive and in which the smallest principal diagonal element is at least twice as large as the largest off-diagonal element has a positive determinant. For

$$m_1 = \min_{k,i}(-B_{k,i}) \text{ and} \tag{4-179}$$

$$M_2 = \max_{k,i}\left[\frac{h_t(DA)_{k-\frac{1}{2},i}}{A_k h_x^2}, \frac{h_t(DA)_{k+\frac{1}{2},i}}{A_k h_x^2}\right] \tag{4-180}$$

a sufficient condition for nonsingularity of K_2 is

$$m_1 \geq 2M_2 \tag{4-181}$$

Similarly, for

$$m_3 = \min_{k,i}(-G_{k,i}) \tag{4-182}$$

and M_2 defined as in equation (4-180), a sufficient condition for nonsingularity of K_3 is

$$m_3 \geq 2M_2 \tag{4-183}$$

From equations (4-143) and (4-179)

$$m_1 = 1 - \frac{h_t K_r}{2} - \frac{2h_t(DA)}{h_x^2 A} \tag{4-184}$$

where:

$$(DA) = \max_{k,i}(DA)_{k,i} \tag{4-185}$$

$$A = \min_k A_k \tag{4-186}$$

Similarly, from equations (4-146) and (4-182)

$$m_3 = 1 - \frac{h_t K_a}{2} - \frac{2h_t(DA)}{h_x^2 A} \tag{4-187}$$

From equation (4-180),

$$M_2 = \frac{h_t (DA)}{h_x^2 A} \qquad (4\text{-}188)$$

where (DA) and A are defined in (4-185) and (4-186), respectively.

Combining (4-181), (4-184) and (4-188) yields

$$1 - \frac{h_t K_r}{2} - \frac{2h_t}{h_x^2} \frac{(DA)}{A} \geq \frac{2h_t}{h_x^2} \frac{(DA)}{A}$$

$$1 \geq \left[\frac{K_r}{2} + \frac{4}{h_x^2} \frac{(DA)}{A} \right] h_t$$

$$\frac{1}{\frac{K_r}{2} + \frac{4(DA)}{Ah_x^2}} \geq h_t \qquad (4\text{-}189)$$

which is a sufficient condition for both nonsingularity of K_2 and numerical stability.

Similarly, one may determine as a sufficient condition for nonsingularity of K_3 the following.

$$\frac{1}{\frac{K_a}{2} + \frac{4(DA)}{Ah_x^2}} \geq h_t \qquad (4\text{-}190)$$

4.4.5 Determination of sufficient stability conitions. To test whether the conditions listed in equations (4-165) through (4-170) are attainable, a simple form is assumed for the submatrices of S_i and the resulting equations are evaluated. To this end, one may assume the following.

$$s_{1,i} = s_{2,i} = s_{3,i} = s_{4,i} = \mathbf{I} \tag{4-191}$$

Then

$$s_{5,i} = K_3^{-1} K_4 \tag{4-192}$$

Substitution of equations (4-191) and (4-192) in equations (4-165) through (4-170) yields:

$$s_{1,i+1} = \rho_1 K_2^{-1} \tag{4-193}$$

$$s_{2,i+1} = \rho_2 K_3^{-1} \tag{4-194}$$

$$s_{3,i+1} = \rho_3 K_1^{-1} \tag{4-195}$$

$$s_{4,i+1} = \rho_4 K_1^{-1} \tag{4-196}$$

$$s_{5,i+1} = \rho_5 K_2^{-1} \tag{4-197}$$

Substitution of equations (4-191) and (4-192) in (4-170) yields

$$S_i^{-1} = \begin{bmatrix} 0 & \mathbf{I} & 0 & 0 \\ \mathbf{I} & 0 & 0 & 0 \\ -K_3^{-1}K_4 & 0 & 0 & \mathbf{I} \\ 0 & 0 & \mathbf{I} & 0 \end{bmatrix} \qquad (4\text{-}198)$$

From equations (4-192) through (4-198)

$$S_{i+1} = \begin{bmatrix} 0 & \rho_1 K_2^{-1} & 0 & 0 \\ \rho_3 K_1^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_2 K_3^{-1} \\ 0 & K_3^{-1}K_4 & \rho_4 K_1^{-1} & 0 \end{bmatrix} \qquad (4\text{-}199)$$

Equations (4-161) and (4-199) in conjunction with equations (4-192) through (4-197) yield:

$$S_{i+1}A(i)S_i^{-1} = \tilde{A} = \begin{bmatrix} 0 & \rho_1 & 0 & 0 \\ \rho_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_2 \\ 0 & \rho_5 & \rho_4 & 0 \end{bmatrix} \qquad (4\text{-}163)$$

The corresponding transformed stationary system, following Freeman(145), is

$$\tilde{\underline{x}}_{i+1} = \tilde{A}\tilde{\underline{x}}_i \qquad (4\text{-}200)$$

where the coefficient matrix $\tilde{A}$ is now time-invariant. Each submatrix of $\tilde{A}$ is assumed to be diagonal, i.e.,

$$\rho_j = \text{diag}(\rho_{j,2}, \ \rho_{j,3}, \ldots, \ \rho_{j,N+1}) \qquad (4\text{-}201)$$

$j=1,2,3,4,5.$

From Freeman[145] the stability of the nonstationary system,

$$\hat{\underline{x}}_{i+1} = A(i)\hat{\underline{x}}_i + B\underline{u}_i \qquad (4\text{-}150)$$

may be determined from the stability of the transformed stationary system expressed in (4-200). Furthermore, a variety of standard stability analyses may be applied to the transformed stationary system.

To facilitate later analysis involving the presence of transport lags, one may employ the z-transform to determine the stability of the transformed stationary system. Taking the z-transform of (4-200) yields:

$$z\tilde{\underline{X}}(z) - \tilde{\underline{x}}(0) \quad - \tilde{A}\tilde{\underline{X}}(z) = 0 \qquad (4\text{-}202)$$

The corresponding characteristic polynomial in the z-domain may be expressed as:

$$\mathrm{Det}(z\mathbf{I} - \tilde{A}) = \left|\begin{array}{cc|cc} z\mathbf{I} & -\rho_1 & 0 & 0 \\ -\rho_3 & z\mathbf{I} & 0 & 0 \\ \hline 0 & 0 & z\mathbf{I} & -\rho_2 \\ 0 & -\rho_5 & -\rho_4 & z\mathbf{I} \end{array}\right| \quad (4\text{-}203)$$

Expansion of this determinant as a determinant of a partitioned matrix (indicated by the dashed lines) results in:

$$\mathrm{Det}(z\mathbf{I} - \tilde{A})$$

$$= \left[z^{2N} - \prod_{k=2}^{N+1} (\rho_{3,k}\,\rho_{1,k})\right] \left[z^{2N} - \prod_{k=2}^{N+1} (\rho_{4,k}\,\rho_{2,k})\right] \quad (4\text{-}204)$$

If

$$\prod_{k=2}^{N+1} (\rho_{3,k}\,\rho_{1,k}) < 1 \quad (4\text{-}205)$$

and

$$\prod_{k=2}^{N+1} (\rho_{4,k}\,\rho_{2,k}) < 1 \quad (4\text{-}206)$$

all of the roots of $\mathrm{Det}(z\mathbf{I} - \tilde{A}) = 0$, the characteristic equation, have magnitudes < 1 and the transformed stationary system,

$$\tilde{\underline{x}}_{i+1} = \tilde{A}\tilde{\underline{x}}_i \quad (4\text{-}200)$$

is stable, which, according to Freeman[145], implies that the nonstationary system,

$$\hat{\underline{x}}_{i+1} = A(i)\hat{\underline{x}}_i + B\underline{u}_i \tag{4-146}$$

is stable for bounded $\underline{u}_i$.

By using the approach of Appendix 12 it can be shown that the scalar components of $\underline{x}_1$, $\underline{x}_2$, $\underline{x}_3$ and $\underline{x}_4$, differ from those of $\hat{\underline{x}}_1$, $\hat{\underline{x}}_2$, $\hat{\underline{x}}_3$ and $\hat{\underline{x}}_4$, respectively, by additive terms. The stability of the system represented by equations involving the first set of vector state variables is implied by the stability of the system involving the second set of vector state variables. In summary, the set of sufficient conditions for stability of the original nonstationary system includes, in addition to equations (4-205) and (4-206), the sufficient condition for nonsingularity of K_1, [inequality (4-172)] , the condition for nonsingularity of K_2, [inequality (4-181)] , the condition for nonsingularity of K_3, [inequality (4-183)] , and the nonsingularity conditions associated with the transformation from $\hat{\underline{x}}_n$ to $\underline{x}_n$ for n=1,2,3,4.

4.4.6 <u>Evaluation of transport lag effects</u>. The z-transform of the stationary system of equation (4-199) may be expanded, with zero initial conditions, to the following form.

$$\begin{bmatrix} z\underline{\tilde{X}}_1 \\ z\underline{\tilde{X}}_2 \\ z\underline{\tilde{X}}_3 \\ z\underline{\tilde{X}}_4 \end{bmatrix} = \begin{bmatrix} 0 & \rho_1 & 0 & 0 \\ \rho_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_2 \\ 0 & \rho_5 & \rho_4 & 0 \end{bmatrix} \begin{bmatrix} \underline{\tilde{X}}_1 \\ \underline{\tilde{X}}_2 \\ \underline{\tilde{X}}_3 \\ \underline{\tilde{X}}_4 \end{bmatrix} \qquad (4\text{-}207)$$

where:

$$\underline{\tilde{X}}_j = (\tilde{X}_{j,2}, \tilde{X}_{j,3}, \ldots, \tilde{X}_{j,N})^T \qquad (4\text{-}208)$$

for j=1,2,3,4.

If a distinct transport lag is introduced for each variable on the right hand side of equation (4-207), then in the place of each $\underline{X}_j$ on this side would appear, following Jury[210],

$$(\underline{\tilde{X}}_{j,2} z^{-\Delta_{j,2}}, \underline{\tilde{X}}_{j,3} z^{-\Delta_{j,3}}, \ldots, \underline{\tilde{X}}_{j,N} z^{-\Delta_{j,N}})^T \qquad (4\text{-}209)$$

Substitution of equation (4-209) into equation (4-207) yields:

$$z\underline{\tilde{X}} = \tilde{\tilde{A}}\underline{\tilde{X}} \qquad (4\text{-}210)$$

where:

$$\tilde{\tilde{A}} = \begin{bmatrix} 0 & \mu_1 & 0 & 0 \\ \mu_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_2 \\ 0 & \mu_5 & \mu_4 & 0 \end{bmatrix} \tag{4-211}$$

$$\mu_{1,k} = z^{-\Delta_{2,k}} \rho_{1,k} \tag{4-212}$$

$$\mu_{2,k} = z^{-\Delta_{4,k}} \rho_{2,k} \tag{4-213}$$

$$\mu_{3,k} = z^{-\Delta_{1,k}} \rho_{3,k} \tag{4-214}$$

$$\mu_{4,k} = z^{-\Delta_{3,k}} \rho_{4,k} \tag{4-215}$$

$$\mu_{5,k} = z^{-\Delta_{2,k}} \rho_{5,k} \tag{4-216}$$

The z-domain characteristic polynomial associated with $\tilde{\tilde{A}}$ may then be expressed as follows.

$$\mathrm{Det}(z\mathbf{I} - \tilde{\tilde{A}})$$

$$= \quad z^{2N-2} - \prod_{k=2}^{N} \left(\rho_{3,k} z^{-\Delta_{1,k}} \rho_{1,k} z^{-\Delta_{2,k}} \right)$$

$$z^{2N-2} - \prod_{k=2}^{N} \left(\rho_{4,k} z^{-\Delta_{3,k}} \rho_{2,k} z^{-\Delta_{4,k}} \right) \tag{4-217}$$

The corresponding characteristic equation, $\mathrm{Det}(z\mathbf{I} - \tilde{\tilde{A}}) = 0$, may then be written in the form:

$$\left(z^{\left[2N-2 + \sum_{k=2}^{N} (\Delta_{1,k} + \Delta_{2,k})\right]} - \prod_{k=2}^{N} (\rho_{3,k} \, \rho_{1,k}) \right)$$

$$\left(z^{\left[2N-2 + \sum_{k=2}^{N} (\Delta_{3,k} + \Delta_{4,k})\right]} - \prod_{k=2}^{N} (\rho_{4,k} \, \rho_{2,k}) \right)$$

$$= 0 \qquad (4\text{-}218)$$

Hence, the conditions for assuring stability of the system without lags given in equations (4-205) and (4-206) also apply to the system with a distinct transport lag associated with each state variable.

4.5 Structure of Subproblem Hierarchy and Computational Efficiency

Recent years have witnessed an ever increasing interest in various types of multilevel hierarchical systems[312]. With the advent of the dedicated minicomputer operating on a control level and being supervised on a higher level by a large-scale machine, real world multilevel control actually is being implemented. Whether the hierarchical structure is real or merely algorithmic, little has been written concerning the relationship between the characteristics of the structure and the efficiency of solution of the subproblems of which it is comprised.

Multilevel structure is an indication of the manner in which an overall control problem is decomposed into subproblems, and these, in turn, are decomposed further in a complete hierarchical system. Thus, the number of levels or system layers often can be greater than that of the typically discussed two-level configuration. Each subsystem feeds up to a lower order subsystem; the ratio of the two state vectors is called the dimensional ratio. Such a ratio is a basic variable of a particular structure that also suggests the amount of coordination necessary. In situations in which a decision is required as to whether or not a simple system should be decomposed into a multilevel structure there exists an upper bound on the dimensional ratio, above which a greater static computational effort occurs with the multilevel configuration.

Most prior work has dealt with simple binary structures. These structures characteristically start at a top level and split into two subsystems at each node on each lower level of the hierarchy. This section considers a more general structural ratio. In its simplest form it is the same as a general radix rather than the radix of two.

The generalized cost referred to in this work is the result of an attempt to quantify in a somewhat general way the total computational effort incurred by a particular multilevel control structure in terms of characteristic variables of the structure. This total effort is defined as the weighted sum of two basic effort terms: the static computational effort and the coordinating effort. The static computational effort can be expressed as a function of the number of levels, the dimensional ratio, and the structural ratio. This is an extension of some prior work by Pearson[359]. The coordination effort can be expressed as a function of the number of levels, the nesting factor, the number of coordination variables, and the number of interlevel iterations. This is a dynamic type of effort in that timing enters into the nesting factor, which is an indication of whether the interlevel iterations of the various levels are disjoint in time. Weighting is incorporated between the two effort terms to allow for a change of emphasis for a particular computer cost situation.

Considerable prior work in multilevel system theory has been of an abstract nature. Where it has been applied in control system theory, the treatment has considered mainly lumped basic systems. However, it has been shown that a simple discretized system can be treated as a multilevel structure directly. That is, the differential-difference equations have a built-in two-level coordinating structure. In this section, the discussion of the two-level distributed system actually is a discussion of the simple distributed parameter system, since the true multilevel distributed parameter structure contains at least three levels. Examples of multilevel distributed structures can be found in environmental and physiological systems.

This section describes the manner in which the total computational effort varies as a function of the characteristic variables and indicates with a series of numerical examples how one might select a particular structural configuration in order to obtain the lowest computational effort subject to a particular set of constraints.

4.5.1 The multilevel structure and the computational effort. The most general subproblem hierarchy considered here consists of L levels of subproblems with one overall coordination subproblem in the top level and N_1 subproblems in the bottom or first level. If n_1 = the dimension of the total state vector for all first level subproblems, the average state vector dimension of one first level subproblems is given by n_1/N_1.

R_i, the structural ratio, is the number of subproblems in level i divided by the number of subproblems in level i + 1 where $1 \leq i \leq L - 1$. N_i, the number of subproblems in the ith level, is:

$$N_i = \prod_{j=i}^{L-1} R_j \tag{4-219}$$

Generalizing the notation of Pearson's paper(359), the dimensional ratio, ϵ_i, is the average number of state vector components passed to a higher level divided by the average number of components in the state vector of a subproblem in the ith level of the hierarchy, $1 \leq i \leq L-1$. If level i passes state vector components only up to level i+1, the average state vector dimension for a subsystem on the ith level may be expressed as

$$\frac{n_i}{N_i} = \frac{n_1}{N_i} \prod_{j=1}^{i-1} \epsilon_j \tag{4-220}$$

The static computational effort for this level is given by

$$E_{si} = N_i K_i \left(\frac{n_i}{N_i} \right), \quad i=1,2,\ldots,L \tag{4-221}$$

where K_i ( ) is a function to be specified.

Under the assumption that the computational effort for a set of simultaneous equations is proportional to the square of its dimension the computational effort for the single level problem consisting of all n_1 first level equations is n_1^2. The static computational effort for each first level subproblem is:

$$K_1\left(\frac{n_1}{N_1}\right) = \left(\frac{n_1}{N_1}\right)^2 \tag{4-222}$$

Subproblems of level 2 and above are coordination subproblems involving direct substitution of variables for which the computational effort is directly proportional to the number of equations involved.

$$K_i\left(\frac{n_i}{N_i}\right) = \frac{n_i}{N_i} \quad \text{for all i such that } 2 \leq i \leq L \tag{4-223}$$

The total static computational effort for all levels of the hierarchy divided by the computational effort for the single level system with the same n_1 is

$$\bar{E}_S = \frac{E_s}{n_1^2} = \frac{1}{N_1} + \frac{1}{n_1^2} \sum_{i=2}^{L} n_i \tag{4-224}$$

Substitution of (4-220) in (4-224) yields

$$\bar{E}_S = \frac{1}{N_1} + \frac{1}{n_1} \sum_{i=2}^{L} \prod_{j=1}^{i-1} \epsilon_j \tag{4-225}$$

The coordination effort for the hierarchy is:

$$E_c = K_n \gamma_M \sum_{i=1}^{L-1} \left(\frac{n_i}{N_i}\right)^2 \tag{4-226}$$

where

K_n = nesting factor for interlevel iterations. If all of the interlevel iterations are disjoint in time $K_n = 1$; if all are simultaneous, $K_n = \frac{1}{L-1}$

γ_M = maximum of γ_i

γ_i = number of iterations between level i and level i+1 of the hierarchy

$$\bar{E}_c = \frac{E_c}{K_n \gamma_M n_1^2} \tag{4-227}$$

Substitution of (4-219), (4-220) and (4-227) in (4-226) yields

$$\bar{E}_c = \frac{1}{N_1^2}\left(1 + \sum_{K=1}^{L-2} \prod_{j=1}^{K} R_j^2 \epsilon_j^2\right) \tag{4-228}$$

The total multilevel computational effort for the hierarchy divided by the computational effort for the single level problem with the same n_1 is

$$\bar{E}_T = \bar{E}_S + \sigma \bar{E}_c \qquad (4\text{-}229)$$

where σ is a weighting factor.

4.5.2 Optimization of total multilevel computational effort. The optimal value of $\bar{E}_T$ is a minimum. Inspection of (4-225) and (4-228) reveals that for minimum $\bar{E}_T$, N_1 should be as close to n_1 as possible ($N_1 \leq n_1$). Since n_1 occurs in $\bar{E}_S$ but not in $\bar{E}_c$, minimization of $\bar{E}_T$ results from maximizing n_1, i.e., the computational advantage of the hierarchy over the corresponding single level problem is more pronounced for larger dimensions.

For the two level hierarchy $N_1 = R_1$ and the maximization of N_1 implies the maximization of R_1. This fixes the value of ϵ_1 in a practical problem.

The three level hierarchy provides more flexibility in the optimization of $\bar{E}_T$ since two structural ratios and two dimensional ratios are involved. Maximization of N_1 is equivalent to maximization of the product of R_1 and R_2.

Evaluation of (4-228) for L = 3 yields

$$\bar{E}_c = \frac{1}{N_1^{\,2}} + \left(\frac{\epsilon_1}{R_2}\right)^2 \qquad (4\text{-}230)$$

From (4-230) it is evident that for a given value of $N_1 = R_1R_2$, the largest value of R_2 corresponds to a minimum of $\bar{E}_c$ and a minimum of $\bar{E}_T$. Once R_1 and R_2 have been determined in a practical three level problem, the values of ϵ_1 and ϵ_2 are fixed.

The ratio of total computational efforts for multi-level and single level problems with the same n_1, $\bar{E}_T$, was evaluated for L = 2 and L = 3 over a range of values of structural ratios, dimensional ratios and σ with a series of digital computer programs. The results obtained confirmed the observations concerning optimization of $\bar{E}_T$ stated above and provided numerical evaluations of the computational efforts associated with the hierarchies in the following examples.

4.5.3 Numerical examples. Example 1 concerns three subproblem hierarchies associated with the pair of interconnected dynamic lumped parameter subsystems discussed by Mesarovic, Pearson and Takahara[309]. These hierarchies are depicted in Figure 4-1. Hierarchy 4-1.1 was presented in the paper cited above. Hierarchy 4-1.2 resulted from discretizing each subproblem of Hierarchy 4-1.1 at four points in time. Hierarchy 4-1.3 was obtained by decoupling the first level costate equations from the state equations in Hierarchy 4-1.2. The three hierarchies of this example are compared in Table 4-2.

Example 2 concerns three subproblem hierarchies

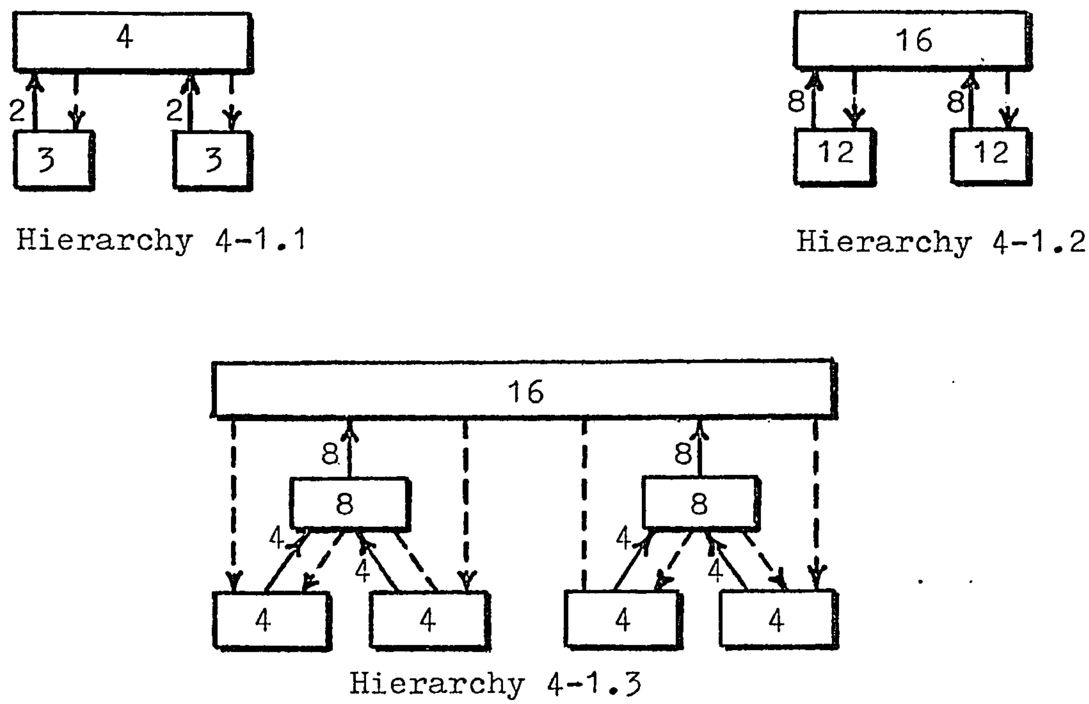


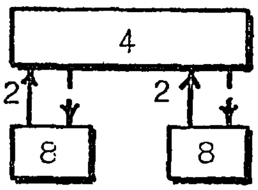
Figure 4-1: Subproblem hierarchies associated with lumped parameter example from the paper by Mesarovic et. al.[309]

associated with the distributed parameter control problem treated in Sections 5.2 and 6.3 of Wismer's dissertation[531]. These hierarchies appear in Figure 4-2. Hierarchy 4-2.1, in which each first level (infimal) subproblem includes four spatial points, was developed in Wismer's dissertation. Hierarchy 4-2.2 resulted from a formulation of the same overall control problem with a larger number of subproblems of smaller dimension in the first level. Hierarchy 4-2.3 was developed by decoupling the state and costate equations in the first level subproblems of Hierarchy 4-2.2. The hierarchies of this example are compared in Table 4-3.

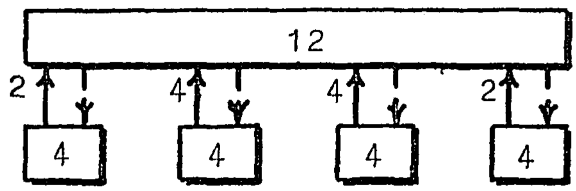
In Figures 4-1 and 4-2 each number enclosed in a box is the number of equations in the corresponding subproblem. Each number associated with a solid arrow is the number of variables sent to a higher level.

This chapter began with a presentation of supplementary boundary conditions for the subproblems comprising the hierarchies developed in Chapters 2 and 3. These boundary conditions, in conjunction with those developed in the chapters cited above, are sufficient for generation of specific solutions for each of the subproblems.

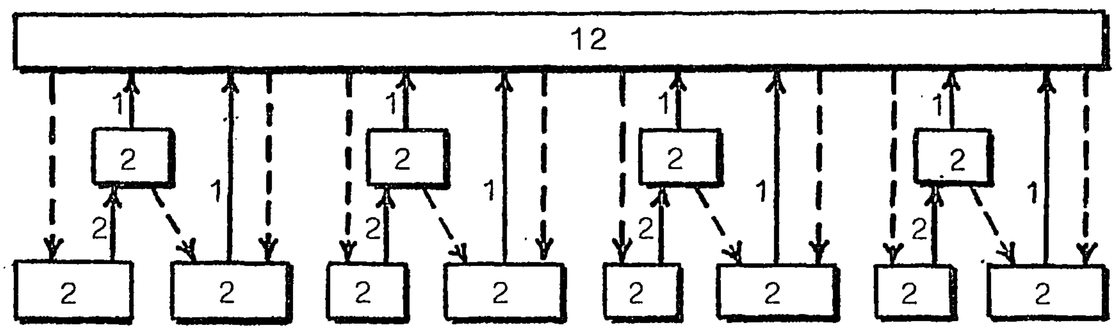
In the second section of this chapter consistency



Hierarchy 4-2.1



Hierarchy 4-2.2



Hierarchy 4-2.3

Figure 4-2: Subproblem hierarchies associated with distributed parameter control problem from Wismer's dissertation and convergence of the solutions of the semidiscretized approximation of the continuous distributed parameter tapered stream water quality model were proved. This model was considered representative of a fairly broad class of continuous distributed parameter water quality models to which the same techniques may be applied in proving consistency and convergence.

In the third section, stability analysis of the semidiscretized continuous distributed parameter tapered stream model with optimal aeration control of Chapter 2 was presented. The model with Kalman regulator control was shown to be asymptotically stable in the large subject to some relatively nonrestrictive conditions. These results were then extended to the same model with gradient control, a spatially and temporally discretized form of the model and a model subjected to transport lags. The tapered stream model to which the stability analysis of this section was applied may be regarded as representative of the class of deterministic continuous distributed parameter water quality models presented in Chapter 2 to which the same approach to stability analysis may be applied.

In the fourth section of this chapter an approach was presented for stability analysis of the tidal river model with optimal aeration control representative of the class of two-step discrete distributed parameter water quality models developed in Chapter 3. The stability of this nonstationary model was established by transforming it to a corresponding stationary system and utilizing an approach presented by Freeman[145]. Sufficient conditions to assure numerical stability of the finite-difference equations comprising the original nonstationary model were then developed. It was also shown that the same conditions assure stability when distinct transport lags are associated with each scalar component of the state vectors of the corresponding stationary model.

In the final section of the chapter, an approach to evaluating the total computational effort associated with solution of an array of subproblems assembled into a hierarchical structure was developed. This approach provides a basis for comparing existing multilevel structures and considering alternate decomposition-coordination schemes that may yield lower computational efforts for the solution of the same original problem.

The next chapter presents a sensitivity analysis of a representative water quality model under multilevel optimal control. Later chapters present numerical examples of the application of multilevel optimal control to selected water quality models developed in Chapters 2 and

3 and an application of the multilevel hierarchical systems analysis approach to a regional water quality control problem with economic constraints.

Hierarchy	n_1	N_1	R_1	R_2	ϵ_1	ϵ_2	$\bar{E}_S$	$\bar{E}_c$	$\bar{E}_T$
Original	6	2	2	-	2/3	-	.611	.250	.861
Time-discretized	24	2	2	-	2/3	-	.529	.250	.779
Decoupled	16	4	2	2	1	1	.375	.312	.688

Table 4-2: Lumped parameter example subproblem hierarchies structural characteristics and effort terms.

Hierarchy	n_1	N_1	R_1	R_2	ϵ_1	ϵ_2	$\bar{E}_S$	$\bar{E}_c$	$\bar{E}_T$
Original	16	2	2	-	1/4	-	.515	.250	.765
Figure 4-2.2	16	4	4	-	3/4	-	.297	.0625	.359
Figure 4-2.3	16	8	2	4	7/8	3/4	.226	.063	.289

Table 4-3: Distributed parameter example subproblem hierarchies structural characteristics and effort terms.

CHAPTER 5

HIERARCHICAL SENSITIVITY MODELS IN A DYNAMIC WATER POLLUTION CONTROL SYSTEM

Two important concepts in effecting optimal control of a system represented by a mathematical model are sensitivities of the state variables of the model and sensitivity of the performance index to changes in the model's parameters. These concepts may be applied to optimal control problems involving any of the water quality models presented in Chapters 2 and 3 of this dissertation. In this chapter they are applied to an optimal dynamic water pollution control problem involving the tapered stream model presented in Chapter 2.

An interesting result is a hierarchical model for generation of trajectory sensitivity coefficients similar to that utilized in the generation of the optimal control contours for the same system. The structures of the two hierarchies are, in fact, the same. The state trajectory sensitivity subproblem hierarchy utilizes space-time contours of the state variables of the original system, optimized in some sense, to generate space-time contours of the state trajectory sensitivity coefficients.

In contrast with the state trajectory sensitivity contours, the performance index sensitivity coefficient yields a single number which facilitates sensitivity comparisons between different systems[367]. Both sensitivity measures vary in direct proportion with the boundary conditions imposed upon the original control problem. A normalized performance index sensitivity function is introduced which is not affected by such changes. Since it is a function of the optimal value of the performance index, its generation requires space-time contours of the optimal control variables as inputs.

5.1 Stream Model, Optimal Control and Performance Indicies

The tapered stream water quality model treated in this chapter is the one represented by equations (2-26) and (2-27) in Chapter 2 with control terms added to both the BOD and DO rate balances.

In order to optimally control the BOD and DO concentrations in the mathematical model of the stream reach, an integral-type measure of performance, the performance index, is required. Two examples of performance indexes for the stream model of this chapter follow.

A performance index suitable for minimizing deviation from a desired level of DO, C_{sp}, with a minimal expenditure of aeration control energy is the following.

$$J = W_1 \int_{t_o}^{t_f} \int_{x_o}^{x_f} \tilde{C}^2 \, dxdt + \Gamma_1 \int_{t_o}^{t_f} \int_{x_o}^{x_f} U_C^2 \, dxdt \tag{5-1}$$

where:

W_1 = constant weighting coefficient.

Γ_1 = constant weighting coefficient.

$\tilde{C} = C_{sp} - C$ = deviation of DO concentration from the desired value.

x_o = location of upstream end of reach.

x_f = location of downstream end of reach.

t_o = initial time.

t_f = final time.

U_C = rate of addition of DO concentration.

The corresponding performance index for waste dumping control is:

$$J = W_2 \int_{t_o}^{t_f} \int_{x_o}^{x_f} \tilde{C}^2 \, dx\, dt + \Gamma_2 \int_{t_o}^{t_f} \int_{x_o}^{x_f} U_L^2 \, dx\, dt \tag{5-2}$$

where:

W_2 = constant weighting coefficient.

Γ_2 = constant weighting coefficient.

U_L = rate of addition of BOD concentration.

Adjustment of the weighting coefficients permits determination of control profiles with different emphases on the relative costs of deviation from the specified level and the expenditure of control energy. The desired level of DO, C_{sp}, may be either the legally required minimum DO or a higher (more conservative) value.

5.2 State Trajectory Sensitivity

From the paper by Kokotovic and Rutman[230] for a state vector V of order n and a parameter vector p of order r, the n x r state trajectory sensitivity matrix is comprised of elements of the following form.

$$S_{ij} = \frac{\partial V_i}{\partial p_j} \tag{5-3}$$

where:

$i = 1,2,\ldots,n$

$j = 1,2,\ldots,r$

V_i = the ith state variable

p_j = the jth parameter

The ith state equation may be written in the general form,

$$F_i(\dot{V}_i,\ V,\ p,\ t) = 0 \tag{5-4}$$

For the spatially discretized tapered stream model BOD equations of Chapter 2, n = N and r = 2,

$$F_k(\dot{L}_k,\ L,\ K_r,\ t) = 0; \quad k = 2,3,\ldots,\ N+1 \tag{5-5}$$

Thus,

$$S_L = \begin{bmatrix} S_{2,L,1} & S_{2,L,2} \\ \vdots & \vdots \\ S_{N+1,L,1} & S_{N+1,L,2} \end{bmatrix} \quad (5\text{-}6)$$

where:

$$S_{1,L,1} = S_{1,L,2} = 0 \quad (5\text{-}7)$$

$$S_{k,L,1} = \frac{\partial L_k}{\partial K_r} ; \quad k = 2,3,\ldots, N+1 \quad (5\text{-}8)$$

$$S_{k,L,2} = \frac{\partial L_k}{\partial K_d} ; \quad k = 2,3,\ldots, N+1 \quad (5\text{-}9)$$

Taking partial derivatives of equation (2-56), with respect to K_r and $K_d = R_d K_r$,

$$\dot{S}_{k,L,1} = - B_k S_{k,L,1} + E_k S_{k-1,L,1} - L_k \quad (5\text{-}10)$$

$$\dot{S}_{k,L,2} = - B_k S_{k,L,2} + E_k S_{k-1,L,2} - \frac{1}{R_d} L_k \quad (5\text{-}11)$$

For the spatially discretized tapered stream model DO equations of Chapter 2, $n = N$, $r = 3$, and

$$F_k \, (C_k, C, L, K_r, K_d, K_a, t) = 0 \quad (5\text{-}12)$$

where: $k = 2,3,\ldots, N+1$

Hence,

$$S_C = \begin{bmatrix} S_{2,C,1} & S_{2,C,2} & S_{2,C,3} \\ \vdots & \vdots & \vdots \\ S_{N+1,C,1} & S_{N+1,C,2} & S_{N+1,C,3} \end{bmatrix} \qquad (5\text{-}13)$$

where:

$$S_{1,C,1} = S_{1,C,2} = S_{1,C,3} = 0 \qquad (5\text{-}14)$$

$$S_{k,C,1} = \frac{\partial C_k}{\partial K_r} ; \quad k = 2,3,\ldots, N+1 \qquad (5\text{-}15)$$

$$S_{k,C,2} = \frac{\partial C_k}{\partial K_d} ; \quad k = 2,3,\ldots, N+1 \qquad (5\text{-}16)$$

$$S_{k,C,3} = \frac{\partial C_k}{\partial K_a} ; \quad k = 2,3,\ldots, N+1 \qquad (5\text{-}17)$$

Taking partial derivatives with respect to K_r, K_d and K_a of equation (2-59),

$$\dot{S}_{k,C,1} = - G_k S_{k,C,1} + E_k S_{k-1,C,1} - K_d S_{k,L,1} - R_d L_k \qquad (5\text{-}18)$$

$$\dot{S}_{k,C,2} = - G_k S_{k,C,2} + E_k S_{k-1,C,2} - K_d S_{k,L,2} - L_k \qquad (5\text{-}19)$$

$$\dot{S}_{k,C,3} = - G_k S_{k,C,3} + E_k S_{k-1,C,3} - K_d S_{k,L,3} - C_k + C_s \qquad (5\text{-}20)$$

The trajectory sensitivity matrix for the aggregation of the BOD and DO equations would have the following form.

$$S = \begin{array}{c} \overbrace{\hphantom{S_L\quad\quad}}^{2} \\ \left[\begin{array}{c:c} & 0 \\ S_L & \vdots \\ & 0 \\ \hdashline \multicolumn{2}{c}{S_C} \\ & \end{array}\right] \\ \underbrace{\hphantom{S_L\quad\quad 0}}_{3} \end{array} \begin{array}{l} \left.\vphantom{\begin{matrix}a\\a\\a\end{matrix}}\right\} N \\ \left.\vphantom{\begin{matrix}a\\a\end{matrix}}\right\} N \end{array} \qquad (5\text{-}21)$$

where the column of zeros corresponds to:

$$\frac{\partial L_k}{\partial K_a} = 0 \text{ for every } k \qquad (5\text{-}22)$$

5.3 Hierarchical Sensitivity Models

The large number of sensitivity equations (5-10), (5-11), (5-18), (5-19) and (5-20) for k = 2,3,..., N+1, can be solved efficiently by the application of the multilevel hierarchical systems analysis techniques of decomposition and coordination to recast the overall problem to be solved into a two-level subproblem hierarchy.

For the BOD equations, (5-10) and (5-11), let:

$$R_{k,L,j} = E_k\, S_{k-1,L,j}\,; \qquad j = 1,2 \qquad (5\text{-}23)$$

Then the BOD sensitivity equations in decomposed form are:

$$\dot{S}_{k,L,1} = - B_k S_{k,L,1} + R_{k,L,1} - L_k \tag{5-24}$$

$$\dot{S}_{k,L,2} = - B_k S_{k,L,2} + R_{k,L,2} - \frac{1}{R_d} L_k \tag{5-25}$$

For the DO equations, (5-18), (5-19) and (5-20), the decomposition (coordination) equations are:

$$R_{k,C,j} = E_k S_{k-1,C,j} - K_d S_{k,L,j} \; ; \quad j = 1,2,3 \tag{5-26}$$

and the decomposed sensitivity equations are:

$$\dot{S}_{k,C,1} = - G_k S_{k,C,1} + R_{k,C,1} - R_d L_k \tag{5-27}$$

$$\dot{S}_{k,C,2} = - G_k S_{k,C,2} + R_{k,C,2} - L_k \tag{5-28}$$

$$\dot{S}_{k,C,3} = - G_k S_{k,C,3} + R_{k,C,3} - C_k + C_s \tag{5-29}$$

With equations (5-23) and (5-26) constituting the coordination subproblems, the state trajectory sensitivity subproblem hierarchy may be represented as in Figure 5-1. Comparison of this hierarchy with the subproblem hierarchy for optimal control, (Figure 2-1 in Chapter 2), reveals that the two hierarchies are of the same form. Furthermore, the equations of which the subproblems are comprised are

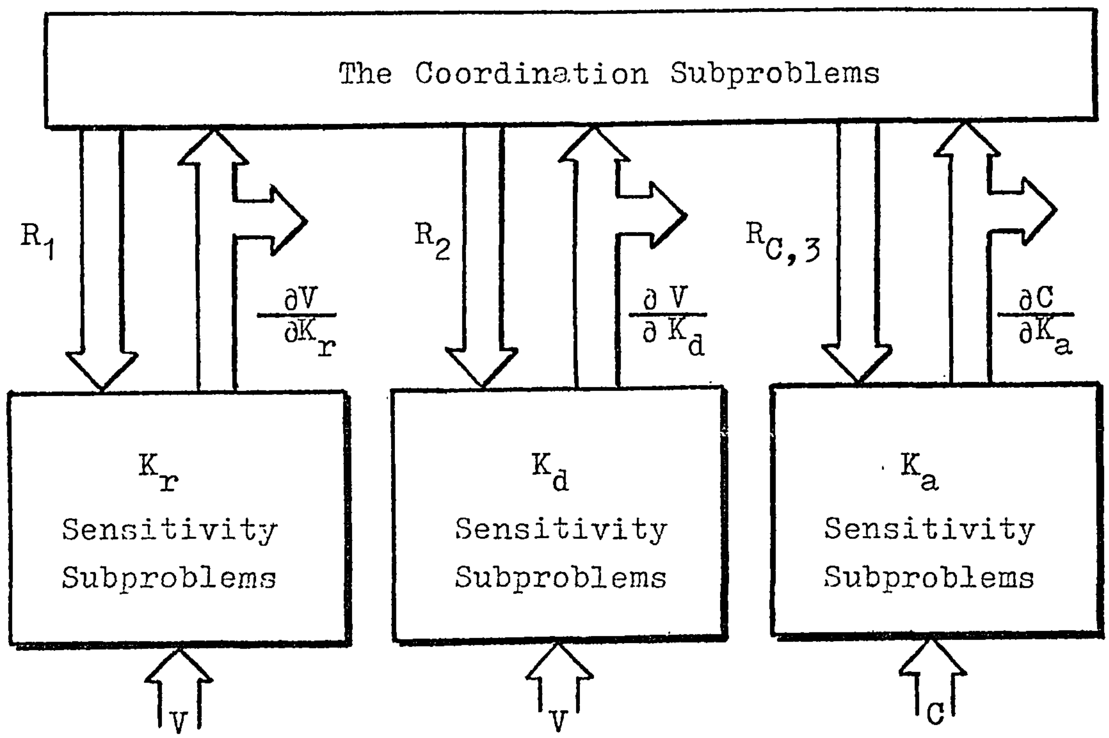


Figure 5-1: State trajectory sensitivity subproblem hierarchy.

also of the same form. This implies that after the optimal control problem has been solved, the same simulation may be used to generate the state trajectory sensitivity coefficient contours with only a reassignment of input and output variables. Such a result is in agreement with prior sensitivity literature[366].

5.4 Performance Index Sensitivity Coefficients and Functions

The performance index sensitivity vector may be written in the following form[367].

$$\frac{\partial J}{\partial \underline{p}} = \left(\frac{\partial J}{\partial p_1}, \frac{\partial J}{\partial p_2}, \ldots, \frac{\partial J}{\partial p_r} \right)^T \tag{5-30}$$

where:

$$\frac{\partial J}{\partial p_j} = \sum_{k=1}^{N+1} \frac{\partial J_k}{\partial p_j} \tag{5-31}$$

$$\frac{\partial J_k}{\partial p_j} = h_k \sum_{i=1}^{n} S_{k,i,j} \frac{\phi_k}{V_{k,i}} \tag{5-32}$$

$$S_{k,i,j} = \frac{\partial V_{k,i}}{\partial p_j} \tag{5-33}$$

The normalized performance index sensivitity function may be expressed as follows[367].

$$S^{J}_{p_j} = \left(\frac{\partial J}{\partial p_j}\right)\left(\frac{p_j}{J}\right) \tag{5-34}$$

The general block diagram for generating the normalized performance index sensitivity functions from the state trajectory sensitivity coefficients appears in Figure 5-2. For the stream model:

$$\phi_k = W_1\tilde{L}^2_k + W_2\tilde{C}^2_k + \Gamma^2_1 u^2_{1,k} + \Gamma^2_2 u^2_{2,k} \tag{5-35}$$

where:

$$\tilde{L}_k = L_{sp,k} - L_k \tag{5-36}$$

$$\tilde{C}_k = C_{sp,k} - C_k \tag{5-37}$$

For $\underline{V} = (\underline{L},\ \underline{C})^T$ (5-38)

$$\underline{L} = (L_1,\ L_2,\ldots,L_{N+1})^T \tag{5-39}$$

$$\underline{C} = (C_1,\ C_2,\ldots,C_{N+1})^T \tag{5-40}$$

$$\underline{u} = (\underline{u}_1,\ \underline{u}_2)^T \tag{5-41}$$

$$\underline{u}_j = (u_{j,1},\ u_{j,2},\ldots,u_{j,N+1})^T \tag{5-42}$$

$$\underline{p} = (p_1,\ p_2,\ldots,p_r)^T \tag{5-43}$$

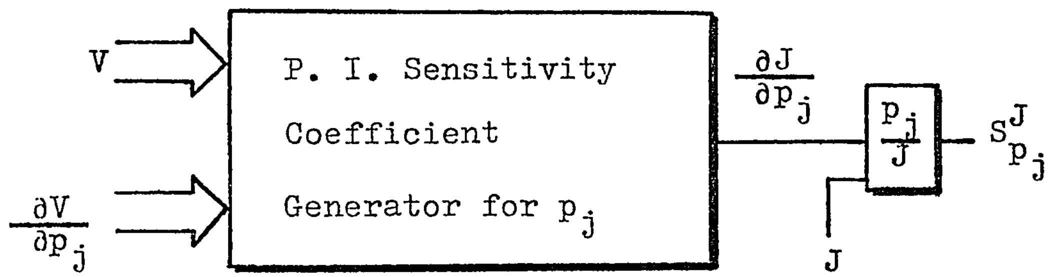


Figure 5-2: Generation of performance index sensitivity functions.

$$\frac{\partial J_k}{\partial p_j} = - 2h_k \left[W_1 \int_{t_o}^{t_f} S_{k,L,j} \tilde{L}_k \, dt \right.$$

$$\left. + W_2 \int_{t_o}^{t_f} S_{k,C,j} \tilde{C}_k \, dt \right] \tag{5-44}$$

But $S_{1,L,j} = S_{1,C,j} = 0$ for all j (5-7) and (5-14)

Hence,

$$\frac{\partial J}{\partial p} = \sum_{k=2}^{N+1} \frac{\partial J_k}{\partial p_j} \tag{5-45}$$

More specifically, applying equations (5-8) and (5-15) and temporal discretization to equation (5-44) and then applying equation (5-34),

$$S^J_{K_r} = \frac{K_r}{J} \frac{\partial J}{\partial K_r} = \frac{K_r}{J} \sum_{k=2}^{N+1} \frac{\partial J_k}{\partial K_r} \tag{5-46}$$

where:

$$\frac{\partial J_k}{\partial K_r} =$$

$$- 2h_k h_t \sum_{i=1}^{I_M} \left(W_1 \tilde{L}_{k,i} \frac{\partial L_{k,i}}{\partial K_r} + W_2 \tilde{C}_{k,i} \frac{\partial C_{k,i}}{\partial K_r} \right) \tag{5-47}$$

h_t = the temporal increment.

By a parallel development,

$$S^{J}_{K_d} = \frac{K_d}{J}\,\frac{\partial J}{\partial K_d} = \frac{K_d}{J}\sum_{k=2}^{N+1}\frac{\partial J_k}{\partial K_d} \tag{5-48}$$

where:

$$\frac{\partial J_k}{\partial K_d} = -\,2h_k h_t \sum_{i=1}^{I_M}\left(W_1 L_{k,i}\frac{\partial L_{k,i}}{\partial K_d} + W_2 C_{k,i}\frac{\partial C_{k,i}}{\partial K_d}\right) \tag{5-49}$$

and

$$S^{J}_{K_a} = \frac{K_a}{J}\,\frac{\partial J}{\partial K_a} = \frac{K_a}{J}\sum_{k=2}^{N+1}\frac{\partial J_k}{\partial K_a} \tag{5-50}$$

where:

$$\frac{\partial J_k}{\partial K_a} = -\,2h_k h_t \sum_{i=1}^{I_M} W_2\tilde{C}_{k,i}\frac{\partial C_{k,i}}{\partial K_a} \tag{5-51}$$

since $\frac{\partial L_{k,i}}{\partial K_a} = 0$ for all values of k and i (5-52)

It has been shown in this chapter that application of spatial discretization followed by hierarchical systems analysis techniques permits direct use of methods of sensitivity analysis developed for lumped parameter systems and efficient solution of the resulting equations. This approach yielded a subproblem hierarchy for the generation of state trajectory sensitivity coefficients from the optimized state variables of the original control problem. It was further shown that if discretization and hierarchical techniques were applied to the original optimal control problem, the resulting subproblem hierarchy would have the same structure as the hierarchy for the generation of the state trajectory sensitivity coefficients. The foregoing was applied to a dynamic water pollution control problem involving a tapered stream.

Methods were developed for generating performance index sensitivity functions from the state trajectory sensitivity coefficients and the optimal space-time control variable contours. These methods were applied to the dynamic water pollution control problem cited above.

CHAPTER 6

COMPUTER PROGRAMS AND NUMERICAL RESULTS

The multilevel dynamic concentrations models presented in Chapters 2 and 3 of this dissertation, except for the two-dimensional regional models, were coded in Fortran for digital computer solution. These models differ from the corresponding models described elsewhere in the literature to the extent that no packaged programs were available a priori to represent them on the computer. Accordingly, new computer programs were designed by combining the coded equations of the models with the logical relationships and the initial, final and boundary conditions necessary for the solution of these equations.

This chapter is divided into two main parts. In the first part, the three most general computer programs utilized in the present research are described briefly. In the second part, representative numerical results obtained with these programs are presented.

6.1 Computer Programs

Due to the evolutionary nature of the development of these concentrations models, models developed later can, with appropriate simplifications, reproduce numerical results obtained by models developed earlier. More specifically, the two-step discrete finite-difference distributed parameter models of Chapter 3 are capable of reproducing all of the numerical results obtained with the discretized continuous distributed parameter models of Chapter 2. Furthermore, the discrete models of Chapter 3 are more versatile than their counterparts of Chapter 2 in that they can accommodate tidal reversals and other temporal changes in the net volume flow rate. For these reasons all of the numerical results displayed in the present chapter were obtained by using three digital computer programs developed from the discrete models of Chapter 3. These computer programs may be associated with their antecedent discrete models as follows. TIDALB is the name of the program based upon the discrete single reach tidal river model; BASIN is a regional multireach extension of TIDALB and ESTUARY corresponds to the discrete two dimensional single reach estuary model. Since appropriate simplifications could reduce either BASIN or ESTUARY to the form of TIDALB, these first two programs are the fundamental members of the set of programs developed in this research.

Although each of the three programs cited above was designed in the form of a main program without any subprograms, each is comprised of modules which are associated as shown in the flow charts of Figures 6-1 through Figure 6-3. TIDALB and ESTUARY share a common overall flow chart because each of these programs corresponds to a single reach.

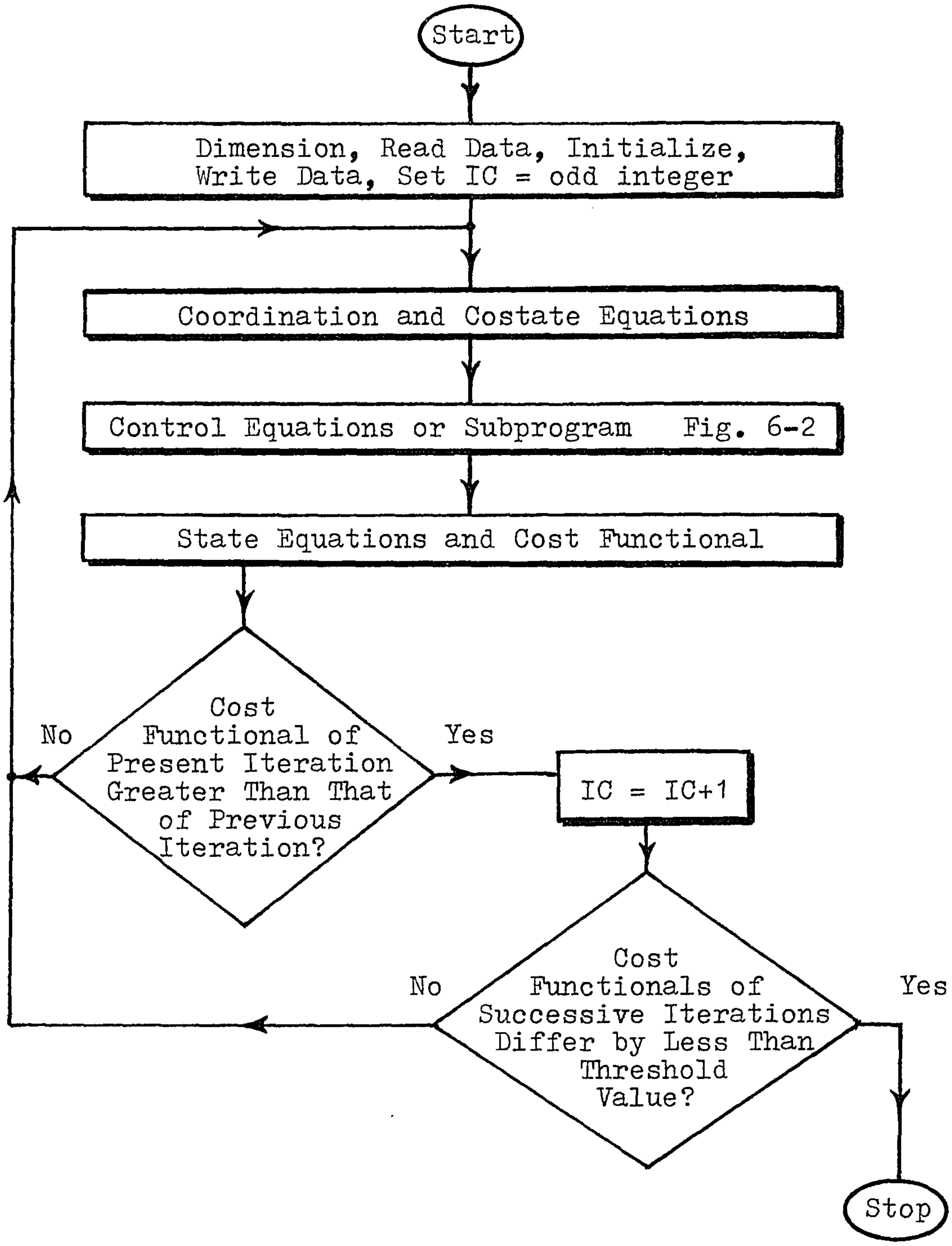


Figure 6-1: TIDALB and ESTUARY program flow chart

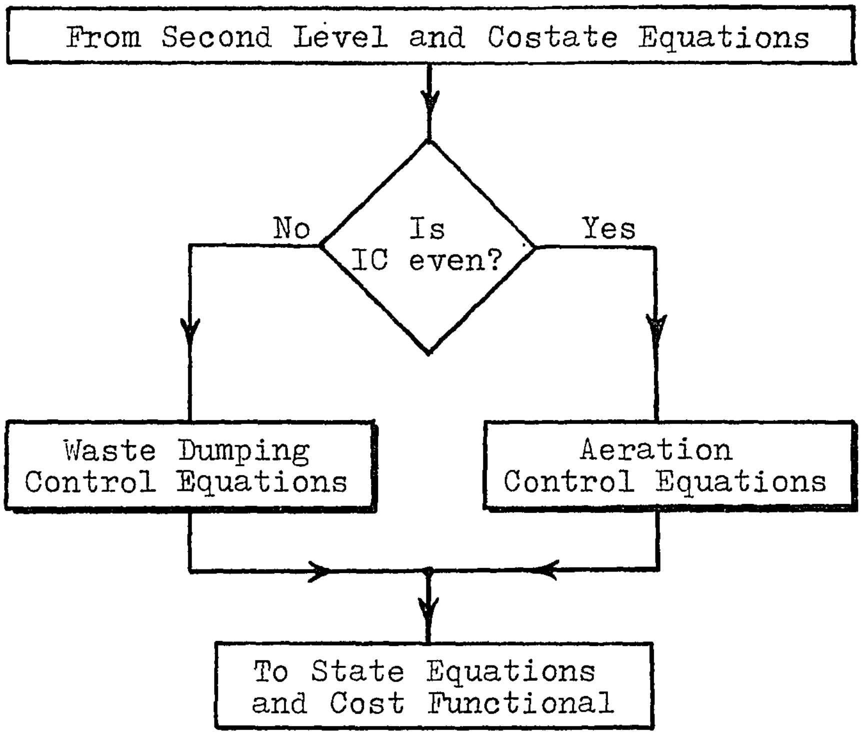


Figure 6-2: Bimodal aeration and waste dumping subprogram flow chart

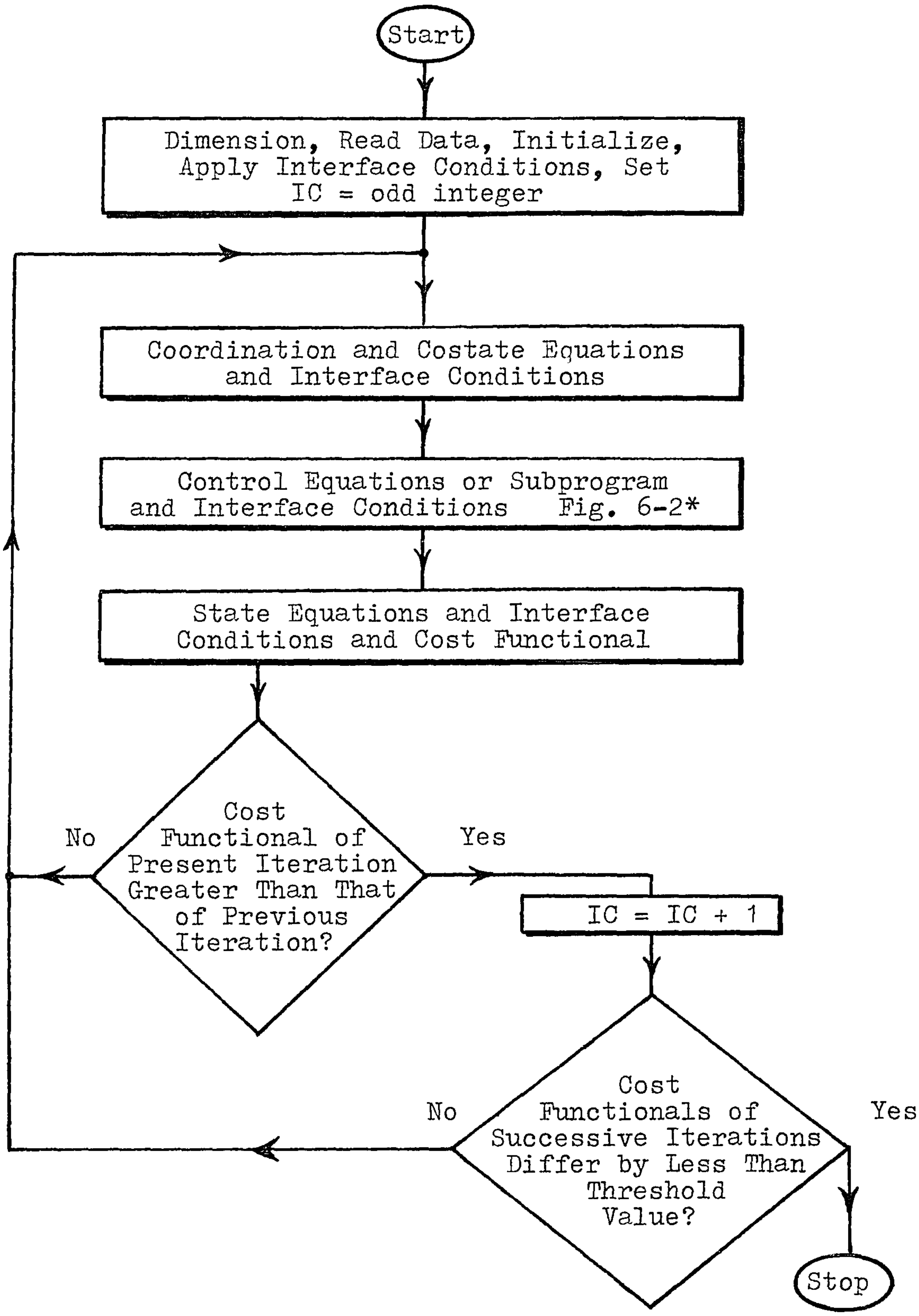


Figure 6-3: BASIN program flow chart.

The numbers in the "Control Equations or Subprogram" block refer to the number of the figure depicting the flow chart for that portion of the overall flow chart when bimodal aeration and waste dumping control is applied to the reach of the waterway. The integer variable, IC, is utilized to provide alternate applications of waste dumping and aeration control to attain an optimum balance between the two modes. If only a single mode of control, such as aeration, waste dumping, or flow augmentation, is applied, the corresponding control equations would replace the "Control Subprogram" and the generation of the switching variable, IC, would be unnecessary.

The overall flow chart associated with BASIN is of the same form as that for TIDALB and ESTUARY, but more complex due to the incorporation of interreach interface conditions in the first four blocks. As indicated in Chapter 3, these interface conditions are quite general in that they can accommodate the addition of BOD and DO concentrations and a volume flow rate at each interface between the contiguous reaches in the regional model to which BASIN corresponds. In practical terms, BASIN is capable of representing on the computer the case in which either a tributary or an effluent source or both discharge into the river at each interface between its constituent reaches. As with the overall flow chart for the single reach models, the numbers in the third box indicate the flow chart which may be substituted for the box in the case of bimodal aeration and waste dumping control. The asterisk associated with these numbers indicates that, for this application, the control equations of Figure 6-2 must be associated with appropriate interface conditions as stated in Chapter 3.

A common characteristic of the three cited programs is that the equations of their corresponding models are expressed as functions of the volume flow rate, Q, and the cross sectional area, A, which in turn, are expressed as functions of spatial location. The three programs thus have the capability of representing on the computer waterways that taper.

6.2 Numerical Results

The numerical results presented in the balance of this chapter were obtained by utilizing the programs described in Section 6.1 in conjunction with an IBM 370/158 digital computer and the computer requirements cited in the present section are predicated upon the use of such equipment. The numerical results are associated with the particular program from which they were generated. The programs themselves are arranged in the order of increasing complexity, beginning with the program representing the single reach tidal river model, progressing through the multireach regional tidal river model and concluding with the single reach two-dimensional estuary model. Since each of the models upon which the programs are based is dynamic, the numerical results presented are instantaneous values. Concentrations are stated in units of mg/l (or ppm).

6.2.1 Single reach tidal river models. Two cases utilizing TIDALB, the program representing a single reach of a tidal river, are presented in this subsection. The first of these is a case in which the concentrations of the reach are controlled by spatially distributed aerators and waste dumping. The computer requirements for this example are: 42.43 seconds execution time, 160K of core and the reading of 355 cards.

The second case is one for which the concentrations of the reach are controlled by spatially distributed waste dumping and a single aerator. The computer requirements for this example are: 48.84 seconds execution time, 160K of core and the reading of 355 cards.

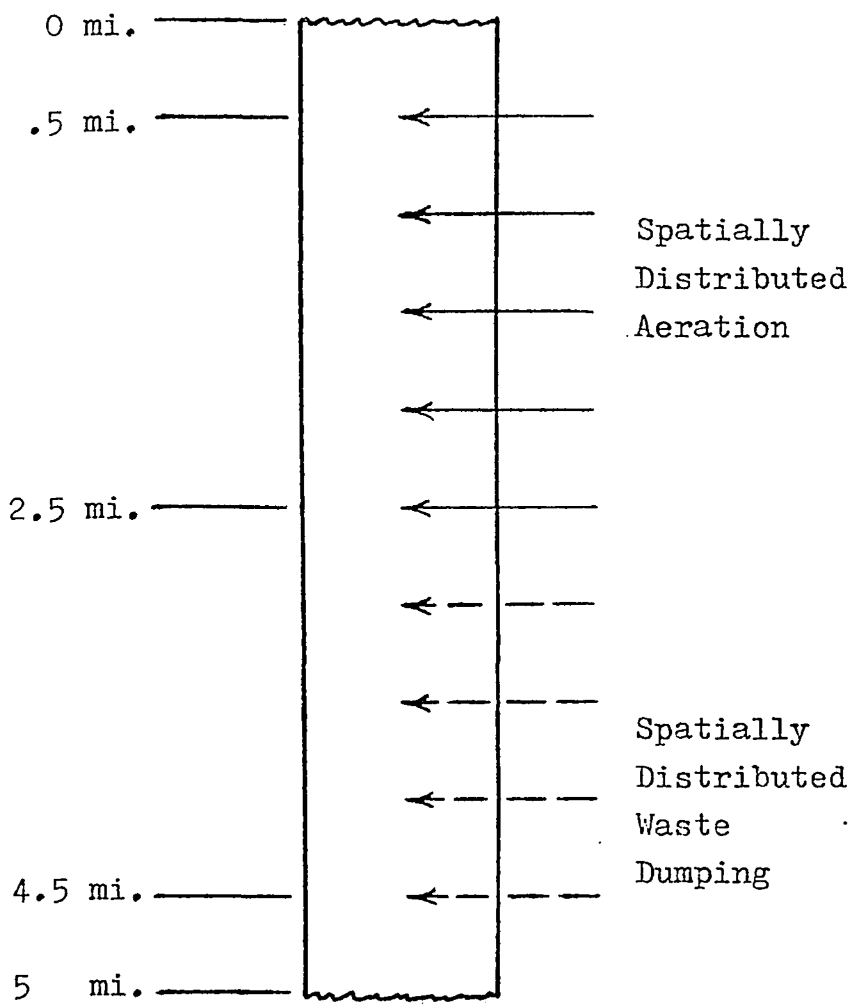


Figure 6-4: Single reach tidal river model with spatially distributed aeration and waste dumping (April 17, 1975).

L_o = 30 mg./l.

C_o = 6 mg./l.

Q_o = .75

Temperature = 290^o

K_r = .164/day

K_d = .164/day

K_a = .658/day

D = .12 mi^2/day

PR = .925 mg/l-day

BD = 0

C_{sp} = 6 mg./l.

C_s = 9.06 mg./l.

Q_T = 0

A = 1.0

W_2 = .40

W_4 = .05

W_5 = 1.0

Table 6-1: Parameter values applied to tidal river model of April 17, 1975.

x (mi)	Time (hr.) 0	15	30	45	60	75	90	105	120
0	30.0	→	→	→	→	→	→	→	30.0
1	23.8	23.9	→	→	→	→	→	→	23.9
2	18.9	19.0	→	→	→	→	→	→	19.0
3	15.0	→	→	→	→	→	→	→	15.0
4	11.9	→	→	→	→	→	→	→	11.9
5	9.42	9.3	→	→	→	→	→	→	9.3

Table 6-2: BOD concentration distributions for tidal river with distributed bimodal control (April 17, 1975 - first iteration).

Time (hr.)

x (mi)	0	15	30	45	60	75	90	105	120
0	6.00	⟶							6.00
1	4.30	4.81	5.38	5.49	5.72	5.71	5.77	5.64	5.53
2	4.74	5.09	5.39	5.55	5.85	5.88	6.00	5.87	5.79
3	5.66	5.79	5.82	5.90	6.06	6.08	6.18	6.10	6.10
4	6.58	6.67	6.59	6.61	6.63	6.63	6.67	6.62	6.62
5	7.35	7.47	7.40	7.40	7.35	7.33	7.33	7.30	7.30

Table 6-3: DO concentration distribution for tidal river with distributed bimodal control (April 17, 1975- 18th iteration).

Time (hr.)

x (mi)	0	15	30	45	60	75	90	105	120
0	30.0	⟶							30.0
1	23.8	23.2	24.0	23.7	24.1	24.0	24.2	24.1	24.1
2	18.9	18.3	19.2	18.7	19.4	19.0	19.5	19.2	19.2
3	15.0	14.6	15.3	14.9	15.5	15.0	15.6	15.2	15.2
4	11.9	11.7	12.4	12.1	12.7	12.3	12.7	12.2	12.1
5	9.42	9.04	9.58	9.39	9.86	9.60	10.0	9.66	9.51

Table 6-4: BOD concentration distribution for tidal river with distributed bimodal control (April 17,1975-18th iteration).

Time (hr.)

x (mi)	0	15	30	45	60	75	90	105	120
0	0	→	→	→	→	→	→	→	0
.5	↓	1.18	1.09	.985	.880	.824	.644	.432	↓
1	↓	1.33	1.22	1.08	.984	.917	.744	.526	↓
1.5	↓	1.21	1.10	.956	.888	.818	.674	.489	↓
2.0	↓	.871	.789	.677	.644	.586	.494	.366	↓
2.5	↓	.427	.375	.309	.313	.280	.255	.200	↓
3.0	0	→	→	→	→	→	→	→	0

Table 6-5: DO control profiles for tidal river model with distributed bimodal control (April 17, 1975 - iteration 18).

x (mi)	Time (hr.) 0	15	30	45	60	75	90	105	120
2.5	0	→	→	→	→	→	→	→	0
3	↓	.306	.315	.256	.195	.054	.017	.001	↓
3.5	↓	.699	.696	.634	.553	.315	.186	.025	↓
4	↓	.782	.773	.733	.676	.472	.330	.065	↓
4.5	↓	.492	.484	.471	.450	.367	.297	.105	↓
5	0	→	→	→	→	→	→	→	0

Table 6-6: BOD control profiles for tidal river model with distributed bimodal control (April 17, 1975 - iteration 18).

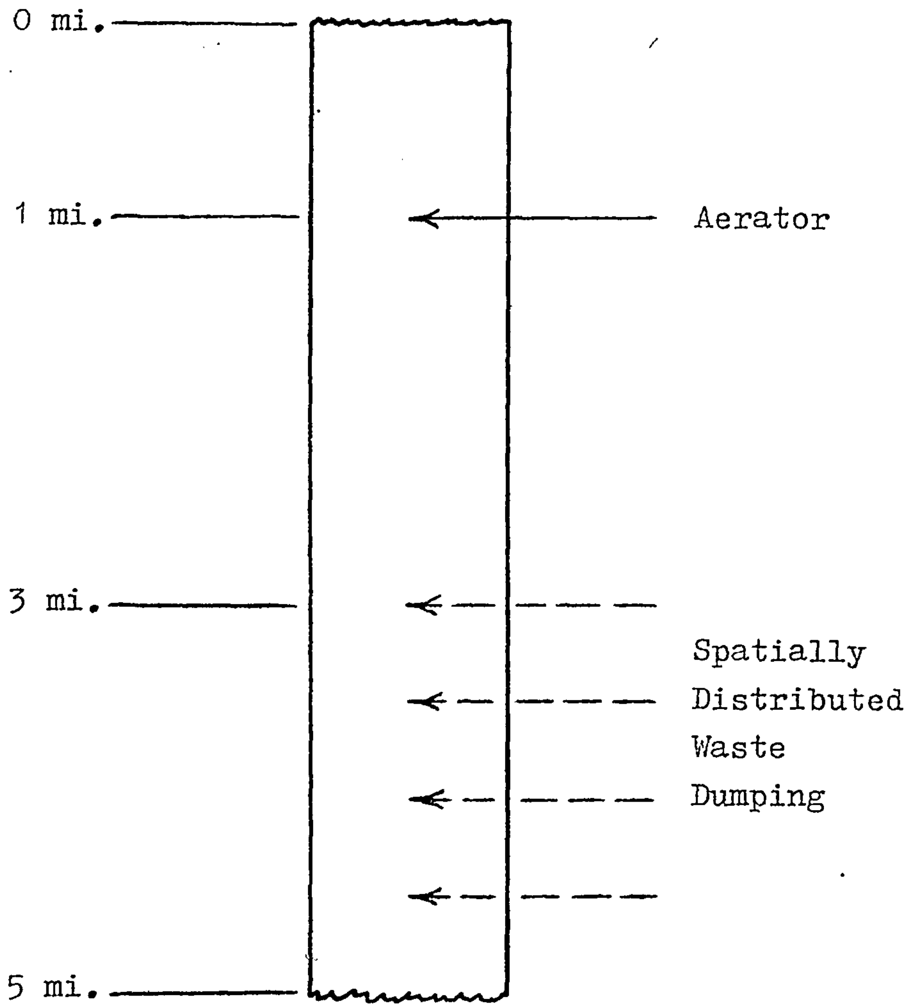


Figure 6-5: Single reach tidal river model with aerator at minimum of DO sag curve and distributed waste dumping (May 21, 1975).

L_o = 30 mg./l.

C_o = 6 mg./l.

Q_o = .75

Temperature = 290^o

K_r = .164/day

K_d = .164/day

K_a = .658/day

D = .12 mi^2/day

PR = .925

BD = 0

C_{sp} = 6 mg./l.

C_s = 9.06 mg./l.

Q_T = .10

A = 1.0

W_2 = .40

W_4 = .05

W_5 = 1.00

Table 6-7: Parameter values applied to tidal river model of May 21, 1975.

Time (hr.)

x (mi)	0	15	30	45	60	75	90	105	120
0	30.0	———	———	———	———	———	———	——→	30.0
1	23.8	24.0	23.8	23.8	23.9	24.0	24.0	23.8	23.8
2	18.9	19.0	18.9	18.9	19.0	19.1	19.0	18.9	18.9
3	15.0	15.1	15.0	15.0	15.0	15.1	15.1	15.0	15.0
4	11.9	12.0	11.9	11.9	11.9	12.0	12.0	11.9	11.9
5	9.42	9.33	9.27	9.26	9.30	9.34	9.33	9.27	9.25

Table 6-8: BOD concentration distributions for tidal river model with aerator at minimum of DO sag curve (May 21, 1975 - 29th iteration).

Time (hr.)

x (mi)	0	15	30	45	60	75	90	105	120
0	6.00	⟶							6.00
1	4.30	4.96	5.51	5.65	5.80	5.73	5.73	5.55	5.46
2	4.74	4.90	5.02	5.15	5.38	5.41	5.55	5.51	5.57
3	5.66	5.77	5.74	5.77	5.81	5.81	5.94	5.92	6.01
4	6.58	6.66	6.60	6.58	6.55	6.52	6.57	6.56	6.62
5	7.35	7.47	7.42	7.40	7.34	7.29	7.29	7.26	7.29

Table 6-9: DO concentration distributions for tidal river model with aerator at minimum of DO sag curve (May 21, 1975 - 29th iteration).

Time (hr.)

x (mi)	0	15	30	45	60	75	90	105	120
0	30.0	⟶							30.0
1	23.8	23.2	23.9	23.7	24.2	24.1	24.1	24.0	24.2
2	18.9	18.4	19.0	18.7	19.4	19.1	19.5	19.2	19.6
3	15.0	14.8	15.4	15.1	15.6	15.3	15.6	15.3	15.7
4	11.9	11.8	12.6	12.5	13.0	12.8	12.9	12.5	12.8
5	9.42	9.04	9.55	9.54	10.2	10.1	10.4	10.1	10.2

Table 6-10: BOD concentration distributions for tidal river model with aerator at minimum of DO sag curve (May 21, 1975 - 29th iteration).

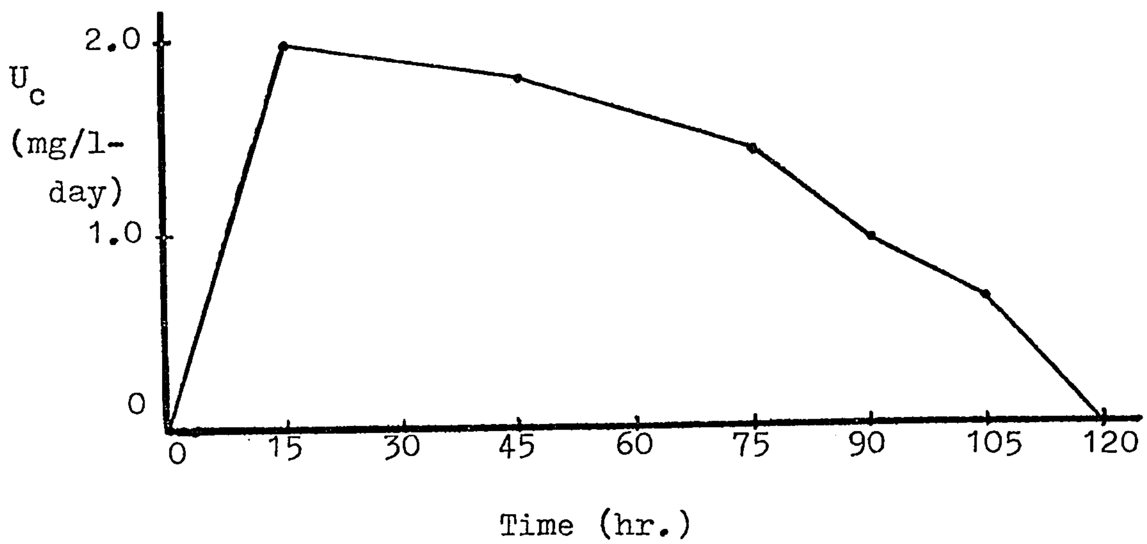


Figure 6-6: DO control profile at x = 1 mile in tidal river model of May 21, 1975 (29th iteration).

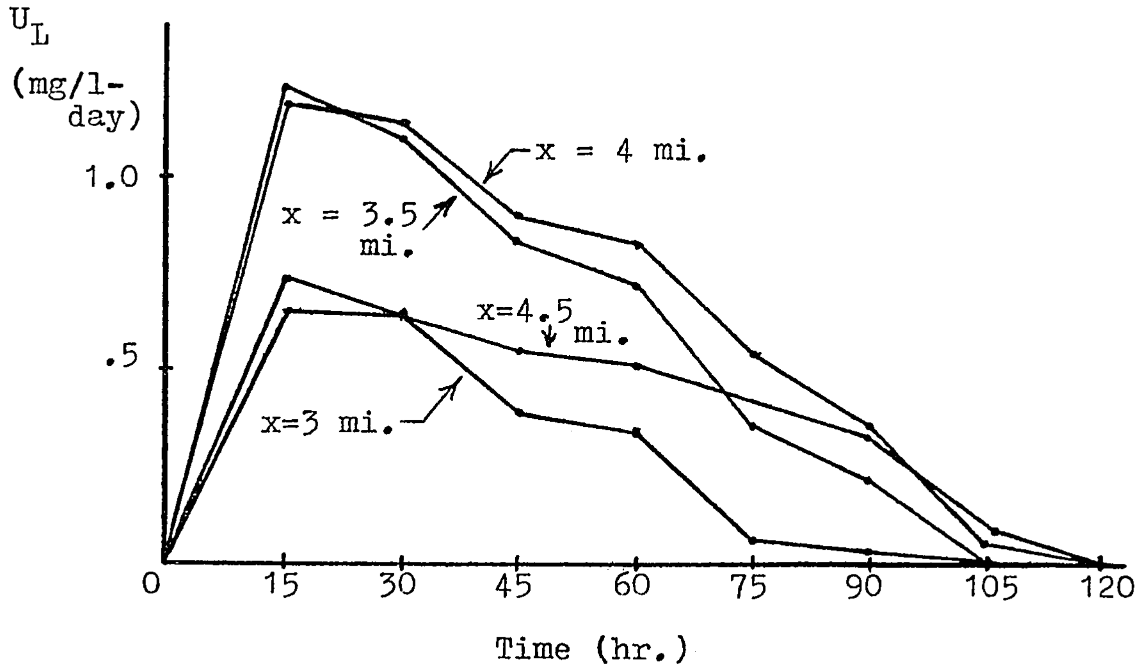


Figure 6-7: BOD control profiles for tidal river model of May 21, 1975 (29th iteration).

6.2.2 Multireach tidal river models. Two cases utilizing BASIN, the program representing a multireach regional model of the concentrations balances in a tidal river are presented in this subsection. The first of these is a four reach model with concentrations controlled by spatially distributed aeration and waste dumping. The computer requirements for this example are 44.3 seconds for central processor units, 8728 kilobytes of core and the reading of 508 cards.

The second case is a six reach tidal river basin model with a linear taper in the two reaches at the downstream end. The concentrations of this model are controlled by spatially distributed aerators. The computer requirements for this example are 34.5 seconds central processor units, 6771 kilobytes of core and the reading of 530 cards.

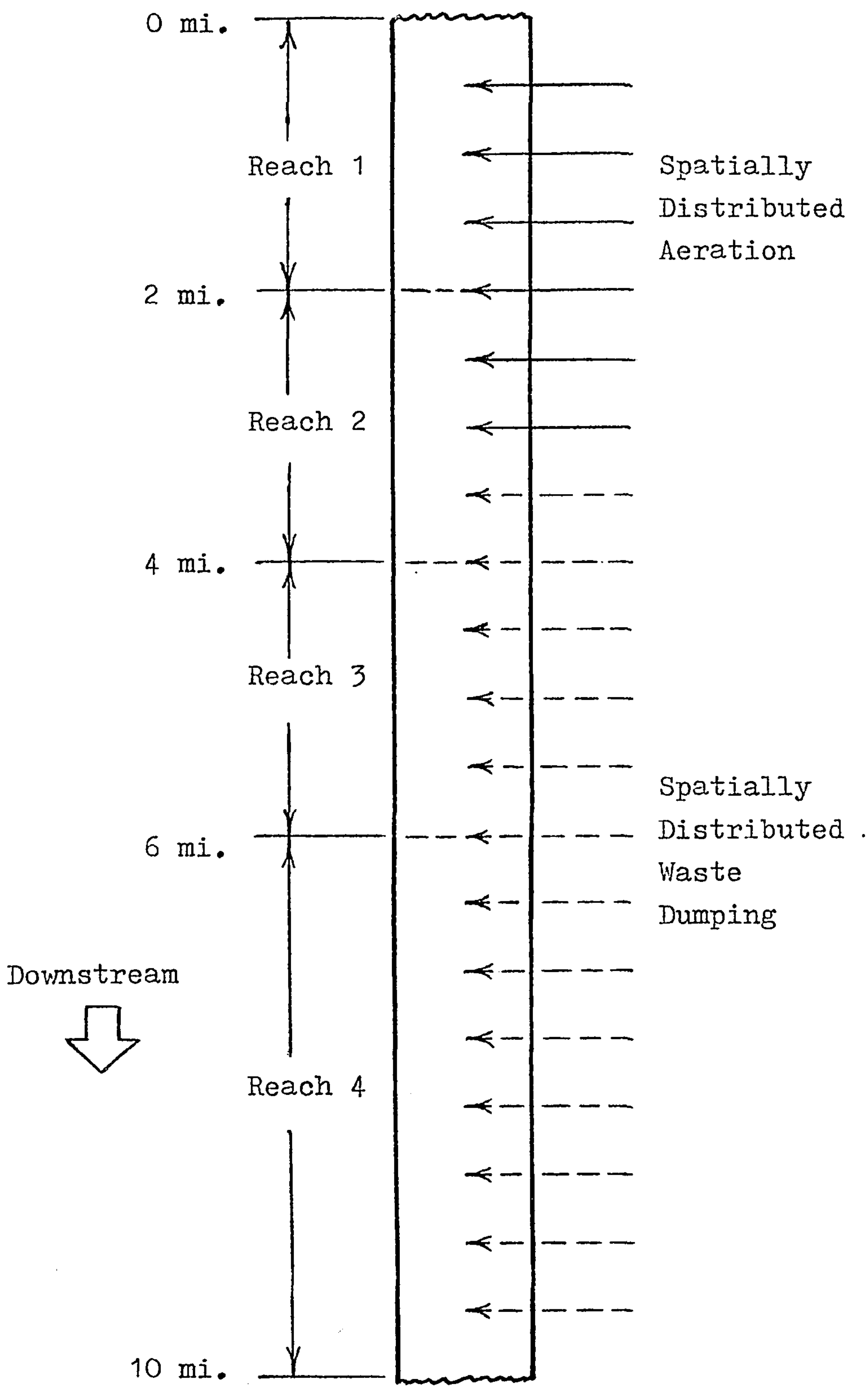


Figure 6-8: Four reach tidal river basin model (December 18, 1975)

No. of reaches = 4

L_o = 30 mg/l

C_o = 6 mg/l

Q_o = .75

Temperature = 290^o

K_r = .164/day

K_d = .164/day

K_a = .658/day

D = .12 mi^2/day

PR = .925 mg/l-day

BD = 0

C_{sp} = 6 mg/l

W_2 = .40

W_4 = .05

W_5 = 1.0

Reach No.	Q_T	A_d	L_a	C_a	Q_a
1	0	1.0	0	0	0
2	.5	1.0	0	0	0
3	1.0	1.0	0	0	0
4	1.5	1.0	0	0	0

Table 6-11: Parameter values applied to river basin model of December 18, 1975.

x (mi)	Time (hr.) 0	3	6	9	12	15	18	21	24
0	6.00	5.87	→	→	→	→	→	→	5.87
1	4.60	4.61	→	→	→	→	→	→	4.61
2	4.89	4.87	→	→	→	→	→	→	4.87
3	5.68	5.66	5.67	5.69	5.69	5.67	5.67	5.69	5.69
4	6.51	6.51	6.53	6.67	6.66	6.52	6.52	6.65	6.68
5	7.25	7.23	7.24	7.28	7.27	7.23	7.23	7.27	7.28
6	7.88	7.86	7.87	7.90	7.90	7.87	7.87	7.89	7.90
7.2	8.49	8.47	8.47	8.51	8.51	8.47	8.47	8.50	8.52
8	8.82	8.80	8.81	8.83	8.84	8.80	8.80	8.83	8.84
9.2	9.06	→	→	→	→	→	→	→	9.06

Table 6-12: DO concentration profiles for river basin (December 18, 1975 - first iteration).

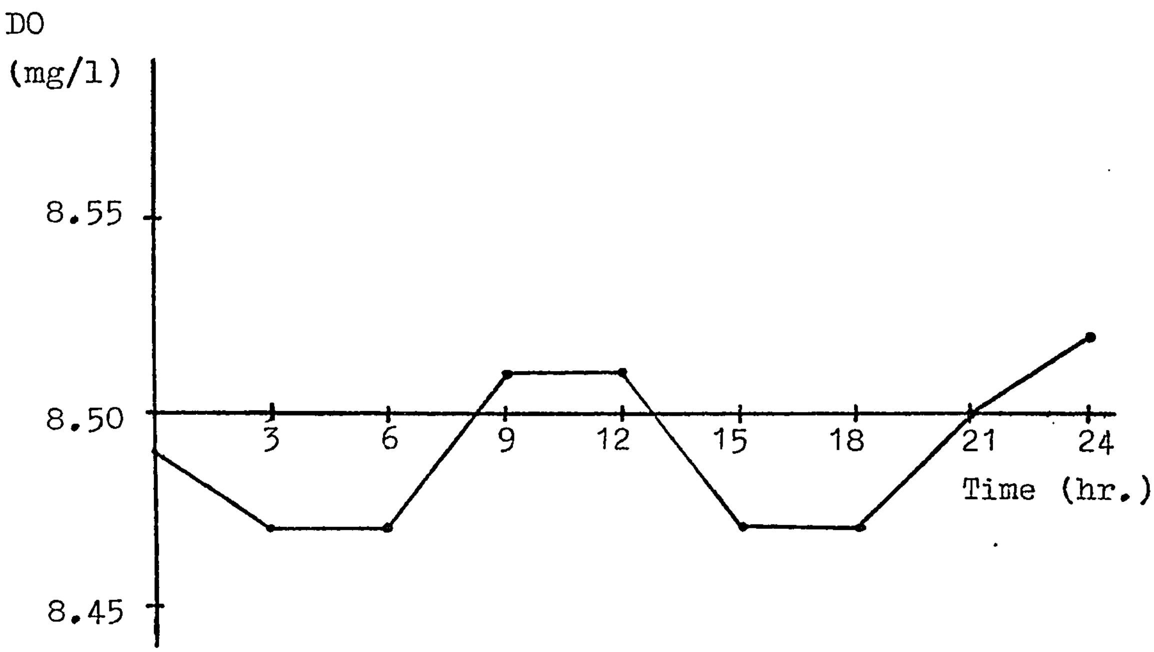


Figure 6-9: Temporal variation of DO concentration at x = 7.2 miles in river basin model of December 18, 1975 (first iteration).

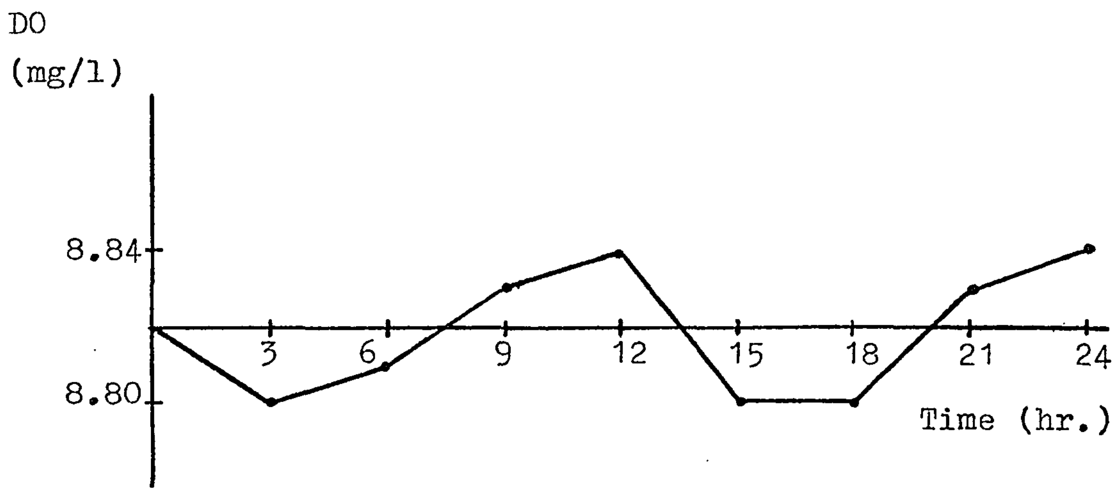


Figure 6-10: Temporal variation of DO concentration at x = 8 miles in river basin model of December 18, 1975 (first iteration).

x (mi)	Time (hr.) 0	3	6	9	12	15	18	21	24
0	30.0	⟶							30.0
1	24.0	⟶							24.0
2	19.2	19.1	⟶						19.1
3	15.4	15.4	15.4	15.3	15.3	15.4	15.4	15.3	15.3
4	12.3	12.3	12.3	12.2	12.2	12.3	12.3	12.2	12.2
5	9.81	9.86	9.90	9.78	9.72	9.83	9.90	9.80	9.72
6	7.84	7.86	7.89	7.80	7.75	7.84	7.89	7.82	7.75
7.2	5.96	6.01	6.04	5.93	5.88	5.98	6.05	5.95	5.87
8	4.96	5.00	5.00	4.94	4.90	4.98	5.04	4.96	4.89
9.2	3.77	3.80	3.82	3.75	3.72	3.79	3.83	3.77	3.72

Table 6-13: BOD concentration profiles for river basin (December 18, 1975 - first iteration).

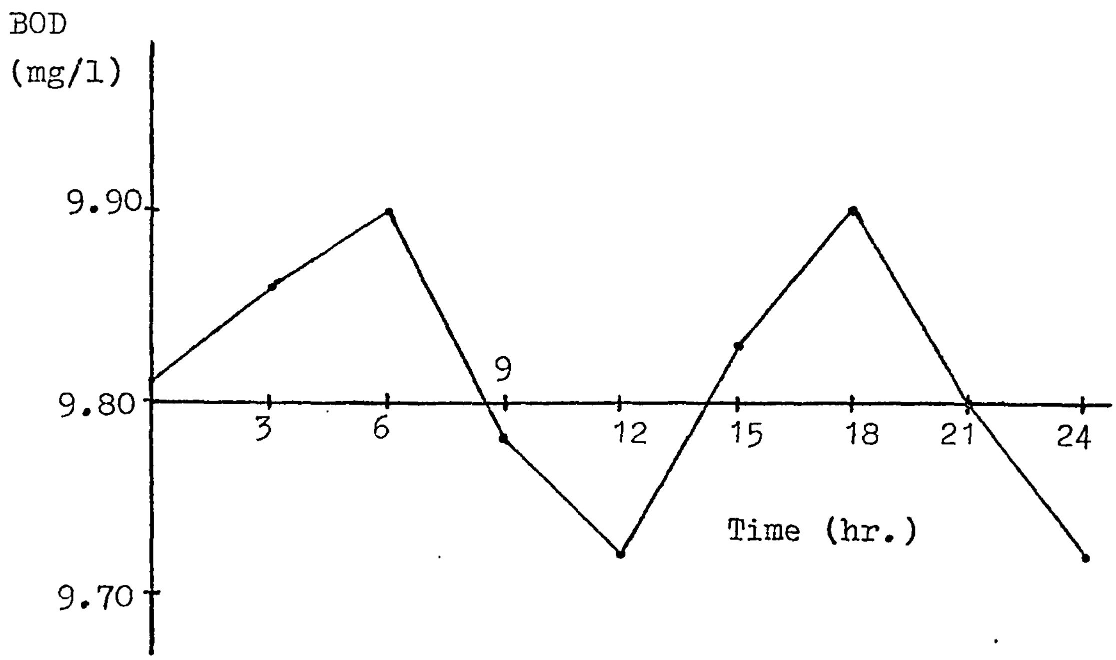


Figure 6-11: Temporal variation of BOD concentration at x = 5 miles in river basin model of December 18, 1975 (first iteration).

x (mi)	Time (hr.) 0	3	6	9	12	15	18	21	24
0	6.00	5.87	5.90	5.90	5.89	5.89	5.89	5.89	5.89
1	4.60	4.73	4.88	4.98	5.03	5.04	5.01	4.96	4.92
2	4.89	4.97	5.06	5.12	5.14	5.14	5.11	5.07	5.03
3	5.67	5.69	5.66	5.67	5.69	5.70	5.85	5.85	5.72
4	6.51	6.51	6.47	6.49	6.53	6.53	6.51	6.51	6.53
5	7.25	7.23	7.13	7.12	7.19	7.18	7.37	7.37	7.24
6	7.88	7.87	7.81	7.84	7.90	7.89	7.86	7.37	7.90
7.2	8.49	8.46	8.30	8.30	8.40	8.41	8.56	8.52	8.46
8	8.82	8.80	8.73	8.75	8.82	8.80	8.80	8.83	8.83
9.2	9.06	→	→	→	→	→	→	→	9.06

Table 6-14: DO concentration profiles for river basin model of December 18, 1975 (26th iteration).

x (mi)	Time (hr.) 0	3	6	9	12	15	18	21	24
0	0	→						→	0
1	↓	1.12	.951	.856	.660	.561	.343	.233	↓
2		.878	.766	.700	.553	.474	.297	.204	
3	↓	.091	.119	.105	.091	.085	.074	.060	↓
4	0	→						→	0

Table 6-15: DO rate control profiles for river basin model of December 18, 1975 (26th iteration).

x (mi)	Time (hr.) 0	3	6	9	12	15	18	21	24
3	0	⟶							0
4	0	.106	.091	.061	.047	.022	.013	.002	0
5	0	.208	.181	.126	.100	.049	.030	.005	0
6	0	.302	.264	.184	.145	.073	.046	.008	0
7.2	0	.378	.334	.235	.185	.094	.058	.011	0
8	0	.427	.377	.265	.208	.107	.067	.012	0
9.2	0	.390	.370	.260	.199	.112	.073	.013	0

Table 6-16: BOD (damping) control profiles for river basin model of December 18, 1975 (26th iteration).

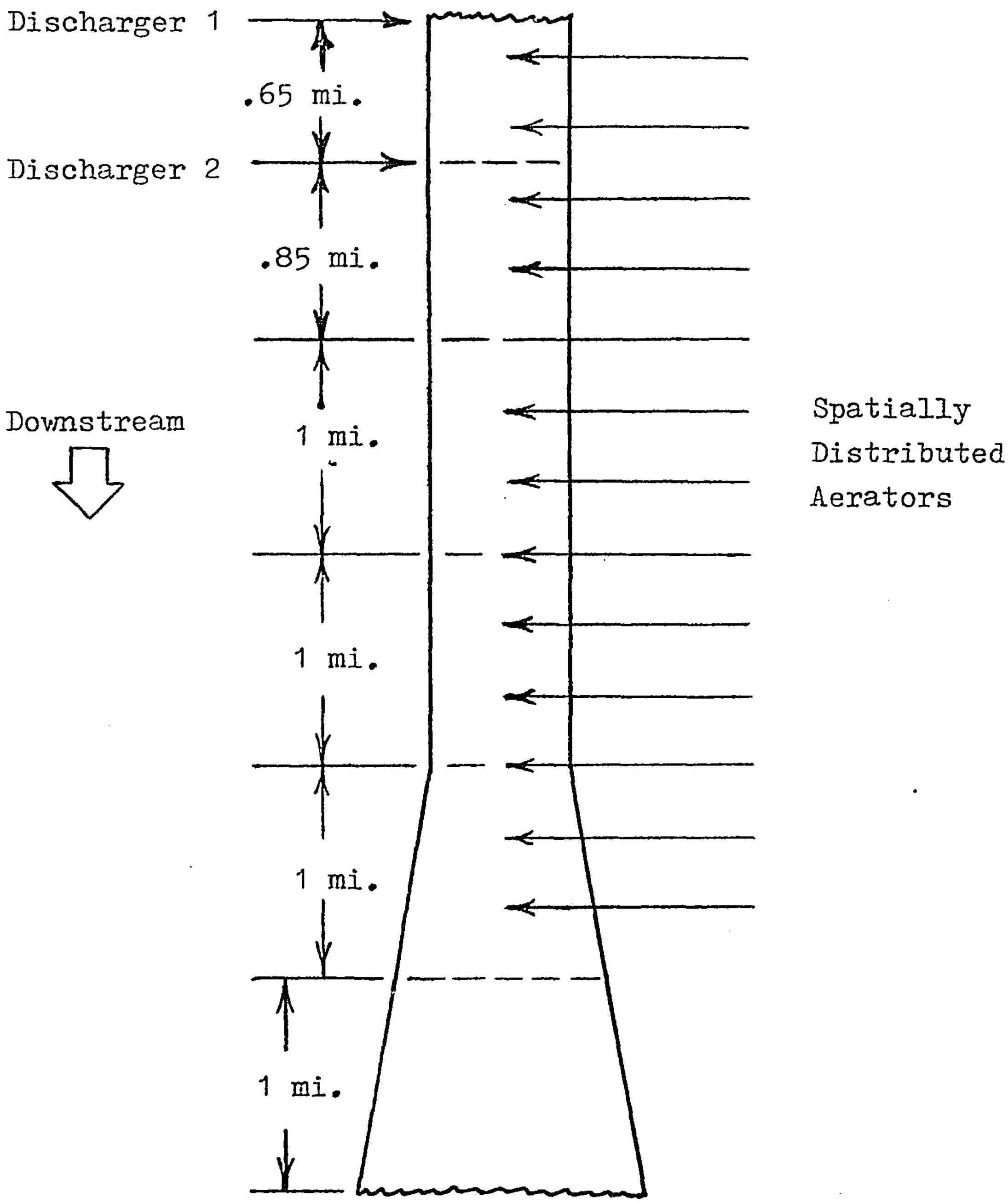


Figure 6-12: Six reach tidal river basin model with taper and distributed aeration control (February 18, 1976).

No. of reaches = 6

L_o = 30

C_o = 6

Q_o = 1.00

Temperature = 290^o

K_r = .164

K_d = .164

K_a = .658

D = .12

PR = .925

BD = 0

C_{sp} = 6.0

W_2 = .4

W_4 = .05

W_5 = 1.0

Reach No.	Q_T	A_d	L_a	C_a	Q_a
1	0	1.0	256	0	.084
2	0	1.0	100	0	.042
3	.13	1.0	0	0	0
4	.13	1.0	0	0	0
5	.13	1.5	0	0	0
6	.13	2.0	0	0	0

Table 6-17: Parameter values used in river basin model of February 18, 1976.

x (mi)	Time (hr.) 0	15	30	45	60	75	90	105	120
0	28.1	⟶							28.1
.43	26.3	26.3	25.5	25.6	⟶				25.6
.93	27.1	25.1	25.2	⟶					25.2
1.5	24.9	25.2	24.4	24.4	24.4	24.4	24.4	24.4	24.4
2.17	22.5	21.9	22.4	22.5	22.7	22.7	22.5	22.4	22.5
2.83	20.4	19.8	20.3	20.4	20.6	20.5	20.3	20.3	20.4
3.5	18.5	17.9	18.2	18.3	18.4	18.3	18.2	18.2	18.3
4.17	16.6	15.9	16.2	16.3	16.4	16.4	16.3	16.2	16.3
4.83	14.4	13.9	14.1	14.2	14.3	14.2	14.1	14.1	14.2
5.5	12.0	11.6	11.9	12.0	12.1	12.1	12.0	11.9	12.0

Table 6-18: BOD concentration profiles for river basin model of February 18, 1976 (5th iteration).

x (mi)	Time (hr.) 0	15	30	45	60	75	90	105	120
0	5.53	→	→	→	→	→	→	→	5.53
.43	5.05	5.33	5.42	→	→	→	5.42	5.32	5.18
.93	4.50	4.94	5.15	5.16	5.16	5.16	5.16	5.09	4.92
1.5	4.31	4.75	5.10	→	→	→	5.10	5.04	4.87
2.17	4.35	4.87	4.97	→	→	→	4.97	4.92	4.77
2.83	4.58	5.05	5.10	→	→	→	5.10	5.06	4.94
3.5	4.91	5.29	5.29	5.29	5.30	5.30	5.30	5.26	5.18
4.17	5.32	5.65	5.62	5.63	5.63	5.64	5.63	5.62	5.57
4.83	5.88	6.07	6.02	6.02	6.03	6.03	6.03	6.02	6.02
5.5	6.55	6.57	6.59	6.59	6.60	6.60	6.60	6.59	6.59

Table 6-19: DO concentration profiles for tidal river basin with distributed aeration control (February 18, 1976 - 5th iteration).

x (mi)	Time (hr.) 0	15	30	45	60	75	90	105	120
0	0	0	0	0	0	0	0	0	0
.43	0	1.45	→	→	→	→	→	.89	0
.93	0	1.41	→	→	→	→	→	1.06	0
1.5	0	1.60	1.59	→	→	→	→	1.27	0
2.17	0	1.33	1.34	1.33	1.32	1.33	1.33	1.07	0
2.83	0	1.07	1.08	1.07	1.06	1.06	1.08	.88	0
3.5	0	.78	.79	.78	.77	.77	.78	.66	0
4.17	0	.38	.39	.38	.37	.37	.38	.34	0
4.83	0	→	→	→	→	→	→	→	0
5.5	0	→	→	→	→	→	→	→	0

Table 6-20: DO rate control profiles for river basin model of February 18, 1976 (5th iteration).

6.2.3 Single reach estuary models. Two cases utilizing ESTUARY, the program representing the single reach two-dimensional estuary model of concentration balances are presented in this subsection. The first of these is a model with concentrations controlled by an aerator 1/2 mile from the upstream end of the reach and spatially distributed waste dumping at the bottom of the reach. The computer requirements for this case are: 4.0 minutes execution time, 300K of core and the reading of 533 cards.

The second case is a model with concentrations controlled by spargers spatially distributed over the bottom of the reach and waste dumping also spatially distributed over the bottom of the reach. The computer requirements for this case are the same as for the first case.

L_o = 30 mg/l

C_o = 6.5 mg/l

Q_o = .25

Temperature = 295°

K_r = .250/day

K_d = .250/day

K_a = .650/day

D_x = .12 mi^2/day

D_z = .0005 mi^2/day

PR = 0

BD = 0

C_{sp} = 6 mg/l

C_s = 9.50 mg/l

Q_T = .10

A = 1.0

W_2 = .40

W_4 = .05

W_5 = 1.00

Table 6-21: Parameter values applied to estuary models of May 21, 1975 and June 13, 1975.

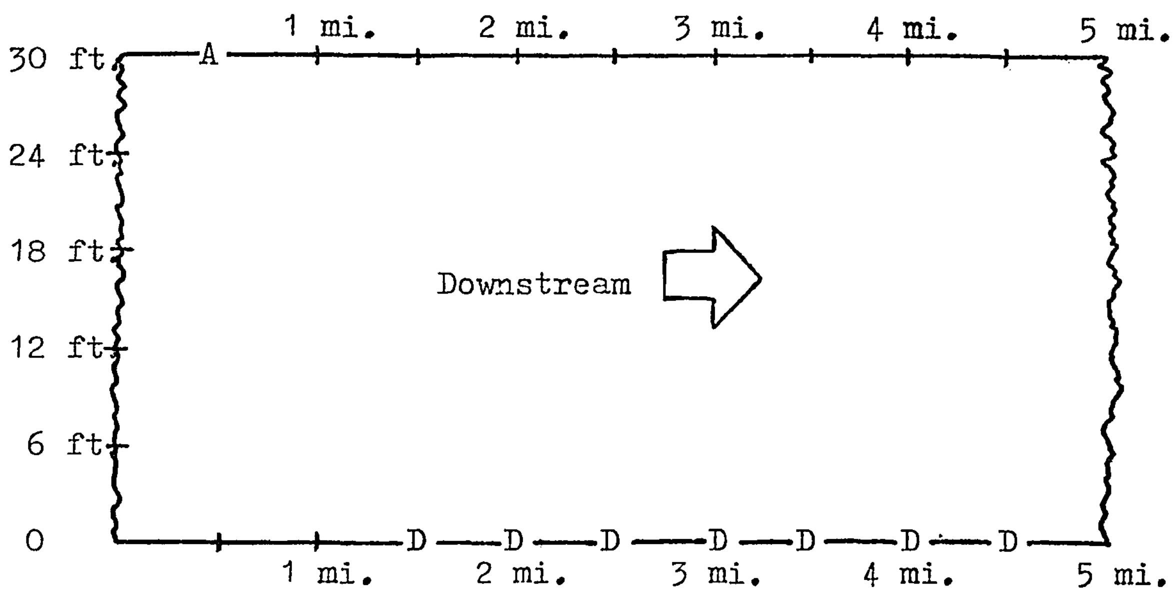


Figure 6-13: Side view of distribution of aeration and dumping control in estuary model of May 21, 1975.

z ft.	x miles 0	1	2	3	4	5
0	30.0	3.9	0.0	0.0	0.0	0.0
6	30.0	4.4	.40	0.0	0.0	0.0
12	30.0	4.8	.96	.15	.02	0.0
18	30.0	5.2	1.5	.50	.18	.04
24	30.0	5.5	2.0	.92	.47	.23
30	30.0	5.8	2.5	1.33	.76	.42

Table 6-22: BOD profiles for uncontrolled estuary (May 7, 1975).

z ft.	x miles 0	1	2	3	4	5
0	6.5	7.8	9.5	9.5	9.5	9.5
6	6.5	7.3	9.3	9.5	9.5	9.5
12	6.5	6.9	9.0	9.4	9.5	9.5
18	6.5	6.5	8.6	9.2	9.4	9.5
24	6.5	6.1	8.2	8.9	9.2	9.4
30	6.5	5.8	7.9	8.7	9.0	9.2

Table 6-23: DO profiles for uncontrolled estuary (May 7, 1975).

z ft.	x miles 0	1	2	3	4	5
0	6.5	6.8	9.5	9.5	9.2	8.7
6	6.5	6.4	9.0	9.5	9.3	9.1
12	6.5	6.0	8.4	9.4	9.5	9.5
18	6.5	5.7	7.8	8.8	9.2	9.3
24	6.5	5.4	7.3	8.3	8.6	8.9
30	6.5	5.1	6.7	7.7	8.2	8.4

Table 6-24: DO profiles with bimodal control (May 21, 1975 - iteration 14).

z ft.	Time (hr.) 15	30	45	60	75	90	105	120
0	2.92	2.44	2.35	1.07	.771	.459	.339	0
6	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0	0
30	0	0	0	0	0	0	0	0

Table 6-25: DO control profiles at x = .5 mile (May 21, 1975 - iteration 14).

x mi.	Time (hr.) 15	30	45	60	75	90	105	120
1	0	0	0	0	0	0	0	0
2	4.14	4.08	4.08	4.10	2.24	1.29	.18	0
3	5.62	5.59	5.58	5.58	3.26	1.97	.31	0
4	4.54	4.57	4.51	4.43	3.09	2.09	.36	0
5	0	0	0	0	0	0	0	0

Table 6-26: BOD control profiles at z = 30 feet (May 21, 1975 - iteration 14).

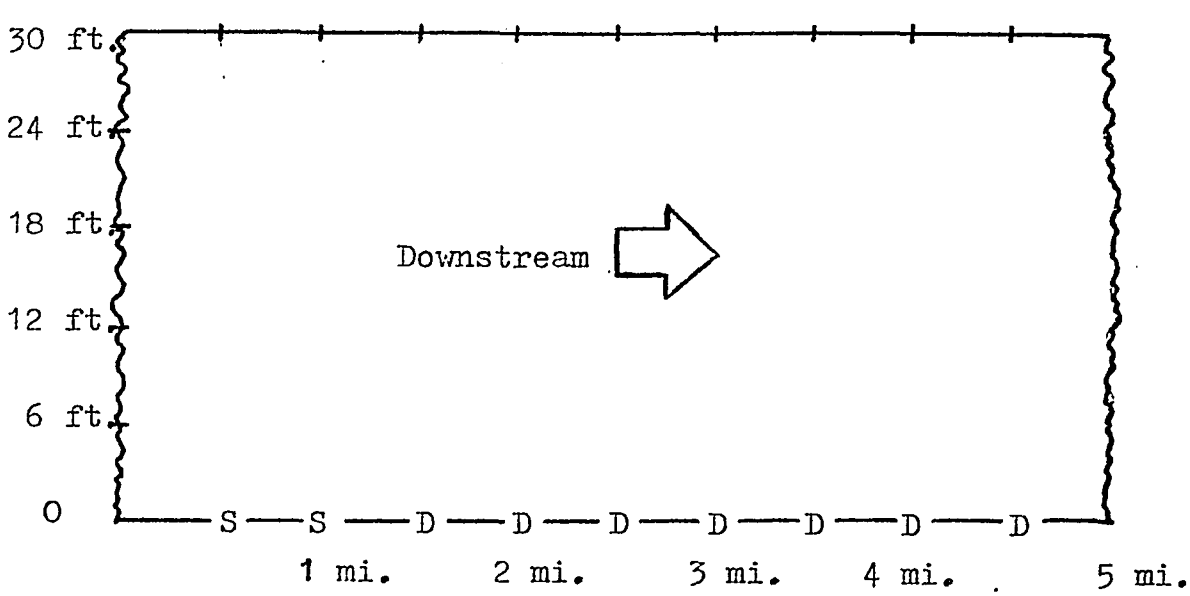


Figure 6-14: Side view of distribution of spargers and waste dumping in estuary model of June 13, 1975.

z ft.	x miles 0	1	2	3	4	5
0	6.5	6.8	9.5	9.5	9.2	8.7
6	6.5	6.4	9.0	9.5	9.3	9.1
12	6.5	6.0	8.5	9.4	9.5	9.5
18	6.5	5.6	7.8	8.9	9.2	9.3
24	6.5	5.3	7.3	8.3	8.7	8.9
30	6.5	5.1	6.7	7.7	8.2	8.4

Table 6-27: DO profiles with bimodal control (June 13, 1975 - iteration 13).

x mi.	Time (hr.) 15	30	45	60	75	90	105	120
.5	2.89	2.61	2.59	1.95	1.49	.809	.525	0
1	.28	.23	.26	.39	.47	.41	.32	0
2	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0

Table 6-28: DO control profiles at z = 30 feet (June 13, 1975 - iteration 13).

x mi.	Time (hr.) 15	30	45	60	75	90	105	120
1	0	0	0	0	0	0	0	0
2	4.14	4.08	4.08	4.10	2.24	1.29	.18	0
3	5.62	5.59	5.58	5.58	3.26	1.97	.31	0
4	4.54	4.57	4.51	4.43	3.09	2.09	.36	0
5	0	0	0	0	0	0	0	0

Table 6-29: BOD control profiles of z = 30 feet (June 13, 1975 - iteration 13).

This chapter has presented selected numerical results and a brief description of the digital computer programs by which they were obtained. The concentrations models antecedent to these computer programs were developed in Chapters 2 and 3 of this dissertation. Several topics of significance relative to the generation of practical solutions for these concentrations models were treated in Chapter 4 while Chapter 5 presented a multilevel hierarchical systems approach to the evaluation of sensitivity. Chapter 7 represents a culmination of the research described by this dissertation in that it describes the formulation of a complex multireach regional water quality model with economic constraints for which representative numerical results are presented.

CHAPTER 7

OPTIMUM DYNAMIC CONTROL OF A TIDAL RIVER WATER QUALITY SYSTEM SUBJECT TO ECONOMIC CONSTRAINTS

The overall objective of a water quality control problem is to achieve and sustain water quality at such levels as to permit beneficial use of the water. It is important, moreover, that this objective be achieved at minimum cost. Earlier work by Kerri[215] presented an economic model which is used to generate the minimum cost of attaining a water quality objective by optimizing effluent treatment costs for multiple waste dischargers taking into account the natural purification capacity of the receiving waters.

The construction of this economic model for minimization of collective effluent treatment costs for dischargers into a river is based upon maintenance of specified water quality levels in a critical reach of the river downstream from the outfalls of all of the dischargers. One major component of Kerri's economic model is a cost matrix displaying the cost of effluent treatment for each discharger affecting the critical reach. This cost matrix is constructed in a form to facilitate minimization of the total collective cost for all dischargers by techniques of linear programming. Once the total amount of effluent that the critical reach can assimilate without violating minimum water quality standards is calculated, it remains fixed.

The other major component of Kerri's economic model is a concentrations balance model of the portion of the river between the discharger located farthest upstream and the downstream end of the critical reach. Since this model includes at least one reach in addition to the critical reach, it actually is a regional model for which a hierarchical structure is especially appropriate. This is a realistic approach because it reflects current establishment of regional water quality management agencies. Moreover, use of a hierarchical formulation of the model improves computational efficiency.

The critical reach model employed in this study is a dynamic finite difference model for dissolved oxygen (DO) and biochemical oxygen demand (BOD) concentration rates in a tidal river water quality model developed by Bella and Dobbins(27). Since this finite-difference model was derived directly from physical considerations, it constitutes the basic distributed parameter model of the rate balances for DO and BOD. Hence, the concentration distributions generated from this model represent the actual concentration distributions more directly than do solutions of finite-difference approximations of continuous distributed parameter models.

The critical reach model is presented in a two-step form such that each concentration rate balance convection is executed first followed by all other applicable processes in a separate equation[106]. While this formulation doubles the number of equations required compared with similar models, it eliminates false dispersive effects that can cause the solutions of many models to converge to incorrect values. In addition, this model remains stable over a broader range of parameter values than do most comparable models. This may be verified by application of the numerical stability criteria of Leendertse[257] to various models under a variety of conditions, especially tidal flow reversal. Addition of cost-optimal aeration feedback control to this critical reach model converts it to an instream treatment cost minimization subproblem hierarchy.

Both the off-line dischargers' treatment cost model and the on-line instream treatment cost model imply the need for measurement of DO and BOD concentrations. DO can be measured on-line continuously; BOD is traditionally a five-day sample test. However, "fast BOD" and calibrated total organic carbon (TOC) measurement systems can be used and have been described in the wastewater treatment literature[413]. A technique for combining these "fast BOD" methods with BOD_5 measurements appears in Okunseinde[340]. In the present chapter it is assumed that measured variables are available using the above cited techniques and discussion is limited to control aspects of the problem.

The minimization subproblems involving the dischargers' treatment cost model and the instream treatment cost model, respectively, are coordinated at a higher level by a supremal coordination subproblem that adjusts the waste load entering the critical reach to minimize the sum of the dischargers' and the instream treatment costs. The dischargers' treatment cost minimization subproblem is constrained by the physical limitations of each discharger's treatment facilities.

This chapter offers the following contributions.

1.) It presents a corrected and more detailed exposition of Kerri's dischargers' treatment cost minimization problem.

2.) It substitutes a dynamic hierarchical model for the steady-state model of concentrations in the critical reach for more accurate representation of the assimilative capacity of the reach.

3.) It adds simulation of a set of optimally controlled aerators to the model of the critical reach to augment the assimilative capacity of the reach.

4.) It aggregates the dischargers' treatment cost minimization problem of Kerri with the instream treatment cost minimization problem to form a subproblem hierarchy to minimize total treatment cost.

5.) It presents an example demonstrating that aggregation of the dischargers' treatment cost minimization problem with the instream treatment cost minimization problem yields substantially lower total treatment cost than Kerri's dischargers' treatment cost minimization problem.

7.1 River Basin Economics Model

7.1.1 Input data. In Kerri's paper[215] DO concentration is used as the measure of water quality and BOD concentration is employed as a measure of the amount of pollution present in the critical reach. To arrive at the minimum total cost of attaining a specified level of DO concentration in the critical reach it is necessary to have a priori data on the relative costs of removing various percentages of BOD concentration from the effluent of each discharger upstream from this reach. Specifically, in order to begin solution of the problem, it is necessary to have a BOD removal cost curve for each such discharger. Tables 7-1 and 7-2 display such information from data given in Kerri's paper where the 100% removal points are included only to establish slopes for high removal percentages.

7.1.2 Dischargers' cost matrix. The dischargers' cost matrix for treatment of effluents to meet DO standards in a critical reach contains the amount of oxygen-consuming wastes passing through the critical reach from each discharger, the amount of waste removed by different levels of treatment and the cost of each level of treatment for each discharger. This matrix is similar to the one in Maass et. al.[280]. An example of the cost matrix for two waste dischargers, each removing between 40% and 90% BOD from its effluent, appears as Table 7-3.

The total amount of waste, measured at the critical reach, that must be removed by n dischargers upstream from the reach may be expressed as follows.

$$\sum_{i=1}^{n} a_i X_i \sum_{j=1}^{3} b_i Y_{ij} = \sum_{i=1}^{n} a_i X_i - P \qquad (7\text{-}1)$$

where:

X_i = rate of production of BOD by ith discharger before treatment.

a_i = proportion of ith discharger's waste entering the critical reach.

b_i = proportion of BOD removed from jth discharger's effluent before it enters the river.

Y_{ij} = interpolation coefficients between breakpoints on dischargers' treatment cost curves.

P = maximum BOD rate that critical reach can accept without violating specified minimum levels of DO concentration.

The first row of the dischargers' treatment cost matrix consists of the coefficients of the Y_{ij}'s on the left hand side of equation (7-1). The next n rows of the dischargers' treatment cost matrix are used to guarantee proper interpolation between the breakpoints on the BOD removal cost curves of Figure 7-1 which is based on data from Tables 7-1 and 7-2.

The bottom row of the dischargers' effluent treatment

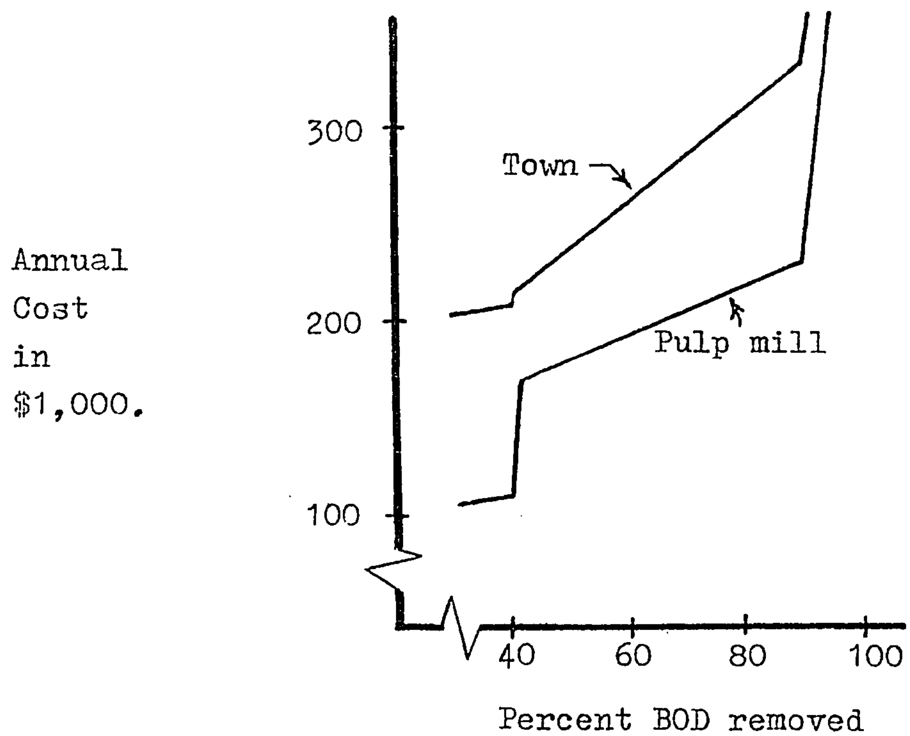


Figure 7-1: Typical dischargers' treatment costs.

cost matrix consists of the costs associated with each breakpoint of the BOD removal cost curve for each discharger. The signs of the costs are negative in order that the linear programming solution will be one of minimum cost.

7.1.3 Dischargers' treatment cost minimization. A summary of the linear programming formulation of dischargers' treatment cost minimization appears in Appendix 13. Linear programming optimization of the treatment cost matrix yields the minimum cost for the dischargers collectively and the amount of waste, in pounds of BOD_5, that each discharger is allocated to release to the river while maintaining specified DO concentration levels in the critical reach. Detailed explanation of the linear programming techniques of this optimization appears in Kenschaft[214].

In addition to the effluent treatment cost curve for each discharger, the dischargers' treatment cost matrix requires the values of P and the a_i's, previously defined following equation (7-1). These parameters may be evaluated using a suitable set of one or more river reach concentrations models.

7.2 Instream Treatment Cost

7.2.1 River reach concentrations models. If both BOD and DO rate balances are represented for the critical reach and all reaches extending upstream to incorporate every discharger, then all of the a_i's and P may be evaluated. The product of the volume flow rate of the river and the BOD concentration at the upstream end of the critical reach is the amount of waste entering the reach from upstream. Assuming that all dischargers are upstream from the critical reach, the a_i's may be evaluated by applying each discharger's output to the concentrations models of the reaches between it and the critical reach in the absence of other waste sources.

Better optimization of overall treatment costs can be attained if the a_i's and P can be varied. This option is added by including optimally controlled instream treatment in the concentrations model for the critical reach. The discrete hierarchical tidal river reach water quality model with optimal aeration control described in Chapter 3 is especially suitable for this application. It includes the following:

1.) variation of the deoxygenation and reaeration coefficients with temperature;

2.) spatial variation of the reach's cross-sectional area (taper);

3.) spatial and temporal variation of volume flow in the reach (tidal effects);

4.) dispersive effects.

The objective of the optimal control for this model is the attainment of a specified level of DO concentration with a minimum expenditure of control energy for instream treatment.

7.2.2 Instream treatment cost subproblem hierarchy. Since the dischargers considered are upstream from the critical reach, the concentrations model for the river involves at least two reaches. This model may be described as a river basin or regional model because it actually represents the aggregation of concentrations models of individual reaches. From Figure 2-1 it is evident that at least the critical reach concentrations model consists of a two-level hierarchy of subproblems. Hence, the river basin concentrations model is a three-level subproblem hierarchy with a coordination or interfacing subproblem in the supremal position and the individual reach concentrations subproblems occupying the lower two levels of the hierarchy as shown in Figure 2-3.

7.2.3 Instream treatment cost minimization. If the minimal cost of instream treatment associated with optimal

BOD and DO concentration profiles is calculated, this model may be used in the solution of a problem to determine minimum instream treatment cost for a given waste load, P. For maintenance of fixed minimum DO concentration levels, this cost increases with increasing P.

7.3 Hierarchical Formulation of the Total Treatment Cost Problem

The fact that both the dischargers' total treatment cost and the instream treatment cost are functions of P implies that the associated cost minimization problems may be coordinated at a higher level by using P as a coordination variable. The corresponding subproblem hierarchy appears in Figure 7-2. This subproblem hierarchy represents the aggregation of the river reach optimal pollution control problem described in Chapter 3 with the river basin economics problem described in Kerri's paper. Total treatment cost for this aggregation is the sum of the total dischargers' treatment cost and the instream treatment cost. The overall treatment cost minimization problem has thus been recast into the form of a four-level hierarchy of subproblems.

A coordination subproblem occupies the supremal position of this hierarchy. This subproblem adjusts P to a value such that the total cost of treatment is minimized

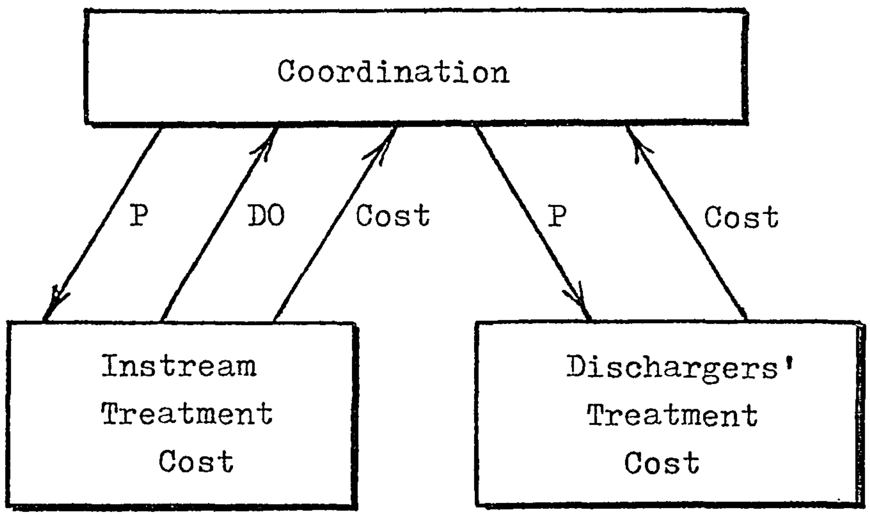


Figure 7-2: Subproblem hierarchy for minimization of total treatment cost.

while the DO concentrations are maintained at or above specified levels within the critical reach.

P is constant throughout each optimization of the instream treatment cost subproblem; its value changes only between optimizations. Hence, the performance indexes, equations (3-87) and (3-103), are minimized only with respect to the control terms, $(U_C)_{k,i}$ or $(U_L)_{k,i}$.

7.4 Example

A critical reach of a tidal river receives waste only from two dischargers located upstream from it as depicted in Figure 7-3. An instream aerator may be installed and operated at the upstream end of the critical reach as shown in the cited figure. The overall objective of this regional economic water quality problem is the minimization of the sum of the cost of the dischargers' effluent treatment and the cost of instream aeration while attaining and maintaining a DO concentration in the critical reach of at least 6 mg/l.

The critical reach is represented by the tidal river model from Chapter 3 joined on the upstream end by a model from O'Connor[334] of the reach within which the outfalls of the dischargers enter the river. The parameter values for both models appear in Table 7-4.

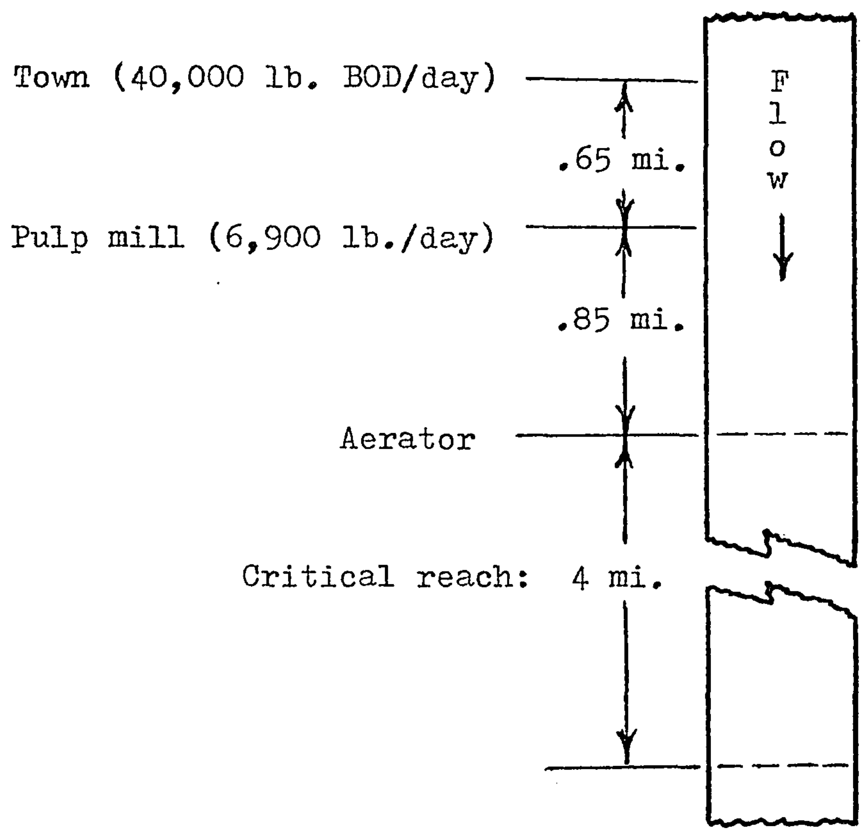


Figure 7-3: Location of dischargers and aerator with respect to the critical reach.

7.4.1 Mathematical model of reach upstream from critical reach. For a continuous pollutant source of rate m, the steady state solution for the BOD concentration profile is:

$$L = \frac{m}{2A\sqrt{K_1 D}} \, e^{-\left(\frac{K_1}{D}\right)^{\frac{1}{2}} x} \qquad (7\text{-}2)$$

where:

A = Cross sectional area of river.

K_1 = Removal coefficient.

D = Coefficient of dispersion.

x = Distance downstream from its outfall.

The corresponding expression for the DO profile is:

$$C = C_s - FL_a \left[e^{-\left(\frac{K_1}{D}\right)^{\frac{1}{2}} x} - \left(\frac{K_1}{K_2}\right)^{\frac{1}{2}} e^{-\left(\frac{K_2}{D}\right)^{\frac{1}{2}} x} \right] \qquad (7\text{-}3)$$

where:

$$F = \frac{K_1}{K_2 - K_1} \qquad (7\text{-}4)$$

$$L_a = \frac{m}{2A\sqrt{K_1 D}} \qquad (7\text{-}5)$$

K_2 = Reaeration coefficient.

7.4.2 <u>Dischargers' treatment cost.</u> In the dischargers' waste treatment cost matrix:

$$a_i = \frac{\text{Amount of waste delivered to critical reach}}{\text{Amount of waste discharged by ith discharger}} \qquad (7\text{-}6)$$

Hence,

$$a_i = \frac{QL}{m_i} = \frac{Q}{2A\sqrt{K_1 D}}\, e^{-\left(\frac{K_1}{D}\right)^{\frac{1}{2}} x_i} = \frac{VEL}{2\sqrt{K_1 D}}\, e^{-\left(\frac{K_1}{D}\right)^{\frac{1}{2}} x_i} \qquad (7\text{-}7)$$

where:

Q = Average volume flow rate of river.

VEL = Average velocity of flow.

x_i = Distance of ith discharger upstream from the critical reach.

Substitution of parameter values from Table 7-5 into equation (7-7) yields:

$$a_i = 3.56\ VELe^{-1.17x_i} = 2.68e^{-1.17x_i} \qquad (7\text{-}8)$$

The results of applying equation (7-8) for each discharger appear in Table 7-5.

Sufficient information now is available to generate all of the coefficients of the dischargers' effluent treatment cost matrix (Table 7-3).

For $a_1 = .416$, $a_2 = .98$, $b_1 = .40$, $b_2 = .41$, $b_3 = .90$, $X_1 = 40$, $X_2 = 6.9$

$b_1X_1 = 16.0$	$a_1b_1X_1 = 6.66$
$b_2X_1 = 16.4$	$a_1b_2X_1 = 6.82$
$b_3X_1 = 36$	$a_1b_3X_1 = 15$
$b_1X_2 = 2.76$	$a_2b_1X_2 = 2.70$
$b_2X_2 = 2.83$	$a_2b_2X_2 = 2.77$
$b_3X_2 = 6.21$	$a_2b_3X_2 = 6.09$

All of the above products are written in units of 1,000 pounds of BOD per day.

The total amount of waste entering the critical reach without treatment by either discharger appears in Table 7-6 at the bottom of the right hand column. The amount to be removed, measured at the critical reach, may be any amount between zero and the total of 23,400 lb./day. The overall percentage of waste removal by the dischargers is given by the following:

$$\% \text{ waste removed} = \frac{\text{BOD removed (lb./day)}}{23{,}400} \qquad (7\text{-}9)$$

Under uniform treatment, the percent waste removed by each discharger is the same as the overall percent waste removal. Under nonuniform treatment, widely different percentages of waste removal by each discharger may be equivalent to a given overall percentage treatment. For consistency of coefficients in the matrix of Table 7-3, the amount of waste to be removed is written in units of 1,000 pounds of BOD per day.

The following treatment costs (in 10^5 dollars) are obtained from Table 7-1 for a flow rate of 10 mgd.

$$C_{1,1} = -2.10$$
$$C_{1,2} = -2.13$$
$$C_{1,3} = -3.35$$

Also from Table 7-2 for a flow rate of 5 mgd,

$$C_{2,1} = -1.07$$
$$C_{2,2} = -1.64$$
$$C_{2,3} = -2.29$$

Using the values calculated above for the coefficients in the cost matrix of Table 7-3, the initial tableau may be constructed for each BOD removal amount to be considered. Since formulation of the dischargers' treatment cost matrix of Table 7-3 was predicated upon a minimum BOD removal of 40% by each discharger, the minimum amount to be removed, from equation (7-9), is 9,360 pounds per day. Various BOD removal rates between 9,360 and 23,400 pounds per day also were inserted in the dischargers' treatment cost matrix of Table 7-3. Techniques of linear programming were then applied to each such cost matrix to yield a tableau of minimum total dischargers' effluent treatment costs. The results are summarized in Table 7-6 and the tableau sets for each amount of BOD removal appear in Appendix 14.

From Table 7-6, it is evident that the cost savings of nonuniform treatment over uniform treatment for removal of a given overall percent BOD is substantial for overall removal percentages greater than 40%. It is also evident from the same table that if a means can be found for meeting minimum DO concentration requirements in the critical reach with the least possible BOD removal by the dischargers, a considerable overall cost saving may be realized. Instream aeration is a particularly promising method for accomplishing this objective.

7.4.3 Application of aeration to critical reach. The one-dimensional tidal river model described in Chapter 3 is used to introduce the benefits of instream aeration to the water quality management problem discussed by Kerri. For the application of this model, it is necessary to know the BOD and DO concentrations at the upstream end of the critical reach.

The BOD concentration at the upstream end of the critical reach may be expressed as:

$$L_o = P/Q \qquad (7\text{-}10)$$

where:

P = waste load entering the critical reach.

Q = mean volume flow rate of river.

In particular, for P expressed in units of 1,000 pounds of BOD per day and $Q = 4.53 \times 10^5 m^3$ per day,

$$L_o \ (mg/l) = P \qquad (7\text{-}11)$$

where:

P = 23.4 - Amount of BOD removed (1,000 lb./day).

The DO concentration of the upstream end of the critical reach may be obtained from equation (7-3). Substitution of the values from Table 7-4 into this equation yields:

$$C_o = 9.06 - .974 \sum_{i=1}^{2} m_i(e^{-1.17X_i} - 1.56\, e^{-2.35X_i}) \qquad (7\text{-}12)$$

where:

m_i = amount of BOD in 1,000 lb./day from ith discharger.

X_i = distance of ith discharger from critical reach.

For $X_1 = 1.5$ miles and $X_2 = .85$ miles equation (7-12) becomes:

$$C_o = 9.06 - .974\ (.167)\ m_1 - .974\ (.346)\ m_2 \qquad (7\text{-}13)$$

The results of applying equations (7-9), (7-11) and (7-13) for selected percentages of uniform effluent treatment by the dischargers appear in Table 7-7.

Inspection of Table 7-7 reveals that the upstream DO concentration is a decisive factor in attaining and maintaining a specified minimum DO level in the critical reach. For a specified minimum of 6 mg/l, the minimum level of overall BOD removal required without aeration is 66%. However, even at 40% overall BOD removal, the BOD concentration is well within generally accepted limits at 14 mg/l. The major role of the instream aeration in this instance, then, is to increase the upstream end of the critical reach DO.

From Table 7-8, it would seem that, without instream aeration, the minimum cost of attaining the specified level of DO of 6 mg/l would be $473,000. per year. However, from Table 7-6, if non-uniform effluent treatment by the dischargers is permitted, the minimum cost to attain this level of DO drops to $409,000. per year. Both of these conditions correspond to a removal of 15,400 pounds of BOD per day by the dischargers. Operation of the digital computer simulation of the discrete tidal river model for the critical reach without aeration control confirms that the minimum values of DO concentration occur at the upstream end. This is depicted in Table 7-8.

If the aerator can be placed at the upstream end of the critical reach, it can increase the upstream DO concentration and permit operation with lower levels of BOD removal while still sustaining a minimum of 6 mg/l of DO in the critical reach. From Table 7-6, it is evident that the potential saving inherent in such a scheme could exceed $100,000. per year depending upon the cost of providing instream aeration.

From Table 7-7, the concentrations at the upstream end of the critical reach with 66% overall (15,400 lb./day) removal of BOD are L_0 = 8.0 mg/l and C_0 = 6.00 mg/l. Removal of any less BOD would result in DO concentrations at the upstream end of the critical reach of less than the specified minimum of 6 mg/l. However, operation of the aerator at the upstream end of the critical reach compensates for low values of the upstream end DO concentration. A number of tests with the mathematical model of the critical reach under optimal aeration control revealed that it is possible to attain DO concentrations of at least 6 mg/l within the critical reach with an initial upstream end DO concentration as low as 4.21 mg/l, corresponding to overall BOD removal of 45% (10,500 lb./day). The resulting DO concentration profiles are presented in Table 7-9 which may be compared directly with Table 7-8.

The corresponding aeration control profiles are presented in Table 7-10. The maximum rate of DO delivery is 458 lb./day while the mean square rate is 46,000 $lb.^2/day^2$. From equations given in Thackston and Speece(476) for estimating the cost of installing and operating an aerator capable of adding 458 lb./day of DO to the river, with adjustments for subsequent inflation, the annual cost of the specified aeration is $1,300.

Use of the aerators permits satisfaction of the DO concentration requirement in the critical reach with an overall BOD removal of only 45% (10,500 lb./day). If the BOD removal requirement of 10,500 lb./day is now substituted into the cost matrix of Table 7-3 and linear programming techniques are applied to determine the optimal distribution of BOD removal costs between the dischargers, Table 7-6 shows that the dischargers' costs can be reduced to $335,000. With the addition of the annual cost of the aerator, the total annual treatment cost is slightly more than $336,000.

Due to the self-cleansing mechanisms in the reaches between the dischargers and the critical reach, the amount of BOD actually entering the critical reach without any treatment is 23,400 lb./day (Table 7-5). Forty-five percent overall BOD removal by the dischargers further reduces the load entering the critical reach to 12,900 lb./day. From Table 7-8 it is evident that up to 458 lb./day of DO is injected into the critical reach. The DO concentration distribution in the first row of Table 7-9 may be regarded as typical of the critical reach without aeration. In order to attain at least 6 mg/l of DO at each point in the reach it is necessary to increase only the concentrations within the first mile of the upstream end.

Kerri's approach alone yields a reduction in annual treatment cost of $64,000. by properly allocating the BOD removal requirements between the dischargers. The methods presented in this chapter in combination with Kerri's approach yield a cost reduction of more than $135,000. per year.

This chapter has described the application of hierarchical systems analysis techniques to an economic river basin water quality problem. The river concentrations portion of the overall problem was recast into the form of a hierarchy of subproblems in order to model more accurately a number of factors affecting concentrations in the river and to incorporate optimal instream treatment of the water and the cost associated with such treatment. The dischargers' total cost of effluent treatment portion of the overall problem was coordinated with the instream treatment cost portion to determine the minimal overall treatment cost subject to maintaining a specified minimum level of DO concentration in the critical reach downstream from the dischargers into the river. This coordination between dischargers' total treatment cost and instream treatment cost provides a cost basis for presenting each discharger a choice between effluent treatment at various levels with corresponding levels of financial support of instream treatment.

The present chapter is a culmination of the development which began with the presentation of two classes of mathematical water quality models in Chapters 2 and 3 and progressed through the treatment of topics significant in the generation of practical numerical solutions of these models in Chapter 4, sensitivity analysis in Chapter 5 and representative numerical results in Chapter 6. This chapter utilizes the models developed in Chapters 2 and 3 and general multilevel hierarchical systems analysis techniques and linear programming to formulate solutions of a multireach river basin water quality problem.

% BOD Removed	Design Flow (mgd) .25	.5	1.0	5.0	10.0
0	0	0	0	0	0
20	10.3	19.3	33.0	100	193
40	10.6	19.7	34.0	107	210
41	11.6	20.5	37.3	123	213
90	15.3	28.0	51.0	183	335
100	32.0	64.0	128.0	640	1280

Table 7-1: Municipal annual BOD removal costs in $1,000.

% BOD Removed	Design Flow (mgd) .25	.5	1.0	5.0	10.0
0	0	0	0	0	0
20	10.3	19.3	33.0	100	193
40	10.6	19.7	34.8	107	210
41	14.8	25.6	46.7	164	267
90	19.1	35.0	63.8	229	421
100	32.0	64.0	128.0	640	1280

Table 7-2: Kraft pulp mill annual BOD removal costs in $1,000.

Row	$Y_{1,1}$	$Y_{1,2}$	$Y_{1,3}$	$Y_{2,1}$	$Y_{2,2}$	$Y_{2,3}$	
1)	$a_1b_1X_1$	$a_1b_2X_1$	$a_1b_3X_1$	$a_2b_1X_2$	$a_2b_2X_2$	$a_2b_3X_2$	= Am't removed
2)	1	1	1	0	0	0	= 1
3)	0	0	0	1	1	1	= 1
4)	$-C_{1,1}$	$-C_{1,2}$	$-C_{1,3}$	$-C_{2,1}$	$-C_{2,2}$	$-C_{2,3}$	= Total Cost

Table 7-3: Treatment cost matrix for two waste dischargers with BOD removal between 40% and 90%

K_1 = .164/day = BOD removal coefficient

K_2 = .658/day = Reaeration coefficient

K_d = .164/day = Carbonaceous deoxygenation coefficient

C_s = 9.06 mg/l = DO concentration at saturation

$\overline{P-R}$ = 0.0 mg/l-day = Average photosynthesis-respiration rate

$\bar{B}$ = 0.0 mg/l = Average benthal deposits demand rate

D = .12 mi^2/day = Diffusion coefficient

Q_o = 4.53×10^5 m^3/day = Average river volume flow rate

Q_T = 6.04×10^4 m^3/day = Peak tidal volume flow rate

A = Cross sectional area of river = 372 m^2

Table 7-4: Example parameters adpated from Okunseinde's Dissertation(340)

Discharger	Distance From Critical Reach (mi)	River Cleansing Ratio	Amount of Waste Entering Critical Reach (Klb. BOD/day)
1. Town	1.5	$a_1 = .416$	16.64
2. Pulp Mill	.85	$a_2 = .98$	6.76
			23.40 TOTAL

Table 7-5: Dischargers' waste entering critical reach without treatment

BOD Removed Evaluated at Critical Reach (lb/day)	Discharger 1 BOD Removal %	Discharger 1 BOD Removal Cost: (K$/year)	Discharger 2 BOD Removal %	Discharger 2 BOD Removal Cost: (K$/year)	Total Cost (K$/yr)
9,360	40	210	40	107	317
10,500	45	223	45	169	392
10,500	47.1	228	40	107	335
12,600	54	246	54	181	427
12,600	59.5	259	40	107	366
15,400	66	274	66	199	473
15,400	76	302	40	107	409

Table 7-6: Dischargers' effluent treatment costs

% BOD Removed	40	45	50	54	66
C_o (mg/l)	3.76	4.21	4.65	5.00	6.00
L_o (mg/l)	14.0	12.9	11.7	10.8	8.00
Cost (K$)	317	392	411	427	473

Table 7-7: Effect of dischargers' effluent treatment on upstream end concentrations of critical reach

Time (days)	Distance (miles) 0	.5	1	2	3	4
0	6.00	7.07	7.77	8.60	9.06	9.06
.625	6.00	6.97	7.69	8.57	9.04	9.06
1.25	6.00	7.02	7.72	8.58	9.05	9.06
1.875	6.00	7.03	7.73	8.59	9.05	9.06
2.50	6.00	6.99	7.70	8.58	9.05	9.06
3.125	6.00	6.96	7.68	8.56	9.04	9.06
3.75	6.00	6.97	7.69	8.57	9.04	9.06
4.375	6.00	7.02	7.72	8.58	9.05	9.06
5.00	6.00	7.03	7.73	8.59	9.05	9.06

Table 7-8: Critical reach DO profiles with 15,400 lb/day removal of BOD by dischargers

(Time increments used in the computations were 1/3 of those entered on the table).

Time (days)	Distance (miles) 0	.5	1	2	3	4
0	4.21	5.54	6.45	7.57	8.27	8.75
.625	5.08	5.75	6.50	7.61	8.29	8.77
1.25	5.14	5.68	6.34	7.48	8.20	8.71
1.875	5.59	6.02	6.50	7.44	8.14	8.66
2.50	5.65	6.01	6.43	7.33	8.06	8.60
3.125	6.03	6.32	6.64	7.38	8.04	8.57
3.75	6.08	6.34	6.64	7.35	8.03	8.56
4.375	6.38	6.61	6.85	7.45	8.06	8.57
5.00	6.36	6.60	6.86	7.45	8.07	8.58

Table 7-9: Critical reach DO profiles with 10,500 lb/day removal of BOD by dischargers and instream aeration

(Time increments used for computation were 1/3 those used on table.)

Distance (miles)

Time (days)	0	.5	1	2	3	4
0	75	0	0	0	0	0
.625	458	0	0	0	0	0
1.25	190	0	0	0	0	0
1.875	262	0	0	0	0	0
2.50	124	0	0	0	0	0
3.125	130	0	0	0	0	0
3.75	80	0	0	0	0	0
4.375	77	0	0	0	0	0
5.00	0	0	0	0	0	0

$\bar{U}^2 = 46{,}300\ \text{lb}^2/\text{day}^2$

Table 7-10: Aeration control profiles in lb./day for critical reach with 10,500 lb./day removal of BOD by dischargers

(Time increments used in computations were 1/3 those entered on table.)

CHAPTER 8

CONCLUSIONS AND RECOMMENDATIONS

8.1 Conclusions

The (approximate) solution of optimal control problems involving two classes of dynamic distributed parameter plants was treated by applying a combination of Pontryagin's minimum principle and multilevel hierarchical systems analysis techniques known as "multilevel control" to them[531]. The first of these classes, linear continuous distributed parameter plants, exemplified by a fairly general dynamic concentrations balance model for streams and rivers, was expressed in the form of a set of simultaneous partial differential equations. These equations were spatially discretized to facilitate the application of Pontryagin's minimum principle for lumped parameter systems. The second class, linear two-step discrete distributed parameter plants, exemplified by a general dynamic concentrations balance model for streams, rivers and estuaries, was expressed in the form of a set of simultaneous finite-difference equations. Optimal control of this class of plants was effected by applying a combination of Pontryagin's minimum principle for discrete systems and multilevel hierarchical systems analysis techniques to each plant.

For members of both classes of distributed parameter plants the application of multilevel control techniques yielded subproblem hierarchies that could be solved iteratively following the imposition of realistic boundary, initial and final conditions. Extensive computer experimentation with the application of several modes of optimal control to these classes of plants supports the conclusion that multilevel hierarchical techniques are both feasible and efficient for these systems' optimization. Some more specific conclusions derived from the study presented in this dissertation are given in the sequel.

Under the spatial and temporal discretization involved in digital computation, the continuous distributed parameter concentrations model of a tapered reach of a waterway requires a ratio of spatial increment to temporal increment that varies spatially, if the mean volume flow rate is time invariant, and both spatially and temporally, if the mean volume flow rate varies temporally, in order to avoid false dispersive effects[106]. This class of plants is therefore not very satisfactory for representing concentrations balances in tapered waterways subject to tidal variations in volume flow rate. The class of discrete distributed parameter plants, exemplified by the model presented by Bella and Dobbins[27], however, readily accommodates variations in volume flow rate without generating false dispersive effects. It is therefore concluded that this latter class of plants is more satisfactory for representing concentrations balances in waterways subject to tidal effects.

Subproblem hierarchies resulting from the application of multilevel optimal control to individual reaches of a waterway may be utilized as modules in the construction of a super hierarchy representing a multireach regional model of a waterway under multilevel optimal control. Extensive computer experience with such models demonstrates their efficiency in the solution of large scale regional optimization problems.

The specific approaches utilized for stability analysis of the subproblem hierarchies resulting from application of multilevel control techniques depends upon the class to which a particular plant belongs. Stability of the spatially discretized continuous distributed parameter plants with optimal control can be proved by formulating the resulting control problem as a linear regulator problem and utilizing the associated performance index as a Liapunov function. Stability of the discrete distributed parameter plants with time-varying mean volume flow rate and optimal control can be proved by formulating each associated control problem as control of a nonstationary plant, transforming each nonstationary system to an equivalent stationary system and applying Liapunov techniques.

Two main conclusions pertaining to sensitivity analysis of distributed parameter plants under multilevel optimal control are the following. Methods of sensitivity analysis developed for lumped parameter systems can be extended to continuous distributed parameter systems by applying spatial discretization followed by multilevel hierarchical systems analysis techniques. In particular, trajectory sensitivity coefficients for the class of linear continuous distributed parameter plants with multilevel optimal control presented in this study can be generated by utilizing a subproblem hierarchy of the same structure as the hierarchy constructed for solution of the optimal control problem.

Three general conclusions can be drawn from the portion of this study concerning the solution of a regional water quality problem subject to economic constraints. Members of the class of discrete distributed parameter concentrations models with multilevel control can be used to generate solutions to instream treatment cost minimization subproblems. Moreover, single reach instream treatment cost minimization subproblems can be aggregated into a multireach regional instream treatment cost minimization subproblem for a waterway. A subproblem hierarchy to solve an overall regional total treatment cost problem therefore can be constructed by utilizing hierarchical multilevel systems analysis techniques to coordinate an instream treatment cost minimization subproblem with a collective dischargers' treatment cost minimization subproblem.

8.2 Recommendations for Further Study.

Fruitful areas for further research include the following.

1) Determination of additional realistic boundary conditions for numerical solution of subproblems in each hierarchy;

2) investigation of applicability of multilevel hierarchical analysis techniques to optimal control of other concentrations that can affect water quality;

3) derivation of a general two-step discrete dynamic distributed parameter concentrations model for three spatial dimensions;

4) development of three-dimensional discrete volume flow rate models for tidal rivers and estuaries;

5) extension of the application of multilevel control techniques to discrete distributed parameter plants;

6) review of the current spectrum of existing digital computer programs for estuary modelling and adaption of the regional estuary model of the present study for use with other existing regional models;

7) development of a computer simulation of the concentration balances in a river, its estuary and its tributaries;

8) extension of the stability analyses of the present study to more general concentrations models;

9) extension of the multilevel hierarchical approach to generation of trajectory sensitivity coefficients to broader classes of distributed parameter plants under multilevel control;

10) investigation of application of multilevel hierarchical optimal control utilizing additional different performance indices;

11) extension of multilevel hierarchical control techniques to optimization of dynamic plants with respect to several different objectives simultaneously.

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APPENDICES

Appendix 1: Literature Survey and Discussion of Numerical Optimization and Choice of Performance Indexes

Numerical techniques presented in the optimal control literature may be classified as follows[465]:

1) function space methods which iterate on entire time functions
   a) function space steepest ascent[47, 97]
   b) function space conjugate gradient[247]
   c) quasilinearization[30]
   d) successive sweep methods[303]
   e) the Ritz method[163, 458]

2) finite dimensional methods which iterate on a small set of parameters that uniquely determine time functions
   a) gradient[213, 371, 566, 202]
   b) conjugate gradient[140]
   c) Fletcher-Powell method[139]
   d) Newton-Raphson method[42, 297, 298]
   e) pattern search[189]
   f) multiple substitution polynomials[200]

Since storage of complete functions may tax the capacity of available computers if state vectors are of large dimension, function space methods usually are applied to continuous systems either by discretizing the the time interval or by representing a function by coefficients of more elementary functions. An advantage of this group of methods is that sensitivity is distributed along the trajectory[462].

Finite dimensional techniques typically involve iteration on the boundary conditions of differential equations. Hence, the sensitivity of the trajectory to these boundary conditions is high. More detailed discussion of these approaches appears in Wilde and Beightler[526], Dyer and McReynolds[116], Wilde[525], Payne[354], and Pierre[371].

The specific form of a performance index results from the definition of desired performance in a particular case. The conventional form of the performance index for minimum error combined with minimum expenditure of control energy, for lumped parameter plant, for example, is:

$$J = \int_{t_o}^{t_f} W_1 (\underline{x}_{sp} - \underline{x})^2 dt + \int_{t_o}^{t_f} W_2 \underline{u}^2 dt \qquad \text{(A1-1)}$$

which is to be minimized in this case. $\underline{x}$ is the vector of state variables, $\underline{x}_{sp}$ is the vector of specified values of the state variables and $\underline{u}$ is the vector of control terms. $\underline{x}$ is expressed in terms of its components in equation (1-2) and $\underline{x}_{sp}$ may be similarly expanded. Also,

$$\underline{u} = (u_1, u_2, \text{---}\ u_m)^T \quad m \leq n \qquad (A1\text{-}2)$$

The expression, $(\underline{x}_{sp}-\underline{x})^2$ represents the magnitude of the differences between the state variables and their pre-specified values. Hence, the first term on the right hand side of equation (1-8) is proportional to the system error. If all of the components of $\underline{x}_{sp}=0$, the associated optimal control problem is a regulator problem; if not, it is a tracking problem. The expression, $W_2\underline{u}^2$, is proportional to the control energy expended. W_1 and W_2 are constant weighting coefficients representing the assignment of relative priorities to minimization of error (maximization of accuracy) and minimization of control energy.

The mathematical reasons for utilizing a performance index of the form of equation (1-8) are enumerated in Tarassov, Perlis and Davidson[470]. Basically, this form provides assurance that the error term is zero whenever $\underline{x} = \underline{x}_{sp}$ for all time. Further, if the control terms u_1, u_2, --- u_m, are properly generated the control term also is zero under the same conditions and $J = 0$ for $\underline{x} = \underline{x}_{sp}$ for all time. Whenever $\underline{x} \neq \underline{x}_{sp}$, the quadratic form of the performance index ensures that it will be positive. Hence, J is positive definite and therefore possesses a relative minimum.

Physical considerations may lead to modification of the quadratic performance index. For example, the magnitude of the quadratic error is a function only of the magnitudes of the differences between the state variables and their specified values and not the polarity of these differences. If, for physical reasons, it is more important to maintain the state variables above the specified values, it would be desirable to increase the magnitude of the weighting coefficient of the error term, W_1, when any state variable falls below its specified value and decrease the magnitude of W_1 when the state variable is above the specified level. The magnitude of the error term then would be switched on the basis of the polarity of the error.

In addition to the quadratic form many other forms, less frequently applied, appear in the optimal control literature each with particular advantages and disadvantages. A selection of publications in this area includes Kryzhanovski and Solodukhin[(237)], Lee[(254)], Mueller and Wang[(323)], Platzman and Athans[(374)], Ramar and Ramaswami[(386)], Reid and Vemurri[(389)], Tihansky[(487)], Willems[(528)], Woods[(536)], and Zadeh[(549)]. The publications by Ramar and Ramaswami and Woods provide bases for comparisons of different performance indexes while the publications of Lee and Tihansky concentrate on performance indices for water quality control problems.

Since the objectives of the optimal control problems treated in this dissertation are minimization of error and minimization of control energy, variants of the performance index described in equation (1-8) are utilized. The modification of the quadratic performance index whereby the magnitude of the error term coefficient is adjusted as a function of the polarity of the error also is applied.

Appendix 2: Literature Survey on Multilevel Hierarchical Systems Analysis Techniques

One of the earliest discussions of breaking a large system into smaller pieces to facilitate its analysis appeared in 1939 in a book by Kron[236] in which he treated the decomposition of complicated electrical networks into component networks that he called simplexes. Philosophies of decomposition were utilized by Bellman[30] in his development of dynamic programming. The concept of utilizing decomposition as a technique for optimization appears to have originated with Dantzig and Wolfe who, in 1960, used this procedure for reducing large linear programming problems to a set of smaller ones. In later publications decomposition was proposed for linear dynamic programs by Dantzig[88] and for nonlinear programs by Wolfe[533], Rosen[393] and Varaiya[502]. A technique similar to decomposition for decoupling interconnected dynamic systems was presented more recently by Kokotovic and Singh[231].

Development of a general theory of multilevel systems was initiated by Mesarovic. An M.I.T. monograph published by him in 1960[307] contained a discussion of multilevel control applied to aggregations of plants. Mesarovic developed a general theory for treating multilevel multigoal systems where the term multigoal implies that the subsystems comprising the multilevel hierarchy may have different goals or objective functions. With respect to a multilevel control hierarchy this implies that each of the infimal subproblems may have a distinct performance index. In the terminology of the general theory, then, Figure 1-2 may be said to represent a two level N-goal hierarchy.

Early development of the multilevel approach was continued by Mesarovic[308, 309, 310] and, his associates at Case-Western Reserve University, Brosilow, Lasdon and Pearson[46], Lasdon and Schoeffler[249], Macko[282], Pearson[356, 357, 358], Sanders[409, 410], Lefkowitz[259a] and Wismer[531]. Other early contributors in this area were Kulikowski[239, 240], Sprague[452], Tel'ksnis[474], Coviello[86] and Varaiya[502].

Brosilow, Lasdon and Pearson introduced the concept of feasible decomposition for the optimization of an interconnected set of static systems. The feasible approach, also known as model coordination or interaction prediction, utilizes a two level hierarchy. The objective of the second level coordination subproblem is the satisfaction of those optimality conditions originally relaxed in the process of decomposition. This approach has the advantage that the set of subproblem solutions obtained from each iteration of the entire hierarchy of subproblems is physically realizable (feasible). Therefore if the iterations must be terminated before optimization is fully attained, a set of physically realizable suboptimal solutions is available.

Lasdon and Schoeffler(249) introduced the idea of nonfeasible decomposition, also known as goal coordination, interaction balance, or the pricing method, which is the dual of feasible decomposition. They applied it to the same class of problems as Brosilow, Lasdon and Pearson used for their presentation of feasible decomposition. Nonfeasible decomposition also was demonstrated utilizing a two level subproblem hierarchy. The distinctive feature of this approach is the initial relaxation of the constraints corresponding to the interconnection of the subsystems. The objective of the second level coordination subproblem in this approach is the coordination of the solutions of the infimal subproblems to gradually satisfy the relaxed interconnection constraints. Each infimal subproblem is thus solved independently and is iteratively adjusted toward reconnection with the other infimal subproblems by the second level coordination subproblem. With this approach only the fully optimized final iteration of the entire hierarchy of subproblems yields a physically realizable set of subproblem solutions. This is an important disadvantage if it is likely that the iterations may be terminated before the multilevel system is fully optimized. Further, if the optimization is executed numerically, the system will generate solutions close to the point of optimality but will not generally attain it exactly. Hence, a combination of nonfeasible optimization and numerical methods may not yield any physically realizable set of solutions. For the above enumerated reasons feasible decomposition is utilized exclusively throughout the present dissertation.

Sprague(452) demonstrated the application of multilevel multigoal systems theory to the study of reticulation (partitioning) of multivariable systems. He developed an ordering relation defined on the set of all possible partitions of the original system. In addition, he applied contraction mapping techniques to evaluate the convergence of control vector sequences to the optimal sequence for different partitionings of the original plant. He defined the optimal reticulation (partitioning) as the one for which the contraction mapping of successive control vector sequences has the smallest mapping contraction factor.

Mesarovic, Pearson and Takahara(309) presented the application of multilevel systems techniques to a classic problem of optimal control, the optimization of a linear lumped parameter dynamic system with respect to a quadratic performance index. In this paper the original control problem was decomposed into N infimal subproblems coordinated by a single second level subproblem. The original problem was thus recast into the form of a two level N-goal subproblem hierarchy as depicted in Figure 1-2. Coordination variables were defined for the infimal subproblems so that the second level coordination subproblem could coordinate their solutions to achieve the integrated solution of the original problem. Necessary conditions of optimal coordination also were presented. This paper, in addition to Wismer's dissertation[531], provided a major portion of the background for the work reported here.

Wismer's dissertation[531] represented the first published application of multilevel systems analysis techniques to the control of distributed parameter systems. It is reviewed in the preceding section on optimal control of distributed parameter plants.

Pearson[356, 357, 358] discussed duality and introduced the evaluation of computational efficiency of different structures of subproblem hierarchies. An extension of this latter topic is presented in Chapter 4 of the present dissertation.

Kulikowski[239, 240] formulated a number of linear multilevel control problems and discussed optimal aggregation. The concepts presented in his discussion of aggregation provided background for the approach utilized to aggregate single reach water quality models into regional multireach models in Chapters 2 and 3 of this dissertation.

Macko[282] extended the techniques of decomposition and coordination to a general class of nonlinear dynamic systems. He utilized the general approach of separating the state equations into subsystems and substituting pseudo control (slack) variables for state and control variables representing coupling in each subsystem. He then optimized the system by using either a feasible method or a nonfeasible method. Computational studies utilizing these decomposition approaches were presented by Baumann, Leondes and Wismer[23].

Lefkowitz[259a] examined the design and synthesis of control systems via multilevel techniques. He proposed a cannonical control structure comprised of four conceptual levels: regulation, optimization, adaptation and self-organization.

In Brosilow, Lasdon and Pearson[46] and in Lasdon and Schoeffler[249] gradient controllers were proposed for the second level control subproblem. Other controllers were presented by other authors. Mesarovic, Pearson and Takahara[309] introduced a direct iteration controller for linear dynamic systems and Wismer[531] presented a Gauss-Seidel controller with sufficient convergence conditions.

Applications of multilevel analysis techniques published during the same period of time (1960-1966) included the following. Himmelblau[184] presented an application of decomposition to multi-step chemical processes. He utilized Boolean network analysis to reduce large-scale systems to their constituent irreducible cyclical nets, i.e., nets which evolved due to feedback.

Sanders[410] presented an application of multilevel control techniques to a two level four goal hierarchy corresponding to a water sypply system comprised of three dams. He used dynamic programming to obtain numerical results for this system. Tel'ksnis[474] discussed the application of multilevel systems analysis to the formulation of a pattern recognition system and showed that the multilevel system potentially was more efficient with respect to cost per observation than the equivalent single level system.

Research in the area of multilevel hierarchical systems analysis has been especially prolific during the past decade. Publications appearing in 1967 through 1971 include: Aoki[8], Baumann[21, 23], Baumann et al.[23], Bensoussen[32], Bronshtein and Tsvirkun[45], Chen and Perlis[74], Donoghue and Lefkowitz[105], Drew[107], Findeisen[134], Haimes[164, 165], Jurdjevic[209], Kokotovic and Singh[231], Lasdon[248], Macko[283], Mesarovic[311], Mesarovic et al.[312], Meyer and Polak[315], Noton[329], Pearson[359, 360], Pliskin[375, 376, 377], Sato and Iehikawa[412], Schoeffler[415], Takahara[466, 467], Takahara and Mesarovic[468], Tomovic[490], Tse and Tether[494] and Wismer[532].

Baumann[21] applied multilevel optimization techniques to classes of trajectories characterized by discontinuities or intermediate boundary conditions. He proposed a two level feasible decomposition with which each original trajectory was subdivided at its points of discontinuity into sequences of smooth arcs. The objectives of the infimal subproblems of the resulting hierarchy were the independent optimizations of their respective arcs subject to boundary conditions which were gradually adjusted via iterative solution of the supremal coordination subproblem. Baumann showed that a second level gradient control was suitable for the coordination of two arcs in a numerical example. Later, using the same example, he applied a Newton-Raphson controller to attain terminal convergence[22].

A number of other applications of multilevel hierarchical systems techniques were published in 1967 through 1971. Chen and Perlis[74] applied multilevel theory to the state estimation problem for a class of water quality models. Drew[107] utilized multilevel techniques in the design of a freeway control system. Haimes[164] used a hierarchical approach in integrating the system identification problem with the system optimization problem for both certain static and dynamic systems. Haimes[165] also proposed a multilevel approach to modeling and control of water resources systems. Noton[329] proposed a two-level form of the recursive (Kalman) filter. Tomovic[490] applied multilevel control to prosthetics. Findeisen[134] developed a synthesis technique for the design of an interconnected thermal power station, sea water desalination plant and reservoir system.

Pliskin[375, 376, 377] published several applications of multilevel hierarchical techniques. He applied decomposition to linear and nonlinear models of chemical production complexes[375]. He also applied hierarchical control techniques to a structurally multilevel complex consisting of hierarchically coupled nonstationary dynamic plants represented by discrete mathematical models[376]. Finally, Pliskin utilized Dantzig-Wolfe decomposition to form optimization algorithms for controlling the production complexes described above and to define the optimal number of levels in a subproblem hierarchy for decompositional (multilevel) optimization[377].

Other publications of 1967 through 1971 treat the structure and coordination of hierarchical systems. The book by Mesarovic, Macko and Takahara[312] presents an intensive development of the theoretical aspects of this subject as does Macko's dissertation[283]. Lasdon's book presents decomposition theory in connection with the mathematical programming approach. Wismer's book[532] consists of a collection of articles by a number of authors presenting applications of multilevel control to large scale systems problems. Pearson's paper[359] demonstrates certain Kuhn-Tucker[238] saddle value conditions and relates them to multilevel control. Takahara's dissertation[466] treats the problem of on-line control in the presence of uncertainty. A later paper by Takahara and Mesarovic[468] discusses the concept of coordinability as it applies to dynamic systems.

Publications in the area of multilevel hierarchical systems analysis during the past five years may be divided into two classes: presentation of applications and development of theory. Applications of multilevel hierarchical systems techniques, other than those pertaining to water quality systems, during the period from 1971 to the present include the following.

Fallside and Perry[129] presented a hierarchical optimization of a water supply network; Cole and Sage[81] demonstrated a multilevel graphical approach to multiperson decision analysis in large-scale systems; Dikarev[98] presented a solution of the problem of determining optimal distribution of reserve equipment and service personnel to maximize cost effectiveness for a hierarchical system of indivisible structure with given construction and operating cost; Rijnsdorp[390] described multilevel control of processes in the petroleum industry.

Two applications to the steel industry were Eaglen, Singh and Coales'[112] description of a hierarchical approach for temperature control of a hot strip roughing process and Sukhorukov and Gorbunov's[463] application of multilevel control to a static hierarchical system representing a steel rolling mill.

Singh and Tamura[433] described hierarchical modelling and control of oversaturated urban road traffic networks. The models representing the dynamic behavior of the traffic networks were linear discrete-time models with inequality constraints on the states and controls and pure time delays in the controls. Optimal control of traffic flow was effected by centralized control of traffic signals in conjunction with a quadratic performance index.

Two applications of multilevel hierarchical techniques to the distribution of electric power were presented in a two level formulation of the economic dispatch optimization problem by Spare(451) and presentation of an algorithm for decomposition of a problem in optimal development and allocation of energy into a set of subproblems by Vakhutinski, Dudkin and Makarov(498). Applications of multilevel hierarchical techniques to determination of optimal trajectories were described in Sugar and Stubberud(461) and Sugar(462). Finally, Vlasyuk and Morosanov(507) developed a hierarchical model representing material flows in large industrial systems.

The literature on development of multilevel hierarchical systems theory has expanded rapidly during the past five years. Following are citations of representative publications.

Cambon and LeLette[69] extended decomposition and other multilevel techniques to the optimization of distributed parameter systems. Javden[201] presented a theory of multilevel control that unifies the general set theoretic approach of Mesarovic with the functional approach of Pearson.

Koplyay[233] investigated specific biological adaptive concepts for hierarchical systems coupled to general environments. He presented a systems model of mathematically tractable aspects of adaptive behavior.

Ozguner[350] developed modelling and control of large-scale composite systems, where a composite system is defined as a system comprised of interconnections of smaller subsystems. Each subsystem and all of the interconnections within each composite system studied were assumed to be linear and time invariant.

Siljak and Sundareshan[431] developed a multilevel control scheme for a class of composite systems. Their approach ensures stability of composite systems subjected to structural perturbations under which the subsystems are disconnected and reconnected during operation.

Vlasyuk and Morosanov[508] presented an approach to construction of a hierarchical control structure for large scale systems predicated upon control efficiency. Their definition of optimality was based upon minimization of magnitudes of losses in material flows in a static multilevel process model.

Warren and Mitter[519] developed necessary conditions for decoupling of large linear time-invariant multivariable systems. Zuev and Fatkin[554] presented an approach to providing optimal control for a hierarchical system comprised of elements specified on different time intervals.

Other contributors to recent literature on the theoretical aspects of multilevel hierarchical systems are: Boychuk[40], Burkov and Opoitsev[52], Dirickx et al.[99], Fatkin[132], Fatkin and Charnyi[132], Grateloup and Titli[152, 153], Gueguen and Manich-Mayol[160], Mahmoud and Bilal[284], Ozguner and Perkins[351], Rosenbrock and Pugh[394], Singh[435, 436, 437, 439], Sutton[464] and Titli, Lefevre and Richetin[488].

Appendix 3: Costate Equations and Remaining Coordination Equations of General Discrete Two-Dimensional Estuary Model

$$(cx)_{1,k,m,i-1} = -B_{k,m,i}(cx)_{7,k,m,i} + E_{k-\frac{1}{2},m,i}(cx)_{7,k-1,m,i} + E_{k+\frac{1}{2},m,i}(cx)_{7,k+1,m,i} + F_{k,m-\frac{1}{2},i}(cx)_{7,k,m-1,i} + F_{k,m+\frac{1}{2},i}(cx)_{7,k,m+1,i} \quad \text{(A3-1)}$$

$$(cx)_{2,k,m,i-1}\Big|_{\substack{Q_{k,m,i} \geq 0 \\ (V_z)_{k,m,i} \geq 0}} = (cx)_{5,k,m,i} + \frac{h_t Q_{k+\frac{1}{2},m,i}}{h_x A_{k,m}}\left[(cx)_{5,k+1,m,i} - (cx)_{5,k,m,i}\right] + \frac{h_t (V_z w)_{k,m+\frac{1}{2},i}}{A_{k,m}}\left[(cx)_{5,k,m+1,i} - (cx)_{5,k,m,i}\right] - h_t (K_d)_{k,m}(cx)_{8,k,m,i} \quad \text{(A3-2)}$$

$$(cx)_{2,k,m,i-1}\Big|_{\substack{Q_{k,m,i} < 0 \\ (V_z)_{k,m,i} \geq 0}} = (cx)_{5,k,m,i} + \frac{h_t Q_{k-\frac{1}{2},m,i}}{h_x A_{k,m}}\left[(cx)_{5,k-1,m,i} - (cx)_{5,k,m,i}\right] + \frac{h_t (V_z w)_{k,m+\frac{1}{2},i}}{A_{k,m}}\left[(cx)_{5,k,m+1,i} - (cx)_{5,k,m,i}\right] - h_t (K_d)_{k,m}(cx)_{8,k,m,i} \quad \text{(A3-3)}$$

$$(cx)_{2,k,m,i-1} \Bigg|_{\substack{Q_{k,m,i} < 0 \\ (V_z)_{k,m,i} < 0}} = (cx)_{5,k,m,i} + \frac{h_t Q_{k-\frac{1}{2},m,i}}{h_x A_{k,m}} \left[(cx)_{5,k-1,m,i} - (cx)_{5,k,m,i} \right] + \frac{h_t (V_z w)_{k,m-\frac{1}{2},i}}{A_{k,m}} \left[(cx)_{5,k,m-1,i} - (cx)_{5,k,m,i} \right] - h_t (K_d)_{k,m} (cx)_{8,k,m,i} \quad \text{(A3-4)}$$

$$(cx)_{2,k,m,i-1} \Bigg|_{\substack{Q_{k,m,i} \geq 0 \\ (V_z)_{k,m,i} < 0}} = (cx)_{5,k,m,i} + \frac{h_t Q_{k+\frac{1}{2},m,i}}{h_x A_{k,m}} \left[(cx)_{5,k+1,m,i} - (cx)_{5,k,m,i} \right] + \frac{h_t (V_z w)_{k,m-\frac{1}{2},i}}{A_{k,m}} \left[(cx)_{5,k,m-1,i} - (cx)_{5,k,m,i} \right] - h_t (K_d)_{k,m} (cx)_{8,k,m,i} \quad \text{(A3-5)}$$

$$(cx)_{3,k,m,i-1} = - G_{k,m,i} (cx)_{8,k,m,i} + E_{k-\frac{1}{2},m,i} (cx)_{8,k-1,m,i} + E_{k+\frac{1}{2},m,i} (cx)_{8,k+1,m,i} + F_{k,m-\frac{1}{2},i} (cx)_{8,k,m-1,i} + F_{k,m+\frac{1}{2},i} (cx)_{8,k,m+1,i} \quad \text{(A3-6)}$$

$$(cx)_{4,k,m,i-1}\Bigg|_{\substack{Q_{k,m,i} \geq 0 \\ (V_z)_{k,m,i} \geq 0}} = (cx)_{6,k,m,i}$$

$$+ \frac{h_t Q_{k+\frac{1}{2},m,i}}{h_x A_{k,m}} \left[(cx)_{6,k+1,m,i} - (cx)_{6,k,m,i} \right]$$

$$+ \frac{h_t (V_z w)_{k,m+\frac{1}{2},i}}{A_{k,m}} \left[(cx)_{6,k,m+1,i} - (cx)_{6,k,m,i} \right]$$

$$- 2h_x h_z h_t W_1 \left[(C_{sp})_{k,m} - X_{4,k,m,i} \right] \qquad \text{(A3-7)}$$

The three additional cases of $(cx)_{4,k,m,i-1}$, depending upon the signs of $Q_{k,m,i}$ and $(V_z)_{k,m,i}$, may be constructed by analogy with equations (A3-2) through (A3-5) and equation (A3-7).

The remaining coordination equations, obtained from equation (3-91), are:

$$(cx)_{5,k,m,i} = (cx)_{1,k,m,i} \qquad \text{(A3-8)}$$

$$(cx)_{6,k,m,i} = (cx)_{3,k,m,i} \qquad \text{(A3-9)}$$

$$(cx)_{7,k,m,i} = (cx)_{2,k,m,i} \Bigg/ \left[1 + \frac{h_t (K_r)_{k,m}}{2} \right] \qquad \text{(A3-10)}$$

$$(cx)_{8,k,m,i} = (cx)_{4,k,m,i} \Bigg/ \left[1 + \frac{h_t (K_a)_{k,m}}{2} \right] \qquad \text{(A3-11)}$$

where $B_{k,m,i}$, $E_{k,m,i}$ and $F_{k,m,i}$ are defined in equations (3-19) through (3-21) and $G_{k,m,i}$ is defined in equation (3-24).

Appendix 4: Boundary, Initial and Final Conditions for Subproblems

Solution of the subproblems in the hierarchy requires a priori information on the boundary, initial and final conditions. Some of these conditions may be stated at the outset; others require some development.

First, it is known that the final time and downstream end conditions on the costate variables are zero[309].

$$(cx)_{n,k,m,I_m} = 0 \quad \text{(A4-1)}$$

for $n = 1,2,3,4;\ k = 1,2,---,N+1;\ m = 1,2,---M_m+1.$

$$(cx)_{n,N+1,m,i} = 0 \quad \text{(A4-2)}$$

for $n = 1,2,3,4;\ m = 1,2,---,M_m+1;\ i = 1,2,---,I_m.$
Also, in the highest layer of the model (water surface) the costate variables are zero.

$$(cx)_{n,k,M_m+1,i} = 0 \quad \text{(A4-3)}$$

for $n = 1,2,3,4;\ k = 1,2,---,N+1;\ i = 1,2,---,I_m.$
The upstream end boundary conditions may be predetermined constants[340].

$$x_{n,1,m,i} = L_o \quad \text{(A4-4)}$$

for $n = 1,2;\ m = 1,2,---,M_m;\ i = 1,2,---,I_m.$

$$x_{n,1,m,i} = C_o \qquad \text{(A4-5)}$$

for $n = 3,4$; $m = 1,2,---,M_m$; $i = 1,2,---,I_m$

As stated in Chapter 2, a distribution of initial concentrations generated from a suitable steady state model generally reduces the number of iterations required to attain the optimal space-time profiles of concentrations. The initial distribution of BOD concentrations may be approximated by the following modified form of equation (2-104).

$$x_{2,k+1,m,1} = \left[B_{k,m}X_{2,k,m,1} - E_{k,m}X_{2,k-1,m,1} - (L_a)_{k,m} \right] / F_{k,m}$$

$k = 1,2,---,N$; $m = 1,2,---,M_m+1$ (A4-6)

where:

$$B_{k,m} = E_{k,m} + F_{k,m} + (Q_{k,m} - Q_{k-1,m})/(A_{k,m}h_x) + (K_r)_{k,m} \qquad \text{(A4-7)}$$

$$E_{k,m} = \frac{DA_{k+1,m}}{h_x^{\,2}A_{k,m}} + Q_{k,m}/(A_{k,m}h_x) \qquad \text{(A4-8)}$$

$$F_{k,m} = D/h_x^{\,2} \qquad \text{(A4-9)}$$

D = coefficient of longitudinal diffusion

$$Q_{k,m} = (Q_{k,m,i} + Q_{k,m,i+1})/2 \qquad \text{(A4-10)}$$

The initial distribution of DO concentrations in the general two-dimensional estuary model is approximated by the following modification of equation (2-105).

$$X_{4,k+1,m,1} = G_{k,m}X_{4,k,m,1} - E_{k,m}X_{4,k-1,m,1} + (K_d)_{k,m}X_{2,k,m,1} - (K_s)_{k,m} \;/F_{k,m} \qquad \text{(A4-11)}$$

$k = 1,2,---,N;\ m = 1,2,---,M_m+1$

where:

$$G_{k,m} = B_{k,m} - (K_r)_{k,m} + (K_a)_{k,m} \qquad \text{(A4-12)}$$

$$(K_s)_{k,m} = (K_a)_{k,m}C_s + \bar{P}_{k,m} - \bar{R}_{k,m} - \bar{B}_{k,m} \qquad \text{(A4-13)}$$

Since control is not applied until after the first temporal increment,

$$(U_C)_{k,m,1} = 0 \qquad \text{(A4-14)}$$

$k = 2,3,---,N+1;\ m = 2,3,---,M_m+1$

If it is further assumed that no control is applied until after the first spatial increments,

$$(U_C)_{1,m,i} = 0 \qquad \text{(A4-15)}$$

$m = 2,3,---,M_m;\ i = 2,3,---,I_m$

$$(U_C)_{k,1,i} = 0 \qquad \text{(A4-16)}$$

$k = 2,3,---,N;\ i = 2,3,---,I_m$

Additional required boundary, initial and final conditions may be obtained by linear extrapolation from internal points of the space-time region of interest.

Details on the method used appear in Okunseinde[340] and Chapter 4 of this dissertation.

Appendix 5: Costate Equations for Two-dimensional Model With Negligible Vertical Velocity Component

$$(cx)_{2,k,m,i-1}\Big|_{Q_{k,m,i}\,\geq\,0}$$

$$= (cx)_{5,k,m,i} - h_t(K_d)_{k,m}(cx)_{8,k,m,i} + \frac{h_t Q_{k+\frac{1}{2},m,i}}{h_x A_{k,m}}\left[(cx)_{5,k+1,m,i} - (cx)_{5,k,m,i}\right] \tag{A5-1}$$

$$(cx)_{2,k,m,i-1}\Big|_{Q_{k,m,i}\,<\,0}$$

$$= (cx)_{5,k,m,i} - h_t(K_d)_{k,m}(cx)_{8,k,m,i} + \frac{h_t Q_{k-\frac{1}{2},m,i}}{h_x A_{k,m}}\left[(cx)_{5,k-1,m,i} - (cx)_{5,k,m,i}\right] \tag{A5-2}$$

$$(cx)_{4,k,m,i-1}\Big|_{Q_{k,m,i}\,\geq\,0}$$

$$= (cx)_{6,k,m,i} - 2h_x h_z h_t W_1\left[(C_{sp})_{k,m} - x_{4,k,m,i}\right] + \frac{h_t Q_{k+\frac{1}{2},m,i}}{h_x A_{k,m}}\left[(cx)_{6,k+1,m,i} - (cx)_{6,k,m,i}\right] \tag{A5-3}$$

$$(cx)_{4,k,m,i-1}\Big|_{Q_{k,m,i}\ <\ 0}$$

$$= (cx)_{6,k,m,i} - 2h_x h_z h_t W_1 \left[(C_{sp})_{k,m} - x_{4,k,m,i} \right]$$

$$+ \frac{h_t Q_{k-\frac{1}{2},m,i}}{h_x A_{k,m}} \left[(cx)_{6,k-1,m,i} - (cx)_{6,k,m,i} \right]$$

(A5-4)

Appendix 6: Costate and Remaining Coordination Equations for Discrete Tidal River Model

$$(cx)_{1,k,i-1} = - B_{k,i}(cx)_{7,k,i} + E_{k-\frac{1}{2},i}(cx)_{7,k-1,i} + E_{k+\frac{1}{2},i}(cx)_{7,k+1,i} \qquad \text{(A6-1)}$$

where

$B_{k,i}$ and $E_{k,i}$ are defined in equations (3-47) and (3-48), respectively

$$(cx)_{2,k,i-1}\Big|_{Q_{k,i} \geq 0} = (cx)_{5,k,m,i} + \frac{h_t Q_{k+\frac{1}{2},i}}{h_x A_k}\left[(cx)_{5,k+1,i} - (cx)_{5,k,i}\right] - h_t (K_d)_k (cx)_{8,k,m,i} \qquad \text{(A6-2)}$$

$$(cx)_{2,k,i-1}\Big|_{Q_{k,i} < 0} = (cx)_{5,k,m,i} + \frac{h_t Q_{k-\frac{1}{2},i}}{h_x A_k}\left[(cx)_{5,k-1,i} - (cx)_{5,k,i}\right] - h_t (K_d)_k (cx)_{8,k,m,i} \qquad \text{(A6-3)}$$

$$(cx)_{3,k,i-1} = - G_{k,i}(cx)_{8,k,i} + E_{k-\frac{1}{2},i}(cx)_{8,k-1,i} + E_{k+\frac{1}{2},i}(cx)_{8,k+1,i} \qquad \text{(A6-4)}$$

$$(cx)_{4,k,i-1}\Big|_{Q_{k,i} \geq 0} = (cx)_{6,k,i} + \frac{h_t Q_{k+\frac{1}{2},i}}{h_x A_k}\left[(cx)_{6,k+1,i} - (cx)_{6,k,i}\right] - 2h_x h_t\ W_1\left[(C_{sp})_k - x_{4,k,i}\right] \qquad (A6\text{-}5)$$

$$(cx)_{4,k,i-1}\Big|_{Q_{k,i} < 0} = (cx)_{6,k,i} + \frac{h_t Q_{k-\frac{1}{2},i}}{h_x A_k}\left[(cx)_{6,k-1,i} - (cx)_{6,k,i}\right] - 2h_x h_t\ W_1\left[(C_{sp})_k - x_{4,k,i}\right] \qquad (A6\text{-}6)$$

The remaining coordination equations for the tidal river model, which may be obtained by omitting subscript, m, from equations (A3-8) through (A3-11), are:

$$(cx)_{5,k,i} = (cx)_{1,k,i} \qquad (A6\text{-}7)$$

$$(cx)_{6,k,i} = (cx)_{3,k,i} \qquad (A6\text{-}8)$$

$$(cx)_{7,k,i} = (cx)_{2,k,i} \Big/ \left[1 + \frac{h_t (K_r)_{k,m}}{2}\right] \qquad (A6\text{-}9)$$

$$(cx)_{8,k,i} = (cx)_{4,k,i} \Big/ \left[1 + \frac{h_t (K_a)_{k,m}}{2}\right] \qquad (A6\text{-}10)$$

Appendix 7: Scalar Components of Generalized Vector-matrix State Equation of Reach j of Regional Two-dimensional Estuary Model

BOD Convection: [from equation (3-4)] :

$$x_{1,j,k,m,i+1} = f_{1,j,k,m,i} = x_{5,j,k,m,i} \qquad \text{(A7-1)}$$

where $x_{5,j,k,m,i}$ is defined by equations (3-5) through (3-8) with subscript, j, added.

BOD Remaining processes: [from equation (3-69)] :

$$x_{2,j,k,m,i+1} = f_{2,j,k,m,i}$$

$$= \left[x_{7,j,k,m,i} + h_t(L_a)_{j,k,m} + h_t(U_L)_{j,k,m,i}\right] \Big/ \left[1 + \frac{h_t(K_r)_{j,k,m}}{2}\right] \qquad \text{(A7-2)}$$

DO Convection: [from equation (3-9)] :

$$x_{3,j,k,m,i+1} = f_{3,j,k,m,i} = x_{6,j,k,m,i} \qquad \text{(A7-3)}$$

where $x_{6,j,k,m,i}$ is defined by equations (3-5) through (3-8) with subscript, j, added and x_4 in the place of x_2.

DO Remaining processes [from equation (3-71)] :

$$x_{4,j,k,m,i+1} = f_{4,j,k,m,i} = \left\{x_{8,j,k,m,i} + h_t\left[(K_3)_{j,k,m} + (PS)_{j,k,m,i} + (U_C)_{j,k,m,i}\right]\right\} \Big/ \left[1 + \frac{h_t(K_a)_{j,k,m}}{2}\right] \quad \text{(A7-4)}$$

Coordination equations in state variable form: [from equation (3-25)] :

$$x_{5,j,k,m,i+1} = f_{5,j,k,m,i} = f_{1,j,k,m} - x_{5,j,k,m,i} \quad \text{(A7-5)}$$

From equation (3-26),

$$x_{6,j,k,m,i+1} = f_{6,j,k,m,i} = f_{3,j,k,m,i} - x_{6,j,k,m,i} \quad \text{(A7-6)}$$

From equation (3-72),

$$x_{7,j,k,m,i+1} = f_{7,j,k,m,i} = -B_{j,k,m,i}x_{1,j,k,m,i} + E_{j,k+\frac{1}{2},m,i}x_{1,j,k+1,m,i} + E_{j,k-\frac{1}{2},m,i}x_{1,j,k-1,m,i} + F_{j,k,m+\frac{1}{2},i}x_{1,j,k,m+1,i} + F_{j,k,m-\frac{1}{2},i}x_{1,j,k,m-1,i} - x_{7,j,k,m,i} \quad \text{(A7-7)}$$

where $B_{j,k,m,i}$, $E_{j,k,m,i}$ and $F_{j,k,m,i}$ are defined in equations (3-19) through (3-21) with the addition of subscript, j.

From equation (3-73),

$$x_{8,j,k,m,i+1} = f_{8,j,k,m,i} = - G_{j,k,m,i}x_{3,j,k,m,i} + E_{j,k-\frac{1}{2},m,i}x_{3,j,k-1,m,i} + E_{j,k+\frac{1}{2},m,i}x_{3,j,k+1,m,i} + F_{j,k,m+\frac{1}{2},i}x_{3,j,k,m+1,i} + F_{j,k,m-\frac{1}{2},i}x_{3,j,k,m-1,i} - x_{8,j,k,m,i} \qquad \text{(A7-8)}$$

where $E_{j,k,m,i}$, $F_{j,k,m,i}$ and $G_{j,k,m,i}$ are defined in equations (3-20), (3-21) and (3-24), respectively.

Appendix 8: Second Level Interface Equations for Regional Discrete Two-dimensional Estuary Model

Forward direction interface equations ($j = 2,3,\ldots,j_M$)

$$x_{5,j,1,m,i}\Big|_{\substack{Q_{j,1,m,i} \geq 0 \\ (V_z)_{j,1,m,i} \geq 0}} = x_{2,j,1,m,i} + h_t\Big[Q_{j-1,N+\frac{1}{2},m,i}x_{2,j-1,N,m,i} - Q_{j,1\frac{1}{2},m,i}x_{2,j,1,m,i} + (V_zA_z)_{j,1,m-\frac{1}{2},i}x_{2,j,1,m-1,i} - (V_zA_z)_{j,1,m+\frac{1}{2},i}x_{2,j,1,m+1,i}\Big] \Big/ \Big[(h_x)_j A_{j,1,m}\Big] \quad \text{(A8-1)}$$

$$x_{5,j,1,m,i}\Big|_{\substack{Q_{j,1,m,i} < 0 \\ (V_z)_{j,1,m,i} \geq 0}} = x_{2,j,1,m,i} + h_t\Big[Q_{j,1\frac{1}{2},m,i}x_{2,j,2,m,i} - Q_{j-1,N+\frac{1}{2},m,i}x_{2,j,1,m,i} + (V_zA_z)_{j,1,m-\frac{1}{2},i}x_{2,j,1,m-1,i} - (V_zA_z)_{j,1,m+\frac{1}{2},i}x_{2,j,1,m+1,i}\Big] \Big/ \Big[(h_x)_j A_{j,1,m}\Big] \quad \text{(A8-2)}$$

$$x_{5,j,1,m,i}\Big|_{\substack{Q_{j,1,m,i} < 0 \\ (V_z)_{j,1,m,i} < 0}} = x_{2,j,1,m,i}$$

$$+ h_t \Big[Q_{j,1\frac{1}{2},m,i} x_{2,j,2,m,i}$$

$$- Q_{j-1,N+\frac{1}{2},m,i} x_{2,j,1,m,i}$$

$$+ (V_z A_z)_{j,1,m+\frac{1}{2},i} x_{2,j,1,m+1,i}$$

$$- (V_z A_z)_{j,1,m-\frac{1}{2},i} x_{2,j,1,m,i} \Big] \Big/ \Big[(h_x)_j A_{j,1,m} \Big]$$

(A8-3)

$$x_{5,j,1,m,i}\Big|_{\substack{Q_{j,1,m,i} \geq 0 \\ (V_z)_{j,1,m,i} < 0}} = x_{2,j,1,m,i}$$

$$+ h_t \Big[Q_{j-1,N+\frac{1}{2},m,i} x_{2,j-1,N,m,i}$$

$$- Q_{j,1\frac{1}{2},m,i} x_{2,j,1,m,i}$$

$$+ (V_z A_z)_{j,1,m+\frac{1}{2},i} x_{2,j,1,m+1,i}$$

$$- (V_z A_z)_{j,1,m-\frac{1}{2},i} x_{2,j,1,m,i} \Big] \Big/ \Big[(h_x)_j A_{j,1,m} \Big]$$

(A8-4)

The interface equations for $x_{6,j,1,m,i}$ are of the same form as equations (A8-1) through (A8-4) except that x_2 is replaced by x_4. Equations (A8-1) through (A8-4) were derived from equations (3-5) through (3-8).

From equation (3-68),

$$x_{7,j,1,m,i} = - B_{j,1,m,i}x_{1,j,1,m,i} + E_{j,1\frac{1}{2},m,i}x_{1,j,2,m,i} + E_{j-1,N+\frac{1}{2},m,i}x_{1,j-1,N,m,i} + F_{j,1,m+\frac{1}{2},i}x_{1,j,1,m+1,i} + F_{j,1,m-\frac{1}{2},i}x_{1,j,1,m-1,i} \qquad (A8-5)$$

From equation (3-70),

$$x_{8,j,1,m,i} = - G_{j,1,m,i}x_{3,j,1,m,i} + E_{j,1\frac{1}{2},m,i}x_{3,j,2,m,i} + E_{j-1,N+\frac{1}{2},m,i}x_{3,j-1,N,m,i} + F_{j,1,m+\frac{1}{2},i}x_{3,j,1,m+1,i} + F_{j,1,m-\frac{1}{2},i}x_{3,j,1,m-1,i} - h_t(K_d)_{1,m}x_{2,j,1,m,i} \qquad (A8-6)$$

$B_{j,k,m,i}$, $E_{j,k,m,i}$, $F_{j,k,m,i}$ and $G_{j,k,m,i}$ are obtained from equations (3-19) through (3-21) and (3-24)

Reverse direction interface equations ($j = 1,2,\ldots,j_M-1$)

$$(cx)_{5,j,N+1,m,i} = (cx)_{1,j+1,1,m,i} \qquad (A8-7)$$

$$(cx)_{6,j,N+1,m,i} = (cx)_{3,j+1,1,m,i} \qquad (A8-8)$$

$$(cx)_{7,j,N+1,m,i} = (cx)_{2,j+1,1,m,i} \Big/ \left[1 + \frac{h_t (K_r)_{j+1,1,m}}{2}\right] \quad \text{(A8-9)}$$

$$(cx)_{8,j,N+1,m,i} = (cx)_{4,j+1,m,i} \Big/ \left[1 + \frac{h_t (K_a)_{j+1,1,m}}{2}\right] \quad \text{(A8-10)}$$

Appendix 9: Scalar Components of Generalized Vector-matrix State Equation of Reach j of Regional Discrete Tidal River Model

BOD convection [from equation (3-45)] :

$$x_{1,j,k,i+1} = f_{1,j,k,i} = x_{5,j,k,i} \qquad \text{(A9-1)}$$

where $x_{5,j,k,i}$ is defined by equations (3-33) and (3-34) with subscript, m, omitted and subscript, j, added.

Remaining BOD processes [from equation (3-77)] :

$$x_{2,j,k,i+1} = f_{2,j,k,i} = x_{7,j,k,i} + h_t \left[(L_a)_{j,k} + (U_L)_{j,k,i} \right] \Big/ \left[1 + \frac{h_t (K_r)_{j,k}}{2} \right] \qquad \text{(A9-2)}$$

DO Convection [from equation (3-49)] :

$$x_{3,j,k,i+1} = f_{3,j,k,i} = x_{6,j,k,i} \qquad \text{(A9-3)}$$

where $x_{6,j,k,i}$ is defined by equations (3-35) and (3-36) with subscript, m, omitted and subscript, j, added.

DO remaining processes [from equation (3-79)] :

$$x_{4,j,k,i+1} = f_{4,j,k,i} = \left\{x_{8,j,k,i} + h_t \left[(K_3)_{j,k} + (PS)_{j,k,i} + (U_C)_{j,k,i}\right]\right\} \Big/ \left[1 + \frac{h_t(K_a)_{j,k}}{2}\right] \quad \text{(A9-4)}$$

Coordination equations in state variable form.

From equation (3-52),

$$x_{5,j,k,i+1} = f_{5,j,k,i} = f_{1,j,k,i} - x_{5,j,k,i} \quad \text{(A9-5)}$$

From equation (3-53),

$$x_{6,j,k,i+1} = f_{6,j,k,i} = f_{3,j,k,i} - x_{6,j,k,i} \quad \text{(A9-6)}$$

From equation (3-84),

$$x_{7,j,k,i+1} = f_{7,j,k,i} = - B_{j,k}x_{1,j,k,i} - x_{7,j,k,i} \quad \text{(A9-7)}$$

From equation (3-85),

$$x_{8,j,k,i+1} = f_{8,j,k,i} = - G_{j,k}x_{3,j,k,i} - h_t(K_d)_{j,k}x_{2,j,k,i} - x_{8,j,k,i} \quad \text{(A9-8)}$$

Appendix 10: Second Level Interface Equations for Regional Discrete Dynamic Tidal River Model

Forward direction interface equations ($j = 2,3,\ldots,j_M$)

$$x_{5,j,1,i}\Big|_{Q_{j,1,i} \geq 0} = h_t(Q_{j-1,N+\frac{1}{2},i}x_{2,j-1,N,i} - Q_{j,1\frac{1}{2},i}x_{2,j,1,i}) \Big/ \left[(h_x)_j A_{j,k}\right] \quad \text{(A10-1)}$$

$$x_{5,j,1,i}\Big|_{Q_{j,1,i} < 0} = h_t(Q_{j,1\frac{1}{2},i}x_{2,j,2,i} - Q_{j-1,N+\frac{1}{2},i}x_{2,j,1,i}) \Big/ \left[(h_x)_j A_{j,k}\right] \quad \text{(A10-2)}$$

$$x_{6,j,1,i}\Big|_{Q_{j,1,i} \geq 0} = h_t(Q_{j-1,N+\frac{1}{2},i}x_{4,j-1,N,i} - Q_{j,1\frac{1}{2},i}x_{4,j,1,i}) \Big/ \left[(h_x)_j A_{j,k}\right] \quad \text{(A10-3)}$$

$$x_{6,j,1,i}\Big|_{Q_{j,1,i} < 0} = h_t(Q_{j,1\frac{1}{2},i}x_{4,j,2,i} - Q_{j-1,N+\frac{1}{2},i}x_{4,j,1,i}) \Big/ \left[(h_x)_j A_{j,k}\right] \quad \text{(A10-4)}$$

From equation (3-76),

$$x_{7,j,1,i} = - B_{j,1,i}x_{1,j,1,i} + E_{j,1\frac{1}{2},i}x_{1,j,2,i} + E_{j-1,N+\frac{1}{2},i}x_{1,j-1,N,i} \quad \text{(A10-5)}$$

From equation (3-78),

$$x_{8,j,1,i} = - G_{j,1,i}x_{3,j,1,i} + E_{j,1\frac{1}{2},i}x_{3,j,2,i} + E_{j-1,N+\frac{1}{2},i}x_{3,j-1,N,i} - h_t(K_d)_{j,k}x_{2,j,k,i} \quad \text{(A10-6)}$$

where $B_{j,k,i}$, $E_{j,k,i}$ and $G_{j,k,i}$ are defined by equations (3-47), (3-48) and (3-51) with subscript, j, added.

Reverse direction interface equations $(j = 1,2,\ldots,j_M-1)$

$$(cx)_{5,j,N+1,i} = (cx)_{1,j+1,1,i} \quad \text{(A10-7)}$$

$$(cx)_{6,j,N+1,i} = (cx)_{3,j+1,1,i} \quad \text{(A10-8)}$$

$$(cx)_{7,j,N+1,i} = (cx)_{2,j+1,1,i} \Bigg/ \left[1 + \frac{h_t (K_r)_{j+1,1}}{2}\right] \qquad \text{(A10-9)}$$

$$(cx)_{8,j,N+1,i} = (cx)_{4,j+1,1,i} \Bigg/ \left[1 + \frac{h_t (K_a)_{j+1,1}}{2}\right] \qquad \text{(A10-10)}$$

Appendix 11: Proof of Convergence

In order to construct the proof of convergence, the following lemma is to be proved first.

Lemma: on every spatial point, x_k, where

$$\frac{2Q_k}{A_k h_k} + K_r \geq 0 , \tag{A11-1}$$

$$Q_{k-1} \geq 0 , \tag{A11-2}$$

$$\frac{2Q_k}{A_k h_k} + K_a \geq 0 , \tag{A11-3}$$

$$K_d \geq 0 , \tag{A11-4}$$

the solution, v_k, of $O_k\left[v_k(t)\right] = (U_L)_k$ is bounded as follows.

$$v_k(t) \leq \frac{2U_L}{K_r} + L_o \ ; \quad \text{where } U_L = \max_k \left|(U_L)_k\right| \tag{A11-5}$$

Similarly, the solution, w_k, of $O'_k\left[v_k(t),\ w_k(t)\right] = (U_C)_k + K_s$ is bounded as follows.

$$w_k(t) \leq \min\left\{C_s, \quad \left[F_2 + \frac{2}{K_a}(U_C + |K_s|)\right]\right\} \tag{A11-6}$$

where: $U_C = \max\limits_k \left|(U_C)_k\right|$

Proof:

Rearranging $O_k\left[v_k(t)\right] = (U_L)_k$ so that all of its coefficients are positive,

$$\frac{dv_k}{dt} + (K_r + \frac{2Q_k}{A_k h_k})v_k = \frac{Q_k v_{k-1}}{A_k h_k} + \frac{v_k Q_{k-1}}{A_k h_k} + (U_L)_k \quad (A11\text{-}7)$$

$$\frac{d\left|v_k\right|}{dt} + (K_r + \frac{2Q_k}{A_k h_k})\left|v_k\right| \le \frac{Q_k}{A_k h_k}\left|v_{k-1}\right| + \frac{Q_{k-1}}{A_k h_k}\left|v_k\right| + \left|(U_L)_k\right| \quad (A11\text{-}8)$$

$$V = \max_k \left|v_k(t)\right| \quad (A11\text{-}9)$$

$$\frac{Q_k V}{A_k h_k} > \frac{Q_k\left|v_{k-1}\right|}{A_k h_k} \quad (A11\text{-}10)$$

Since Q_k is downstream from Q_{k-1} , $Q_k \ge Q_{k-1}$

$$\frac{Q_k V}{A_k h_k} \ge \frac{Q_{k-1}\left|v_k\right|}{A_k h_k} \quad (A11\text{-}11)$$

Applying (A11-5), (A11-10) and (A11-11) to (A11-8), an upper bound for V is given by:

$$\frac{dV}{dt} + K_r V = U_L \quad (A11\text{-}12)$$

Let $F_1 = \max_{k} \left| f_1(x_k) \right|$ (A11-13)

where $V(0) = f_1(x_k) \leq F_1 = L_o$ (A11-14)

Solving (4-75),

$$V = B_1 e^{-K_r t} + B_2 \qquad \text{(A11-15)}$$

$$\frac{dV}{dt} = - K_r B_1 e^{-K_r t} \qquad \text{(A11-16)}$$

$$\frac{dV}{dt} + K_r V = K_r B_2 = U_L \qquad \text{(A11-17)}$$

$$V = \frac{U_L}{K_r}(1 - e^{-K_r t}) + L_o e^{-K_r t} \qquad \text{(A11-18)}$$

$$v_k(t) \leq V \leq L_o + \frac{2U_L}{K_r} \qquad \text{(A11-19)}$$

Rearranging $O_k' \left[v_k(t), w_k(t) \right] = (U_C)_k + K_s$ so that all coefficients are positive,

$$\frac{dw_k}{dt} + K_d v_k + (K_a + \frac{2Q_k}{A_k h_k}) w_k = \frac{Q_k w_{k-1}}{A_k h_k} + \frac{Q_{k-1} w_k}{A_k h_k} + (U_C)_k + K_s \qquad \text{(A11-20)}$$

$$W(t) = \max_k |w_k(t)| \tag{A11-21}$$

$$\frac{Q_k W}{A_k h_k} > \frac{Q_k |w_{k-1}|}{A_k h_k} \tag{A11-22}$$

Since $Q_k \geq Q_{k-1}$, $Q_k > 0$ and $A_k > 0$,

$$\frac{Q_k W}{A_k h_k} \geq \frac{Q_{k-1} |w_k|}{A_k h_k} \tag{A11-23}$$

Also,

$$\frac{d|w_k|}{dt} + (K_a + \frac{2Q_k}{A_k h_k})|w_k| < \frac{d|w_k|}{dt} + (K_a + \frac{2Q_k}{A_k h_k})|w_k| + K_d|v_k| \tag{A11-24}$$

Applying (4-62), (A11-21), (A11-22), (A11-23) and (A11-24) to equation (A11-20), an upper bound for W is given by:

$$\frac{dW}{dt} + K_a W = U_C + |K_s| \tag{A11-25}$$

$$\text{Let } F_2 = \max_k |f_2(x_k)| \tag{A11-26}$$

$$\text{where: } W(0) = f_2(x_k) \leq F_2 \tag{A11-27}$$

Solving (4-90),

$$W = B_3 e^{-K_a t} + B_4 \tag{A11-28}$$

$$B_4 = \frac{1}{K_a}(U_C + |K_s|) \tag{A11-29}$$

$$B_3 = F_2 - \frac{1}{K_a}(U_C + |K_s|) \tag{A11-30}$$

$$W = \left[F_2 - \frac{1}{K_a}(U_C + |K_s|)\right] e^{-K_a t} + \frac{1}{K_a}(U_C + |K_s|) \tag{A11-31}$$

$$w_k(t) \leq W \leq F_2 + \frac{2}{K_a}(U_C + |K_s|) \tag{A11-32}$$

$$w_k(t) \leq W \leq \min \left\{ C_s, \left[F_2 + \frac{2}{K_a}(U_C + |K_s|)\right] \right\} \tag{A11-33}$$

and the proof of the lemma is completed. The proof of convergence continues in the sequel.

From equation (4-35),

$$O_k \left[v(x_k, t)\right] = (U_L)_k \tag{4-35}$$

from equation (4-16),

$$O \left[L(x_k, t)\right] = U_L(x_k, t) \tag{A11-34}$$

and, from equation (4-27),

$$U_L(x_k, t) = (U_L)_k \tag{4-28}$$

Subtracting equation (4-101) from (4-35),

$$O_k \left[v(x_k,t)\right] - O \left[L(x_k,t)\right] = 0 \tag{A11-35}$$

Similarly,

$$O'_k \left[v(x_k,t),\ w(x_k,t)\right] - O' \left[C(x_k,t),\ L(x_k,t)\right] = 0 \tag{A11-36}$$

Adding and subtracting $O_k\left[L(x_k,t)\right]$ from equation (A11-35),

$$O_k \left[v(x_k,t)\right] - O_k \left[L(x_k,t)\right] + O_k \left[L(x_k,t)\right] - O \left[L(x_k,t)\right] = 0 \tag{A11-37}$$

Since O_k is a linear operator,

$$O_k \left[v(x_k,t)\right] - O_k \left[L(x_k,t)\right] = O_k \left[v(x_k,t) - L(x_k,t)\right] \tag{A11-38}$$

Substituting equation (A11-38) in equation (A11-37),

$$O_k \left[v_k(t) - L_k(t)\right] + (O_k \left[L_k(t)\right] - O \left[L_k(t)\right]) = 0 \tag{A11-39}$$

From the proof of consistency,

$$O \left[L_k(t)\right] - O_k \left[L_k(t)\right] = \frac{Q_k}{A_k} \eta_k^{(1)} + \frac{L_k}{A_k} \eta_k^{(3)} \tag{4-47}$$

But $(e_1)_k(t) = v_k(t) - L_k(t)$ (4-60)

Substituting equations (4-48) and (4-61) in equation (A11-39),

$$O_k \left[(e_1)_k\right] = \frac{Q_k}{A_k}\eta_k^{(1)} + \frac{L_k}{A_k}\eta_k^{(3)} \qquad \text{(A11-40)}$$

Similarly,

$$O_k' \left[(e_2)_k\right] = \frac{Q_k}{A_k}\eta_k^{(2)} + \frac{C_k}{A_k}\eta_k^{(3)} \qquad \text{(A11-41)}$$

The errors, $(e_1)_k$ and $(e_2)_k$, equal zero initially and on the boundary so one need consider only the errors at the internal points of the space-time domain. If h_k satisfy equations (4-64) and (4-66), then expanding equation (A11-40),

$$\frac{d(e_1)_k}{dt} + K_r(e_1)_k + \frac{Q_k}{A_k h_k}\left[(e_1)_k - (e_1)_{k-1}\right]$$

$$+ \frac{(e_1)_k}{A_k h_k}(Q_k - Q_{k-1}) = \frac{Q_k}{A_k}\eta_k^{(1)} + \frac{L_k}{A_k}\eta_k^{(3)} \qquad \text{(A11-42)}$$

$$E_1 = \max_{k,t}\left|(e_1)_k\right| \qquad \text{(A11-43)}$$

$$Q = \max_k |Q_k| \qquad \text{(4-55)}$$

$$a = \min_k |A_k| \neq 0 \qquad \text{(4-56)}$$

$$L = \max |L_k| \qquad \text{(A11-44)}$$

Since $\frac{Q_k E_1}{A_k h_k} > \frac{Q_k \left|(e_1)_{k-1}\right|}{A_k h_k}$ (A11-45)

and $\frac{Q_k E_1}{A_k h_k} \geq \frac{Q_{k-1} \left|(e_1)_k\right|}{A_k h_k}$ (A11-46)

an upper bound on E_1 may be obtained from the following equation.

$$\frac{dE_1}{dt} + K_r E_1 \leq \frac{Q}{a}\left[\max_{k,t} \left|\eta_k^{(1)}\right|\right] + \frac{L}{a}\left[\max_{k,t} \left|\eta_k^{(3)}\right|\right] \tag{A11-47}$$

Similarly, for $E_2 = \max\limits_{k,t} \left|(e_2)_k\right|$ (A11-48)

and for $C = \max\limits_{k,t} \left|C_k\right|$ (A11-49)

an upper bound on E_2 may be obtained from

$$\frac{dE_2}{dt} + K_a E_2 < \frac{Q}{a}\left[\max_{k,t} \left|\eta_k^{(2)}\right|\right] + \frac{C}{a}\left[\max_{k,t} \left|\eta_k^{(3)}\right|\right] \tag{A11-50}$$

Solving equation **(A11-47),**

$$\left|(e_1)_k\right| \leq E_1 \leq \frac{Q}{aK_r}\left[\max_{k,t} \left|\eta_k^{(1)}\right|\right] + \frac{L}{aK_r}\left[\max_{k,t} \left|\eta_k^{(3)}\right|\right] \tag{A11-51}$$

Solving equation (A11-50),

$$\left|(e_2)_k\right| \leq E_2 \leq \frac{Q}{aK_a}\left[\max_{k,t}\left|\eta_k^{(2)}\right|\right] + \frac{C}{aK_a}\left[\max_{k,t}\left|\eta_k^{(3)}\right|\right] \qquad \text{(A11-52)}$$

From the proof of consistency, equations (4-48), (4-49), and (4-51),

$$\eta_k^{(1)} \propto h_k \qquad \text{(A11-53)}$$

$$\eta_k^{(2)} \propto h_k \qquad \text{(A11-54)}$$

$$\eta_k^{(3)} \propto h_k \qquad \text{(A11-55)}$$

Applying (A11-53) and (A11-55) to equation (A11-51),

$$\lim_{h_k \Rightarrow 0} \left|(e_1)_k\right| = 0 \qquad \text{(4-62)}$$

Applying equations (A11-54) and (A11-55) to (A11-52),

$$\lim_{h_k \Rightarrow 0} \left|(e_2)_k\right| = 0 \qquad \text{(4-63)}$$

Thus the solution, v_k, of the spatially discretized BOD equation, $O_k\, v_k(t) = 0$, converges to the solution, $L(x_k,t)$, of the original BOD equation at every spatial point, $x = x_k$, as h_k approaches zero. The corresponding result also has been proved for the DO equations.

Appendix 12: Transformation of Discretized Tapered Stream Model to the Form $\dot{\underline{x}} = A\underline{x} + B\underline{u}$

The vector-matrix state equations of the model given by equations (4-71) through (4-78) can be written in the standard state equation form given above by means of the following transformations.

BOD equations:

At the upstream end of the reach

$$x_1 = L_o \tag{A12-1}$$

From equation (4-74),

$$\dot{L}_2 = - B_2L_2 + E_2L_o + L_a = - B_2(L_2 - \frac{E_2L_o + L_a}{B_2}) \tag{A12-2}$$

For $x_2 = L_2 - \dfrac{E_2L_o + L_a}{B_2}$ (A12-3)

$$\dot{x}_2 = - B_2x_2 \tag{A12-4}$$

By a similar process the substitution,

$$x_3 = L_3 + \frac{E_3}{B_3}(x_2 - L_2) - \frac{L_a}{B_3}$$

$$= L_3 - \frac{E_3E_2}{B_3B_2} L_o - \frac{E_3L_a}{B_3B_2} - \frac{L_a}{B_3} \tag{A12-5}$$

yields:

$$\dot{x}_3 = - B_3x_3 + E_3x_2 \tag{A12-6}$$

For k = 4,5,...,N+1

$$x_k = L_k + \frac{E_3}{B_3}(x_2 - L_2) \prod_{r=4}^{k} \frac{E_r}{B_r} - \frac{L_a}{B_k} - \frac{E_kL_a}{B_kB_{k-1}} \cdots - \frac{L_a}{B_3} \prod_{r=4}^{k} \frac{E_r}{B_r} \tag{A12-7}$$

yields:

$$\dot{x}_k = - B_kx_k + E_kx_{k-1} \tag{A12-8}$$

<u>DO equations:</u>

At the upstream end of the reach

$$x_{N+2} = C_o \tag{A12-9}$$

From equation (4-75),

$$\dot{C}_2 = - G_2C_2 + K_s + E_2C_o - K_dL_2 + (U_C)_2 \tag{A12-10}$$

$$= - G_2 \left[C_2 - \frac{K_s + E_2C_o}{G_2} - \frac{K_d(x_2 - L_2)}{G_2}\right] - K_dx_2 + (U_C)_2$$

$$= - G_2 \left[C_2 - \frac{K_s + E_2C_o}{G_2} + \frac{K_dE_2}{G_2B_2} L_o\right] - K_dx_2 + (U_C)_2$$

The substitution,

$$x_{N+3} = C_2 \frac{K_s + E_2C_o}{G_2} - \frac{K_d(x_2 - L_2)}{G_2} \tag{A12-11}$$

reduces equation (A12-11) to the form:

$$\dot{x}_{N+3} = - G_2 x_{N+3} - K_d x_2 + (U_C)_2 \qquad \text{(A12-12)}$$

Similarly, for the equation,

$$\dot{C}_3 = - G_3 C_3 + K_s + E_3 C_2 - K_d L_3 + (U_C)_3$$

$$= - G_3 \left[C_3 - \frac{K_s}{G_3} + \frac{E_3}{G_3}(x_{N+3} - C_2) - \frac{K_d}{G_3}(x_3 - L_3)\right]$$

$$+ E_3 x_{N+3} - K_d x_3 + (U_C)_3 \qquad \text{(A12-13)}$$

the substitution,

$$x_{N+4} = C_3 - \frac{K_s}{G_3} + \frac{E_3}{G_3} (X_{N+3} - C_2) - \frac{K_d}{G_3} (x_3 - L_3)$$

(A12-14)

reduces it to the form:

$$\dot{x}_{N+4} = G_3 x_{N+4} + E_3 x_{N+3} - K_d L_3 + (U_C)_3 \qquad \text{(A12-15)}$$

For k = 4,5,...,N+1 it can be shown that the substitution,

$$x_{N+k+1} = C_k - \frac{K_s}{G_k} + \frac{E_k K_s}{G_k G_{k-1}} - \frac{E_k E_{k-1} K_s}{G_k G_{k-1} G_{k-2}} + \cdots\cdots$$

$$+ (-1)^k \frac{K_s}{G_3} \prod_{r=4}^{k} \frac{E_r}{G_r} + (-1)^{k-1} \frac{E_3}{G_3}(x_{N+3} - C_2) \prod_{r=1}^{k} \frac{E_r}{G_r}$$

$$+ (-1)^k \frac{K_d}{G_3} (x_3 - L_3) \prod_{r=4}^{k} \frac{E_r}{G_r} + (-1)^{k-1} \frac{K_d}{B_4} (x_3 - L_3) \prod_{r=4}^{k} \frac{E_r}{G_r}$$

$$+ \cdots\cdots + (-1)^{k-1} \frac{K_d}{G_k}(x_3 - L_3) \frac{\prod_{r=4}^{k} E_r}{\prod_{r=4}^{k-1} B_r} \qquad \text{(A12-16)}$$

yields the scalar equation:

$$\dot{x}_{N+k+1} = - G_k x_{N+k+1} + E_k x_{N+k} - K_d x_k + (U_C)_k \qquad \text{(A12-17)}$$

Appendix 13: Linear Programming Formulation of Treatment Cost Minimization for "n" Dischargers

Minimize:

$$\sum_{i=1}^{n} \sum_{j=1}^{3} C_{ij} Y_{ij} = \text{Total dischargers' treatment cost} \qquad \text{(A13-1)}$$

Subject to:

$$\sum_{i=1}^{n} a_i X_i \sum_{j=1}^{3} b_j Y_{ij} = \sum_{i=1}^{n} a_i X_i - P \qquad \text{(A13-2)}$$

$$\sum_{j=1}^{3} Y_{ij} = 1 \quad \text{for } i = 1,2,\ldots,n \qquad \text{(A13-3)}$$

Appendix 14: Linear Programming Tableaux Used In Chapter 7 Example

BOD removed: 10,500 lb./day

Tableau 1 (in Phase 1)

	y_{13}	y_{14}	y_{22}	y_{23}	r_1	r_2	r_3	Solutions
r_1	6.82	(15)	2.70	2.77	1	0	0	10.5
r_2	1	1	0	0	0	1	0	1
r_3	0	0	1	1	0	0	1	1
-Z	7.82	16	3.70	3.77	0	0	0	12.5

Tableau 2 (in Phase 1)

	y_{13}	y_{14}	y_{22}	y_{23}	r_1	r_2	r_3	Solutions
y_{14}	.455	1	.18	.185	.067	0	0	.7
r_2	.545	0	-.18	-.185	-.067	1	0	.3
r_3	0	0	(1)	1	0	0	1	1
-Z	.545	0	.82	.81	-1.067	0	0	1.3

Tableau 3 (in Phase 1)

	y_{13}	y_{14}	y_{22}	y_{23}	r_1	r_2	r_3	Solutions
y_{14}	.455	1	0	.005	.067	0	-.18	.52
r_2	(.545)	0	0	-.005	-.067	1	.18	.48
y_{22}	0	0	1	1	0	0	1	1
-Z	.545	0	0	-.01	-1.067	0	-.82	.48

BOD removed: 10,500 lb./day

Tableau 4 (in Phase 1) and Tableau 1 (in Phase 2)

	y_{13}	y_{14}	y_{22}	y_{23}	r_1	r_2	r_3	Solutions
y_{14}	0	1	0	.009				.12
y_{13}	1	0	0	-.009				.88
y_{22}	0	0	1	1				1
-Z	0	0	0	0	-1	-1	-1	0
$-C_j$	-2.13	-3.35	-1.07	-1.64				
z_j	-2.13	-3.35	-1.07	-1.08				
C_j-z_j	0	0	0	-.56				

COST: .40
1.88
1.07
3.35

BOD removed: 15,400 lb./day

Tableau 1 (in Phase 1)

	y_{13}	y_{14}	y_{22}	y_{23}	y_{24}	s_1	s_2	s_3	Solutions
r_1	6.82	15	2.70	2.77	6.09	1	0	0	15.4
r_2	1	(1)	0	0	0	0	1	0	1
r_3	0	0	1	1	1	0	0	1	1
-Z	7.82	16	3.70	3.77	7.09	0	0	0	17.4

BOD removed: 15,400 lb./day

Tableau 2 (in Phase 1)

	y_{13}	y_{14}	y_{22}	y_{23}	y_{24}	r_1	r_2	r_3	Solu-tions
r_1	-8.18	0	2.70	2.77	6.09	1	-15	0	.4
y_{14}	1	1	0	0	0	0	1	0	1
r_3	0	0	1	1	1	0	0	1	1
-Z	-8.18	0	3.70	3.77	7.09	0	-16	0	1.4

Tableau 3 (in Phase 1)

	y_{13}	y_{14}	y_{22}	y_{23}	y_{24}	r_1	r_2	r_3	Solu-tions
y_{24}	-1.34	0	.44	.45	1	.16	-2.46	0	.066
y_{14}	1	1	0	0	0	0	1	0	1
r_3	1.34	0	.56	.55	0	-.16	2.46	1	.934
-Z	1.34	0	.56	.55	0	-1.16	1.46	0	.934

Tableau 4 (in Phase 1) and Tableau 1 (in Phase 2)

	y_{13}	y_{14}	y_{22}	y_{23}	y_{24}	r_1	r_2	r_3	Solu-tions
y_{24}	0	0	1	1	1				1
y_{14}	0	1	-.417	-.41	0				.303
y_{13}	1	0	.417	.41	0				.607
-Z	0	0	0	0	0	-1	-1	-1	0
C_j	-2.13	-3.35	-1.07	-1.64	-2.29				
z_j	-2.13	-3.35	-1.78	-1.78	-2.29				
-C	0	0	.71	.15	0				

BOD removed: 15,400 lb./day

Tableau 2 (in Phase 2)

	y_{13}	y_{14}	y_{22}	y_{23}	y_{24}	Solutions
y_{22}	0	0	1	1	1	1
y_{14}	0	1	0	.007	.417	.72
y_{13}	1	0	0	-.007	-.417	.28
-C	0	0	0	-.56	-3.00	

COST: 1.07
2.41
.60
4.08