WATER RESOURCES MODELING BY QUASILINEARIZATION AND INVARIANT IMBEDDING

by

IRVING KEAO HWANG

B.S.(Ind. Mgt.), Cheng Kung University
Tainan, Taiwan, China, 1966

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Major Professor

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CHAPTER 1

INTRODUCTION

The mathematical models which represent the complex blending of biological, chemical, and physical factors are not simple. In general, they must be represented by complicated differential equations, and these equations cannot be solved analytically when a fairly complicated system is involved. In order to establish these equations, the reaction and diffusion rate constants must be estimated from the actual experimental data. In other words, these constants or parameters must be estimated directly from the set of differential equations based on the measured concentrations with respect to time or space. This estimation problem forms a two-point or multipoint nonlinear boundary-value problem in which the conditions are not all given at one point. This type of nonlinear boundary-value problem is subtle and diffcult to solve.

The purpose of this work is to use two powerful techniques which have been recently developed for obtaining numerical solutions to water resources problems of the boundary-value type. Quasilinearization and invariant imbedding represent two completely different approaches to these problems. The quasilinearization technique, also known as the generalized Newton-Raphson method, represents an iterative approach combined with linear approximations; while the invariant imbedding approach, or the invariant principle, reformulates the original boundary-value problem into a family of initial value problems by introducing new variables or parameters.

Emphasis is placed upon computational instead of analytical aspects throughout this work. Most of the discussions are concerned with the actual convergence rates and computational requirements. Various numerical examples are solved and detailed computational procedures and results are given. General discussions concerning the stream quality models are also given but are not in detail.

In Chapter 2, the quasilinearization technique is introduced; the generalized Newton-Raphson formula, and the principle of superposition are discussed briefly.

Chapter 3 is devoted to the application of the quasi-linearization technique to various estimation problems in stream quality modeling. Many details concerning the computational procedure, and the convergence rates of the results are given in this chapter. It is shown that the quasilinearization technique appears to be a powerful tool for the stream quality modeling.

The invariant imbedding approach is described in Chapter 4. In this chapter, not only the basic concept but also the non-linear filtering theory is discussed.

In Chapter 5, the invariant imbedding approach is applied to solve some boundary-value problems which result from the identification or estimation of both state and parameters in dynamic stream pollution modeling.

CHAPTER 2

QUASILINEARIZATION

2.1 INTRODUCTION

The quasilinearization technique, also known as the generalized Newton-Raphson method was developed by Bellman and Kalaba [4, 5, 8], and has been applied extensively to various chemical engineering problems by Lee [20-23, 26] for obtaining numerical solutions of two-point or multipoint nonlinear boundary-value problems. Lee and his co-workers have also extended the application of the technique successfully to various problems in the fields of industrial management systems [18, 38], applied mechanics [27], water resources research [28], etc.

Conceptually, the quasilinearization technique, is very similar to the Newton-Raphson root finding method; however, the unknowns to be determined in this technique are functions and are not fixed values (roots) as in Newton-Raphson method. Thus, both the computational and theoretical aspects are much more complicated.

In general, most engineering problems are nonlinear boundary-value problems whose numerical solutions cannot be obtained easily, and there is a need for a method which can solve this type of problem efficiently. However, there are no severe difficulties in solving linear boundary-value problems, so whenever a nonlinear boundary-value problem is encountered, there is a natural temptation to try to linearize the nonlinear problem. However, the approximate linearized equations are often unsatisfactory for many application purposes. By the use of the quasilinearization technique, not only the original nonlinear equations can be linearized, but even more important, a sequence of functions which converges rather rapidly to the solution of the original nonlinear equations can be provided. For most practical problems, an initial approximation for the unknown function can be obtained from engineering experience and intuition. With this initial approximation, the solution of the original equations can be obtained through a sequence of functions.

2.2 GENERALIZED NEWTON-RAPHSON FORMULA

To apply the quasilinearization technique, consider the following general system of nonlinear differential equations

$$\frac{dx_i}{dt} = f_i(x_1, x_2, \ldots, x_M, t) \qquad i = 1, 2, \ldots, M. \tag{2.1}$$

where the x_i represents the dependent variable and t is the independent variable. In vector form, this system of equations can be represented by

$$\frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{f}(\underset{\sim}{x}, t) \tag{2.2}$$

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where $\underset{\sim}{x}$ and $\underset{\sim}{f}$ represent M-dimensional vectors with components $x_1, x_2, \ldots, x_M$ and $f_1, f_2, \ldots, f_M$, respectively. Eq. (2.2) can be linearized by the recurrence vector equation [8, 20-23].

$$\frac{d\underset{\sim}{x}_{k+1}}{dt} = \underset{\sim}{f}(\underset{\sim}{x}_k, t) + \underset{\sim}{J}(\underset{\sim}{x}_k)(\underset{\sim}{x}_{k+1} - \underset{\sim}{x}_k) \tag{2.3}$$

where $\underset{\sim}{x}_{k+1}$ and $\underset{\sim}{x}_k$ represent M-dimensional vectors with components $x_{1,k+1}, x_{2,k+1}, \ldots, x_{M,k+1}$ and $x_{1,k}, x_{2,k} \ldots, x_{M,k}$, respectively. The Jacobian matrix $\underset{\sim}{J}(\underset{\sim}{x}_k)$ is

$$\underset{\sim}{J}(\underset{\sim}{x}_k) = \begin{bmatrix} \frac{\partial f_1}{\partial x_{1,k}}, & \frac{\partial f_1}{\partial x_{2,k}}, & \ldots, & \frac{\partial f_1}{\partial x_{M,k}} \\ \frac{\partial f_2}{\partial x_{1,k}}, & \frac{\partial f_2}{\partial x_{2,k}}, & \ldots, & \frac{\partial f_2}{\partial x_{M,k}} \\ & & \vdots & \\ \frac{\partial f_M}{\partial x_{1,k}}, & \frac{\partial f_M}{\partial x_{2,k}}, & \ldots, & \frac{\partial f_M}{\partial x_{M,k}} \end{bmatrix}. \tag{2.4}$$

Note that Eq. (2.3) is essentially the Taylor series expansion with the second and higher order terms neglected. If $\underset{\sim}{x}_k$ is assumed to be the known value and is obtained from previous calculations and $\underset{\sim}{x}_{k+1}$ is the unknown value, Eq. (2.3) will always be linear.

2.3 PRINCIPLE OF SUPERPOSITION

In general, it is not an easy task to solve a two-point or multipoint nonlinear boundary-value problem. However, if the performance equations are linear, the superposition principle can be used [20-21].

Assume that the boundary conditions for Eq. (4) are

$$x_{j,k+1}(t_f) = x_j^f \qquad j = 1, 2, \ldots, m \tag{2.5a}$$

$$x_{L,k+1}(t_0) = x_L^0 \qquad L = m+1, m+2, \ldots, M. \tag{2.5b}$$

Now consider how the system of Eqs. (2.3) and (2.5) can be solved. Generally, the system cannot be solved in closed form. However, since Eq. (2.3) is linear, the system can be solved numerically by the use of the principle of superposition; and a numerical integration technique such as the Runge-Kutta integration scheme [20, 35] for initial value problems can be used. It is well known that for M simultaneous linear equations, their general solutions can be represented by one set of particular solutions and M sets of homogeneous solutions [20-21]. Thus, the general solutions of Eq. (2.3) are

$$\underset{\sim}{x}_{k+1}(t) = \underset{\sim}{x}_{p,k+1}(t) + \sum_{j=1}^{M} a_{j,k+1}\underset{\sim}{x}_{hj,k+1}(t) \tag{2.6}$$

$$t_0 \leq t \leq t_f$$

where $\underset{\sim}{x}_{p,k+1}(t)$ and $\underset{\sim}{x}_{hj,k+1}(t)$ are M-dimensional column vectors with components $x_{1p,k+1}(t)$, $x_{2p,k+1}(t)$, ..., $x_{Mp,k+1}(t)$ and $x_{1hj,k+1}(t)$, $x_{2hj,k+1}(t)$, ..., $x_{Mhj,k+1}(t)$, respectively. The $a_{j,k+1}$, $j = 1, 2, \ldots, M$, represent the M scalar integration constants to be determined from the boundary conditions.

The one set of particular solutions and M sets of homogeneous solutions must be obtained numerically. However, since they can be any solutions of Eq. (2.3) as long as the homogeneous solutions are nontrivial and distinct, any set of initial conditions can be used to obtain the particular solutions; and any M sets of initial conditions, as long as they are nontrivial and distinct, can be used to obtain the M sets of homogeneous solutions. Furthermore, if these M+1 sets of initial conditions are chosen in such a way that they satisfy the given initial conditions as given in Eq. (2.5b), only m sets of homogeneous solutions are needed with m integration constants, $a_{j,k+1}$, $j = 1, 2, \ldots, m$. Thus, Eq. (2.6) can be reduced to

$$\underset{\sim}{x}_{k+1}(t) = \underset{\sim}{x}_{p,k+1}(t) + \sum_{j=1}^{m} a_{j,k+1} \, \underset{\sim}{x}_{hj,k+1}(t). \tag{2.7}$$

$$t_0 \leq t \leq t_f$$

In vector form, the set of algebraic equations (2.7) can be represented by

$$\underset{\sim}{x}_{k+1}(t) = \underset{\sim}{x}_{p,k+1}(t) + \underset{\sim}{x}_{h,k+1}(t)\, \underset{\sim}{a}_{k+1} \tag{2.8}$$

where $\underset{\sim}{a}_{k+1}$ is the m-dimensional integration constant vector with components $a_{1,k+1}$, $a_{2,k+1}$, ..., $a_{m,k+1}$, respectively. The symbol $\underset{\sim}{x}_{h,k+1}(t)$ represents the homogeneous solution matrix

$$\underset{\sim}{x}_{h,k+1}(t) = \begin{bmatrix} x_{1h1,k+1}(t) & x_{1h2,k+1}(t) & \cdots & x_{1hm,k+1}(t) \\ x_{2h1,k+1}(t) & x_{2h2,k+1}(t) & \cdots & x_{2hm,k+1}(t) \\ & & \cdot & \\ & & \cdot & \\ & & \cdot & \\ x_{mh1,k+1}(t) & x_{mh2,k+1}(t) & \cdots & x_{mhm,k+1}(t) \end{bmatrix}. \tag{2.9}$$

Once the particular and homogeneous solutions are obtained, the integration constant, $\underset{\sim}{a}_{k+1}$ can be obtained from Eq. (2.8). With $\underset{\sim}{a}_{k+1}$ known, the general solution $\underset{\sim}{x}_{k+1}(t)$ of Eq. (2.3) can be obtained. Once $\underset{\sim}{x}_{k+1}(t)$, $t_0 \leq t \leq t_f$, is obtained, an improved solution vector $\underset{\sim}{x}_{k+2}(t)$ can be obtained. The procedure is continued until the process converges and the desired accuracy is obtained.

2.4 DISCUSSION

In the quasilinearization technique, the solution of the nonlinear equation is obtained by solving a sequence of linear equations. In general, the solutions of this sequence of linear equations converge rapidly to the solution of the original nonlinear equation provided that the process converges. The main advantage of this technique is that if the procedure converges, its convergence would be quadratic. Quadratic convergence means that the error in the current iteration tends to be proportional to the square of the error in the previous iteration. The advantage of quadratic convergence, of course, lies in the rapidity of convergence.

The principle of superposition provides a fairly routine procedure for solving the linear equations of the boundary-value problems on modern computers. However, in spite of all the advantages, the ill-conditioning phenomenon which is the main difficulty encountered in the use of this technique can make the superposition principle useless. Another difficulty is the convergence problem. If the initial approximation is not within the domain of convergence a solution generally cannot be obtained. Further discussions of convergence properties can be found in the literature [20].

CHAPTER 3

STREAM QUALITY MODELING AND ESTIMATION BY QUASILINEARIZATION

3.1 INTRODUCTION

Modeling and estimating the response of a river or stream to any proposed pollution abatement action is one of the most complex problems facing the sanitary engineers. The mathematical models which must represent a complex blending of biological, chemical, and physical factors are not simple and must be represented by complicated differential equations. In order to establish these equations, the reaction and diffusion parameters must be estimated from actual experimental measurements. For a fairly complicated system these equations cannot be solved analytically. Furthermore, the reaction, diffusion, and mixing constants cannot be measured directly. They must be calculated from the measured change of concentrations with respect to time or space. Thus, these constants or parameters must be estimated directly from the set of differential equations based on the experimental data.

In this chapter, the computational aspects of estimation process by the quasilinearization technique will be discussed with respect to its application in stream quality modeling and estimation. The estimation problem is treated as a two-point or multipoint boundary-value problem.

3.2 HYDROLOGICAL BACKGROUND

Water comes in contact with many different substances during its natural passage from the air, over and through the ground, through the various uses of the municipalities and industries back to the stream, lake and to the sea, and from there to the air again. In the surface runoff stage of the cycle, water may carry with it soil, chemical contaminants, vegetation, and micro-organisms. In the ground water stage, water will contain many dissolved minerals; this is usually the stage at which man encounters water.

Man's use of water for domestic, municipal, and industrial purposes introduces a further degradation of water quality. The wastes discharged into the stream from municipal and industrial treatment plants generally consist of a large variety of chemical compounds, of which a large portion is bio-degradable and oxygen demanding. When this waste substance is placed in a watercourse, it undergoes biochemical oxidation by micro-organisms for food. When sufficient dissolved oxygen is contained in the water, the dominant organisms are aerobic. The dissolved oxygen is used to complete the oxidation reaction, resulting in the production of carbon dioxide and water. However, if there is insufficient dissolved oxygen available, then anaerobic organisms predominant and end up with undesirable products such as putrid odors, septic conditions, and even fish kills, etc.

Due to the fact that there are various oxygen-demanding

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organisms contained in wastes, and the importance of the dissolved oxygen content of streams, it is therefore more common to measure the "strength" of wastes in terms of their biochemical oxygen demand (BOD) rather than to analyze for the chemical constituents of the waste. For this reason stream quality standards usually specify minimun dissolved oxygen (DO) concentrations for the streams.

The dissolved oxygen content of a stream is generally governed by two major factors: One is the utilization of oxygen by biochemical oxidation, and the other is the supply of oxygen by absorption of atmospheric oxygen, artificial aeration, and photosynthesis.

The biochemical oxygen demand of the polluted water consists of two reaction stages: The first is concerned with the relatively earlier acting oxidation of carbonaceous material, while the second is concerned with the later and slower acting nitrification process. In practical cases, engineering investigations are carried out using only first stage demand. Thus, only the first stage demand has been satisfactorily generalized in mathematical terms.

In the following section, the commonly used mathematical models will be discussed.

3.3 THE MATHEMATICAL MODELS

The most widely used mathematical model of the dissolved oxygen relationships in a stream is that proposed by Streeter and Phelps [40]. It is an one dimensional model and is in terms of two competing parameters: One is the biochemical oxygen demand, and the other is the dissolved oxygen. The model describes biochemical oxidation as a very simple first order differentical equation

$$\frac{dB}{dt} = -K_1 B \qquad (3.1)$$

where B is the first stage biochemical oxygen demand in parts per million (ppm), t is the time in days, and K_1 is a reaction rate constant for deoxygenation in day^{-1} which depends not only on the characteristics of the waste but also on the water temperature.

In the Streeter-Phelps model, the reaeration is also presented as a first order process depending upon the difference between the dissolved oxygen concentration, and the saturation concentration:

$$\frac{dC}{dt} = -K_2(S-C) \qquad (3.2)$$

where C is the dissolved oxygen concentration in ppm, S is the satuation concentration in ppm, and K_2 is the reaeration rate constant in day^{-1}.

By combining the rates of the two reactions, the resulting equation in terms of the dissolved oxygen deficit is obtained:

$$\frac{dD}{dt} = K_1B - K_2D \tag{3.3}$$

where D = S - C.

The Streeter-Phelps formulation describes the behavior of the dissolved oxygen concentration in a single reach of a stream. It considers only the oxygen uptake of dissolved organic material and the absorption of atmospheric oxygen, but it fails to account for the effects of photosynthesis, sedimentation, bottom scour, and surface runoff on the dissolved oxygen balance.

Furthermore, since the capacity of the stream to assimilate bio-degradable wastes is determined by such factors as BOD and DO concentrations, stream flow and temperature, and the physical and biological properties of the stream that affect settling rates, reaeration, and BOD addition due to runoff and scour, etc. A number of modifications of this work have been proposed by several people [10], [13], [30], [41].

In the present study, a modified Streeter-Phelps model which has been developed by Camp [10] and Dobbins [13] is considered.

In addition to the two rate constants, deoxygenation and reaeration, three more constants which represent the BOD addition due to runoff and scour, oxygen production or reduction by plants or bottom deposits, and sedimentation appear in the Camp-Dobbins model. In the present case, Eqs. (3.1) and (3.3) become

$$\frac{dB}{dt} = -(K_1 + K_3)B + R \tag{3.4}$$

$$\frac{dD}{dt} = K_1 B - K_2 D - A \tag{3.5}$$

where B, D, K_1, K_2, and t remain the same as in Eqs. (3.1) and (3.3), R represents the BOD addition rate due to runoff and scour in ppm per day, A is the rate of oxygen production or reduction due to plant photosynthesis and respiration in ppm per day, and K_3 is the sedimentation and absorption rate constant in day^{-1}.

The Camp-Dobbins equations do not satisfactorily describes the complex biological, chemical and physical phenomena of streams. However, they do account for the effects of introduction of some unstable bio-degradable and oxygen demanding wastes on the oxygen resources of streams. It is, therefore, the model commonly used by state and federal officials as means of water pollution control. Letting B_0 be the initial (t = 0) BOD, the BOD concentration B_t at any point (corresponding to a time, t) downstream can be obtained by integrating Eq. (3.4).

$$B_t = \left(B_0 - \frac{R}{K_1+K_3}\right)e^{-(K_1+K_3)} + \frac{R}{K_1+K_3} \tag{3.6}$$

Substituting for B_t from Eq. (3.6), and letting D_0 be the initial oxygen deficit, Eq. (3.5) can be integrated to determine the DO deficit D_t at any point downstream.

$$D_t = \frac{K_1}{K_2-(K_1+K_3)} (B_0 - \frac{R}{K_1+K_3}) (e^{-(K_1+K_3)t} - e^{-K_2 t})$$
$$+ \frac{K_1}{K_2} (\frac{R}{K_1+K_3} - \frac{A}{K_1}) (1 - e^{-K_2 t}) + D_0 e^{-K_2 t} . \quad (3.7)$$

A graph of D_t versus t results in the typical oxygen "sag curve", shown in Figure 1. The point of maximum DO deficit (or minimum DO concentration) is called the critical point. The critical deficit D_c, and the critical time t_c, occur at the critical point. In Region A, the rate of deoxygenation exceeds the reaeration rate. While in Region B, the reverse is true. Further discussions of water pollution models, BOD and DO relationships in streams, can be found in the references [14-15, 30-32, 34, 39, 41-42].

3.4 PARAMETER ESTIMATION

The purpose of this section is to illustrate how the quasilinearization technique can be applied to the estimation problems in stream quality modeling. A number of examples are solved to illustrate the technique.

3.4.1 A Simple Estimation Problem

To illustrate the approach, consider the simple representation of stream quality proposed by Camp and Dobbins, described earlier in Eqs. (3.4) and (3.5).

In actual experimental situations, the reaction rate

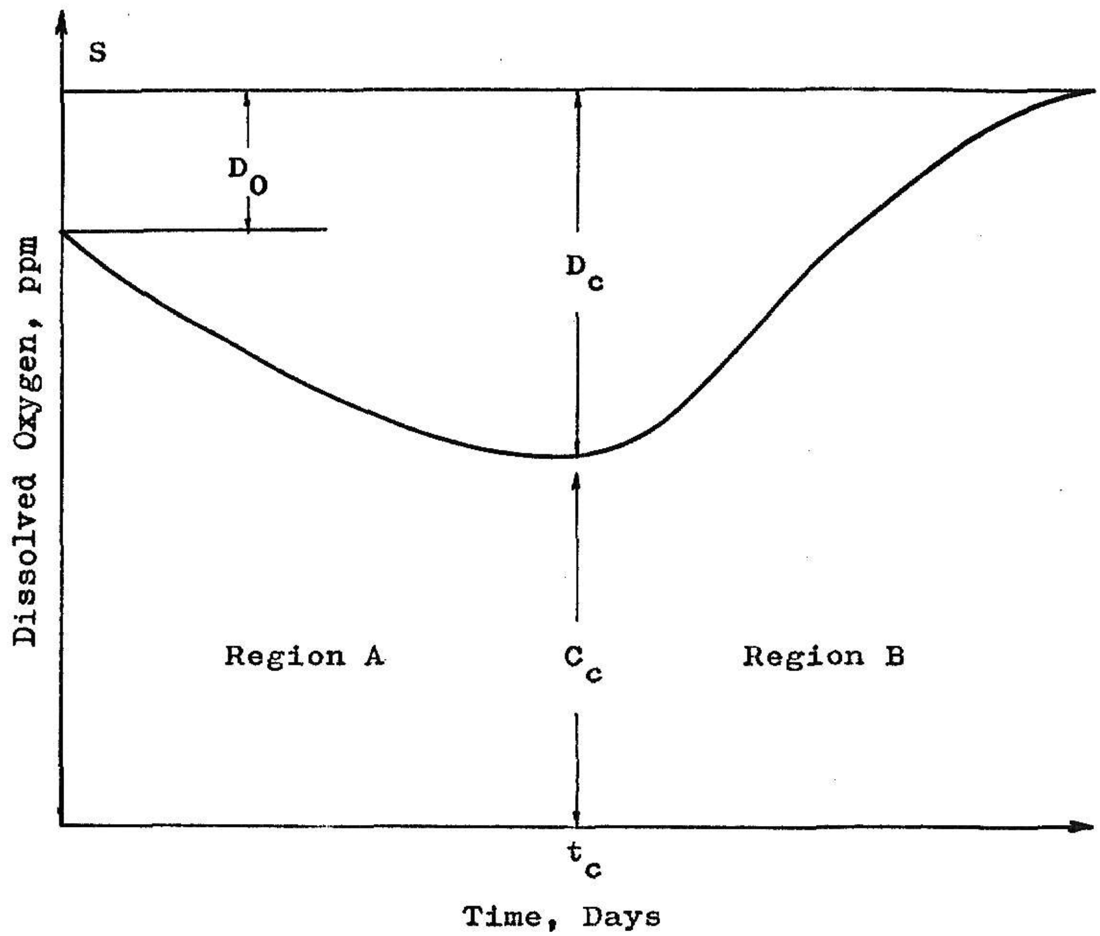

Fig. 1. Oxygen Sag Curve

constants K_1, K_2, and K_3 cannot be measured directly. Only B and D can be measured at various values of t. The rate constants must be estimated from these experimental values. Since Eqs. (3.4) and (3.5) can be solved in closed form, the estimation of these rate constants is not very difficult. However, it must be noted that Eqs. (3.4) and (3.5) are a simplified representation of the actual stream situation. The use of a more realistic model would make the differential equations more complicated and unsolvable analytically. The estimation of these rate constants from the experimental data becomes very difficult when closed form solutions for the equations representing the process cannot be obtained. Furthermore, even if closed form solutions for the process model could be obtained, as in Eqs. (3.4) and (3.5), the present approach of directly estimating the parameters from the differential equations still has distinct advantages. Note that the parameters or rate constants appear nonlinearly in the resulting analytical solutions of Eqs. (3.4) and (3.5). The estimation of parameters from nonlinear algebraic equations is not simple. The quasilinearization technique appears to be much more powerful than the commonly used nonlinear regression or nonlinear least squares estimation techniques.

The problem can be stated as follows: Estimate the rate constants or parameters K_1, K_2, and K_3 for Eqs. (3.4) and (3.5) with the following measured or experimental data

$$B^{(exp)}(t_s) = b_s, \qquad s = 1, 2, \ldots, S.$$
$$D^{(exp)}(t_r) = d_r, \qquad r = 1, 2, \ldots, R. \tag{3.8}$$

where $S + R \geq 3$, $t_0 \leq t_s \leq t_f$, and $t_0 \leq t_r \leq t_f$. The initial conditions for Eqs. (3.4) and (3.5) are

$$B(t_0) = B^0$$
$$D(t_0) = D^0. \tag{3.9}$$

The quantities b_s and d_r are known values and are obtained by measuring B and D experimentally at various values of t. The number of the experimental values must be greater or equal to the number of the unknown constant parameters. The superscript, (exp), denotes that the values of B and D are experimental values. Note that t_s and t_r are not necessarily the same. Although experimental data for both the state variables B and D are assumed, the approach can be used in the same way if only one of the variable has experimental measurements.

3.4.2 Computational Consideration

First, the case in which $S + R = 3$ is considered. It is assumed that only the following three data points are available for estimating the rate constants

$$B^{(exp)}(t_1) = b_1$$

$$B^{(exp)}(t_2) = b_2 \tag{3.10}$$

$$D^{(exp)}(t_1) = d_1.$$

Further assume that the experimental errors resulting from obtaining the experimental data are very small and thus these experimental values can be considered as the true values of B and D at the given values of t. To estimate the rate constants, it is convenient to consider the unknown parameters K_1, K_2 and K_3 as dependent variables parallel to B and D, and as functions of the independent variable t. Since these funotions do not change with time t, they can be written as:

$$\frac{dK_1}{dt} = 0 \tag{3.11}$$

$$\frac{dK_2}{dt} = 0 \tag{3.12}$$

$$\frac{dK_3}{dt} = 0 \tag{3.13}$$

Now, the system has five simultaneous differential equations, Eqs. (3.4), (3.5), (3.11)-(3.13). The five equations can be solved by the use of the boundary conditions as given in (3.9) with $t_0 = 0$ and

$$\begin{aligned} B(t_1) &= b_1 \\ B(t_2) &= b_2 \\ D(t_1) &= d_1 \end{aligned} \tag{3.14}$$

where t_1 and t_2 are two discrete values of t within the interval $0 \leq t \leq t_f$. Note that the experimental data are used as the boundary conditions. Since these boundary conditions are not all given at one point, the problem is therefore a multipoint boundary-value type. Furthermore, since both the rate constants K_1, K_2 and K_3, and the original variables B and D are considered as unknown functions, Eqs. (3.4) and (3.5) are nonlinear equations. Thus, the system represented by Eqs. (3.4), (3.5), (3.11)-(3.13) is a multipoint nonlinear boundary-value problem.

3.4.3 The Least Squares Approach

For nearly all parctical situations, the experimental data are not exact and always have experimental or measurement errors. It is therefore desirable to obtain a fairly large amount of data instead of just three data points. For $S + R > 3$, the classical least squares criterion can be used, the object is to determine the constant parameters so that the sum of the squares of the deviations is minimized. Instead of using boundary conditions (3.14), one can obtain these three conditions by minimizing the following least squares expression

$$Q = \sum_{s=1}^{S} [B(t_s) - b_s]^2 + \sum_{r=1}^{R} [D(t_r) - d_r]^2 \qquad (3.15)$$

where the minimization is over the constant parameters K_1, K_2 and K_3. $B(t_s)$ and $D(t_r)$ are obtained by solving Eqs. (3.4) and (3.5).

Note that the above problem is equivalent to the optimization problem of minimizing the expression (3.17) subject to the conditions (3.4), (3.5) and (3.9). The minimization is over the three unknown initial values $K_1(0)$, $K_2(0)$ and $K_3(0)$.

3.4.4 Computational Procedure

The estimation problem for the simple stream quality model can now be approached by the quasilinearization technique. The system of equations (3.4), (3.5), (3.11)-(3.13) can be easily linearized by using the generalized Newton-Raphson formula of Eq. (2.3) as developed in Chapter 2 with M = 5. These linearized equations are

$$\frac{dB_{k+1}}{dt} = -(K_{1,k} + K_{3,k})B_{k+1} - B_k K_{1,k+1} - B_k K_{3,k+1} + B_k K_{1,k} + B_k K_{3,k} + R \tag{3.16}$$

$$\frac{dD_{k+1}}{dt} = K_{1,k} B_{k+1} - K_{2,k} D_{k+1} + B_k K_{1,k+1} - D_k K_{2,k+1} - K_{1,k} B_k + K_{2,k} D_k - A \tag{3.17}$$

$$\frac{dK_{1,k+1}}{dt} = 0 \tag{3.18}$$

$$\frac{dK_{2,k+1}}{dt} = 0 \tag{3.19}$$

$$\frac{dK_{3,k+1}}{dt} = 0. \tag{3.20}$$

The two given boundary conditions are

$$B_{k+1}(0) = B^0 \tag{3.21}$$

$$D_{k+1}(0) = D^0. \tag{3.22}$$

The other three boundary conditions can be obtained either by using Eqs. (3.14) or by minimizing the least squares equation (3.15). Since the use of least squares is a more practical problem, the case of minimizing Eq. (3.15) is considered.

Eqs. (3.16)-(3.20) are linear equations with variable coefficients. In general, they cannot be solved in closed form. However, since they are linear, the principle of superposition as described earlier in Chapter 2 can be used. The general solution vector equation for the system of equations (3.16) through (3.20), which corresponds to Eq. (2.8), can be represented by

$$\underset{\sim}{x}_{k+1}(t) = \underset{\sim}{x}_{p,k+1}(t) + \underset{\sim}{x}_{h,k+1}(t)\ \underset{\sim}{a}_{k+1} \tag{3.23}$$

where $0 \leq t \leq t_f$. The state vector $\underset{\sim}{x}_{k+1}(t)$ and the particular solution vector $\underset{\sim}{x}_{p,k+1}(t)$ are defined as

$$\underset{\sim}{x}_{k+1}(t) = \begin{bmatrix} B_{k+1}(t) \\ D_{k+1}(t) \\ K_{1,k+1}(t) \\ K_{2,k+1}(t) \\ K_{3,k+1}(t) \end{bmatrix} \tag{3.24}$$

and

$$\underset{\sim}{x}_{p,k+1}(t) = \begin{bmatrix} B_{p,k+1}(t) \\ D_{p,k+1}(t) \\ K_{1p,k+1}(t) \\ K_{2p,k+1}(t) \\ K_{3p,k+1}(t) \end{bmatrix} . \tag{3.25}$$

The integration constant vector is

$$\underset{\sim}{a}_{k+1} = \begin{bmatrix} a_{1,k+1} \\ a_{2,k+1} \\ a_{3,k+1} \end{bmatrix} \tag{3.26}$$

and the homogeneous solution matrix is defined as

$$\underset{\sim}{x}_{h,k+1}(t) = \begin{bmatrix} B_{h1,k+1}(t) & B_{h2,k+1}(t) & B_{h3,k+1}(t) \\ D_{h1,k+1}(t) & D_{h2,k+1}(t) & D_{h3,k+1}(t) \\ K_{1h1,k+1}(t) & K_{1h2,k+1}(t) & K_{1h3,k+1}(t) \\ K_{2h1,k+1}(t) & K_{2h2,k+1}(t) & K_{2h3,k+1}(t) \\ K_{3h1,k+1}(t) & K_{3h2,k+1}(t) & K_{3h3,k+1}(t) \end{bmatrix}. \tag{3.27}$$

The particular and homogeneous solutions are chosen in such a way that they satisfy the two given initial conditions in (3.21) and (3.22). Thus, only three sets of homogeneous solutions and three integration constants are needed. In actual calculations, the set of particular solutions are obtained by integrating Eqs. (3.16)-(3.20) with the following initial values:

$$\underset{\sim}{x}_{p,k+1}(0) = \begin{bmatrix} B^0 \\ D^0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{3.28}$$

The homogeneous form of Eqs. (3.16) through (3.20) is

$$\frac{dB_{k+1}}{dt} = -(K_{1,k} + K_{3,k})B_{k+1} - B_k K_{1,k+1} - B_k K_{3,k+1} \tag{3.29}$$

$$\frac{dD_{k+1}}{dt} = K_{1,k}B_{k+1} - K_{2,k}D_{k+1} + B_kK_{1,k+1} - D_kK_{2,k+1} \tag{3.30}$$

$$\frac{dK_{1,k+1}}{dt} = 0 \tag{3.31}$$

$$\frac{dK_{2,k+1}}{dt} = 0 \tag{3.32}$$

$$\frac{dK_{3,k+1}}{dt} = 0 \tag{3.33}$$

The initial values used to obtain the homogeneous solutions are

$$x_{h,k+1}(0) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 0.2 \\ 0 & 1 & 0 \\ 0.5 & 0 & 1 \end{bmatrix}. \tag{3.34}$$

Note that the initial values in (3.28) and (3.34) are chosen in such a way that at $t = 0$, the general solutions of B and D in Eq. (3.23) satisfy the given initial conditions (3.21) and (3.22) and only three sets of homogeneous solutions are needed. Note also that three simple linear relationships between the integration constants $a_{j,k+1}$, $j = 1, 2, 3$ and the constant parameters $K_{j,k+1}$, $j = 1, 2, 3$, can be obtained from the general solutions of K_1, K_2 and K_3 in Eq. (3.23) and the initial conditions (3.28) and (3.34). These linear relationships are as follows:

$$K_{1,k+1}(t) = a_{1,k+1} + a_{2,k+1} + 0.2\, a_{3,k+1} \tag{3.35}$$

$$K_{2,k+1}(t) = a_{2,k+1} \tag{3.36}$$

$$K_{3,k+1}(t) = 0.5\, a_{1,k+1} + a_{3,k+1} \tag{3.37}$$

Since the two given boundary conditions, Eqs. (3.21) and (3.22), have already been used in choosing the initial conditions for obtaining the particular and homogeneous solutions. The remaining three integration constants, $a_{j,k+1}$, $j = 1, 2, 3$, can be obtained from the remaining three boundary conditions. For the case $S + R > 3$, these three conditions can be obtained by minimizing Eq. (3.15). At various positions of t_s and t_r($s = 1, 2, \ldots, S$; $r = 1, 2, \ldots, R$), the following $S + R$ equations can be obtained from the general solutions of B and D in the vector equation (3.23)

$$B_{k+1}(t_s) = B_{p,k+1}(t_s) + \sum_{j=1}^{3} a_{j,k+1}\, B_{hj,k+1}(t_s) \tag{3.38}$$

$$D_{k+1}(t_r) = D_{p,k+1}(t_r) + \sum_{j=1}^{3} a_{j,k+1}\, D_{hj,k+1}(t_r) \tag{3.39}$$

Substitution of the above two equations into Eq. (3.15) yields,

$$Q_{k+1} = \sum_{s=1}^{S}\Big[B_{p,k+1}(t_s) + \sum_{j=1}^{3} a_{j,k+1}\, B_{hj,k+1}(t_s) - b_s\Big]^2$$

$$+ \sum_{r=1}^{R} [D_{p,k+1}(t_r) + \sum_{j=1}^{3} a_{j,k+1} D_{hj,k+1}(t_r) - d_r]^2. \quad (3.40)$$

Since the particular and homogeneous solutions at the various positions of t are known and are obtained numerically by using the initial values in (3.28) and (3.24), the only unknowns on the right-hand side of Eq. (3.40) are the three integration constants, $a_{j,k+1}$, $j = 1, 2, 3$. Thus, the problem is now changed into an optimization problem of determining the values of these three integration constants such that the value of Q_{k+1} is minimized.

There are many techniques which can be used to minimize Eq. (3. 40). However, for this work, partial differentiation will be used to obtain the extreme values. By differentiating (3.40) with respect to $a_{j,k+1}$, $j = 1, 2, 3$, respectively, and setting the results equal to zeros, the following three algebraic equations are obtained:

$$\begin{aligned} \frac{Q_{k+1}}{a_{i,k+1}} &= 2 \sum_{s=1}^{S} B_{hi,k+1}(t_s)[B_{p,k+1}(t_s) \\ &\quad + \sum_{j=1}^{3} a_{j,k+1} B_{hj,k+1}(t_s) - b_s] \\ &\quad + 2 \sum_{r=1}^{R} D_{hi,k+1}(t_r)[D_{p,k+1}(t_r) \\ &\quad + \sum_{j=1}^{3} a_{j,k+1} D_{hj,k+1}(t_r) - d_r] \\ &= 0 \end{aligned} \quad (3.41)$$

$$i = 1, 2, 3.$$

These three equations form the remaining three boundary conditions. Since the variables $B(t_s)$, $D(t_r)$, b_s and d_r ($s = 1, 2, \ldots, S$; $r = 1, 2, \ldots, R$) are all known values, the integration constants $a_{j,k+1}$, $j = 1, 2, 3$, can now be obtained by solving the above three algebraic equations. Once the integration constants are known, the general solutions for $B_{k+1}(t)$, $D_{k+1}(t)$, $K_{1,k+1}(t)$, $K_{2,k+1}(t)$, and $K_{3,k+1}(t)$ can be obtained from Eq. (3.23). Since the estimated parameters $K_{1,k+1}$, $K_{2,k+1}$, and $K_{3,k+1}$ are constants, they can be obtained either from the general solutions (3.23) or by the linear relationships represented by Eqs. (3.35)-(3.37).

With B_{k+1}, D_{k+1}, $K_{1,k+1}$, $K_{2,k+1}$, and $K_{3,k+1}$ known, an improved set of values can be obtained in the same way by making $k = k+1$ in (3.16)-(3.20). The iterative procedure is continued until the desired results are obtained provided that the process converges.

The computational procedure can now be summarized as follows:

1. Linearize the system of equations (3.4), (3.5), (3.11)-(3.13) using the generalized Newton-Raphson formula (2.3).
2. Assume a set of reasonable initial functions for $B(t)$, $D(t)$, $K_1(t)$, $K_2(t)$, and $K_3(t)$. Let these initial functions be $B_{k=0}(t)$, $D_{k=0}(t)$, $K_{1,k=0}(t)$, $K_{2,k=0}(t)$, and $K_{3,k=0}(t)$.
3. Integrate Eqs. (3.16)-(3.20) numerically using (3.28) as the initial value with $k = 0$.

4. Integrate the homogeneous equations (3.29)-(3.33) three times using (3.34) as the initial value with $k = 0$.

5. Solve Eq. (3.41) for the integration constants $a_{j,k+1=1}$, $j = 1, 2, 3$, using the newly obtained particular and homogeneous solutions from Steps 3 and 4, and using the given experimental data, b_s and d_r ($s = 1, 2, \ldots, S$; $r = 1, 2, \ldots, R$).

6. Calculate $B_{k+1=1}(t)$, $D_{k+1=1}(t)$, $K_{1,k+1=1}(t)$, $K_{2,k+1=1}(t)$, and $K_{3,k+1=1}(t)$ using Eq. (3.23) or obtain $K_{1,k+1=1}$, $K_{2,k+1=1}$, and $K_{3,k+1=1}$ from Eqs. (3.35) through (3.37).

7. Repeat Steps 3 through 5 with $k = 1, 2, \ldots,$ until no further improvement on the values of $B(t)$, $D(t)$, K_1, K_2, and K_3 can be obtained.

Note that the best available initial functions should be used for Step 2.

3.4.5 A More General Estimation Problem

In practical situations, the oxygen production or reduction rate A, and the BOD addition rate R, cannot be measured directly for most of the cases. Thus, a practically important problem is: Given experimental data on B and D along the stream and assume that the pollution model of the stream can be represented by Eqs. (3.4) and (3.5), obtain the best estimates for the parameters K_1, K_2, K_3, A, and R. This problem can be solved in essentially the same way as before except for the presence of five unknown parameters. This system can be represented by Eqs. (3.4), (3.5), (3.11)-(3.13) and

$$\frac{dA}{dt} = 0 \tag{3.42}$$

$$\frac{dR}{dt} = 0 \tag{3.43}$$

These seven equations can be linearized in the same way as that discussed for the estimation of three parameters. Since A and R appear linearly in these equations, the linearization operation does not influence these two parameters. Using the principle of superposition, a system of seven equations for the general solutions can be obtained. By using the initial values listed in Table 1 to obtain the particular and homogeneous solutions, only five sets of homogeneous solutions are needed. Eq. (3.41) remains essentially the same except that $i = 1, 2, \ldots, 5$ and $j = 1, 2, \ldots, 5$.

Note that since $A_k(t)$ and $R_k(t)$ do not appear in the linearized equations, the initial functions for $A_{k=0}(t)$ and $R_{k=0}(t)$ are not needed in Step 2 in the previously discussed computational procedure.

3.5 NUMERICAL RESULTS

To test the effectiveness of this approach, the constants or coefficients in Eqs. (3.4) and (3.5) are estimated from a given set of data. These given data are obtained numerically by solving Eqs. (3.4) and (3.5) using the following numerical values:

Table 1.

Initial Values Used for Obtaining the Particular and Homogeneous Solutions

Variable	Particular Solution	Homogeneous Solutions 1	2	3	4	5
$B_{k+1}(0)$	7.0	0	0	0	0	0
$D_{k+1}(0)$	5.7	0	0	0	0	0
$K_{1,k+1}(0)$	0	1	1	0.2	0.3	0
$K_{2,k+1}(0)$	0	0	1	0	0	0
$K_{3,k+1}(0)$	0	0.5	0	1	0.5	0
$A_{k+1}(0)$	0	0	0	0	1	0
$R_{k+1}(0)$	0	0	0	0	0.2	1

$$B^0 = 7.0, \quad D^0 = 5.7, \quad t_f = 1, \tag{3.44}$$

$$R = 0.15, \quad A = 0.85, \tag{3.45}$$

$$K_1 = 0.31, \quad K_2 = 1.02, \quad K_3 = 0.03. \tag{3.46}$$

Eqs. (3.4) and (3.5) are integrated numerically with the Runge-Kutta integration scheme. The step size which was used in this integration is $\Delta t = 0.01$. Part of the results from this integration are listed in Table 2 and plotted in Figure 2 which are used as the experimental data. Note that 21 ($S = R = 21$) data points are used and $t_s = t_r$ for this particular problem. Note also that the experimental profile of D used as shown in Figure 2 is just a portion of the complete "oxygen sag" curve which has been described in Section 3.3.

3.5.1 Estimation of Two Parameters

First, parameters K_1 and K_2 are estimated using the values listed in Table 2 as the experimental data. In other words, K_1 and K_2 are considered as the unknown parameters which must be estimated from the given data listed in Table 2, the given model represented by Eqs. (3.4) and (3.5), and the given values represented by Eqs. (3.44), (3.45) and $K_3 = 0.03$.

The system of equations for this problem is represented by Eqs. (3.4)-(3.5), and (3.11)-(3.12). These four equations can be linearized in the same way as before except that K_3 is considered as a given constant.

Table 2.

Numerical Values Used as Experimental Data

t_s	s	$B^{(exp)}(t_s) = b_s$	$D^{(exp)}(t_s) = d_s$
0.00	1	7.0000	5.7000
0.05	2	6.8894	5.4801
0.10	3	6.7807	5.2695
0.15	4	6.6739	5.0677
0.20	5	6.5688	4.8743
0.25	6	6.4655	4.6890
0.30	7	6.3640	4.5113
0.35	8	6.2642	4.3410
0.40	9	6.1660	4.1776
0.45	10	6.0695	4.0209
0.50	11	5.9746	3.8706
0.55	12	5.8814	3.7262
0.60	13	5.7897	3.5877
0.65	14	5.6995	3.4547
0.70	15	5.6109	3.3269
0.75	16	5.5237	3.2042
0.80	17	5.4380	3.0863
0.85	18	5.3538	2.9729
0.90	19	5.2710	2.8639
0.95	20	5.1896	2.7591
1.00	21	5.1095	2.6583

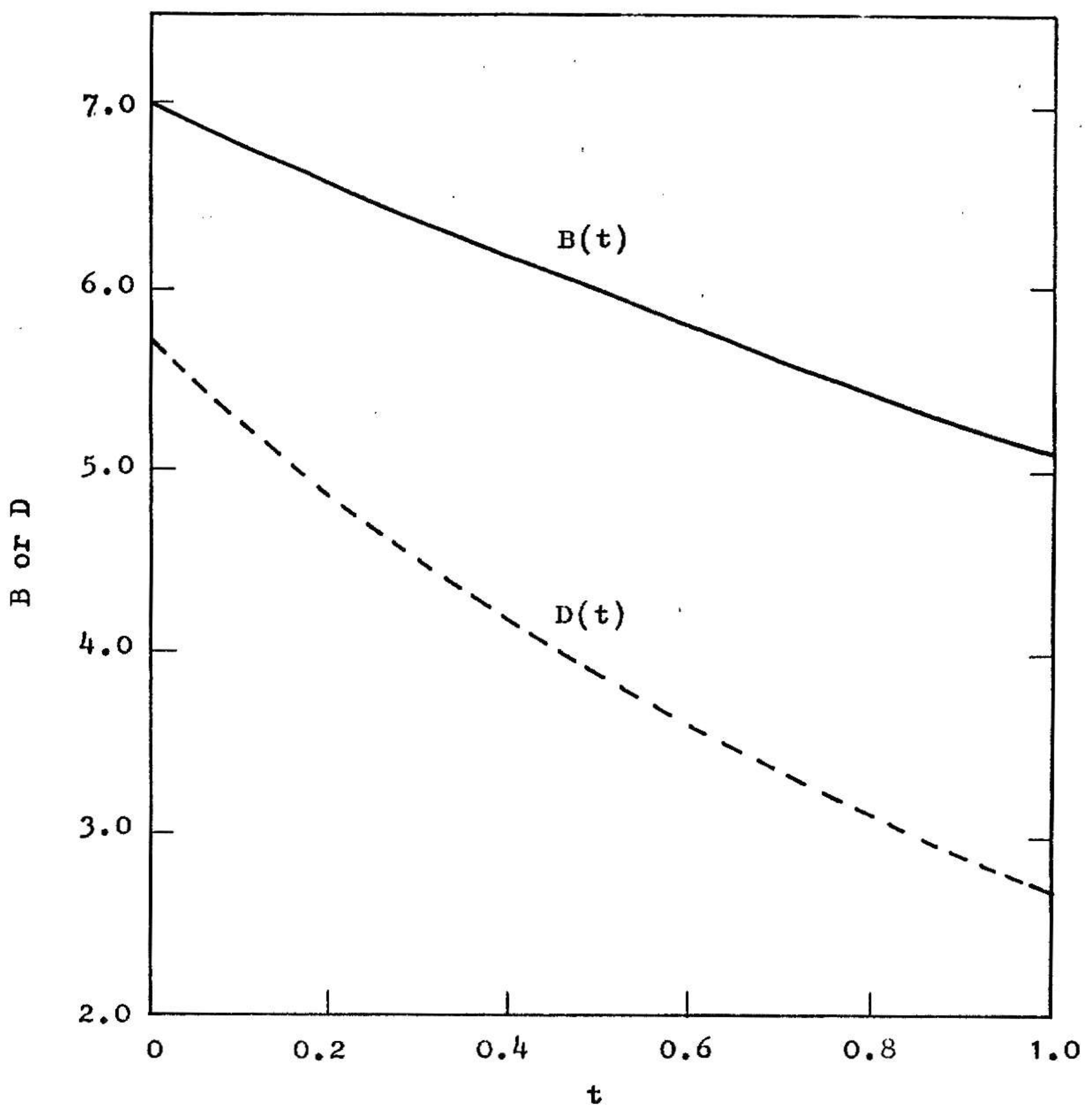

Fig. 2. B and D Profiles

The initial values used to obtain the one set of particular and two sets of homogeneous solutions are listed in Table 3. Note that the initial values are chosen in such a way that they satisfy the given initial conditions in (3.21) and (3.22). Thus only two sets of homogeneous solutions are needed. This problem is solved by using the same computational procedure discussed earlier except that only two parameters are being estimated and the initial values used for obtaining the particular and homogeneous solutions are given by Table 3. The Runge-Kutta integration scheme is used with the step size $\Delta t = 0.01$. To test the influence of the initial functions used in Step 2 in the computational procedure, the following three different sets of initial functions are used for the unknown parameters K_1 and K_2:

$$\begin{aligned}
&(1)\quad K_{1,k=0}(t) = 0.1, \qquad K_{2,k=0}(t) = 0.1 \\
&(2)\quad K_{1,k=0}(t) = 0.5, \qquad K_{2,k=0}(t) = 0.5 \\
&(3)\quad K_{1,k=0}(t) = 1.0, \qquad K_{2,k=0}(t) = 1.0
\end{aligned} \tag{3.47}$$

for $0 \leq t \leq t_f = 1$. The following constant functions are used as the initial functions for B and D for all the calculations:

$$B_{k=0}(t) = 7.0, \qquad D_{k=0}(t) = 5.7 \tag{3.48}$$

for $0 \leq t \leq t_f = 1$. In other words, instead of the experimental data given in Table 2, the initial conditions in (3.21) and (3.22) are used as the initially assumed constant functions for B and D. Notice that in order to increase the convergence rate, either the experimental data or the actual solutions of B and D should be used as the initially assumed functions in practical solutions.

The problem converges rapidly to the correct solutions for all three sets of initially assumed functions. The convergence rates for B and D with the initially assumed functions $K_{1,k=0}(t) = 0.1$ and $K_{2,k=0}(t) = 0.1$ are shown in Figure 3. Notice that a great amount of improvement has been obtained during the first iteration. The convergence rates for B and D with the second and third sets of initial functions as shown in (3.47) are approximately the same as that shown in Figure 3. The convergence rates for the unknown parameters K_1 and K_2 are shown in Table 4. It can be seen that a six-digit accuracy is obtained in only three or four iterations. It should be noted that the initially assumed functions as given by Eq. (3.47) are very far removed from the correct solutions.

3.5.2 Estimation With Experimental Errors-Two Parameters

In practical situations, the data obtained almost always have measurement or experimental errors. To test the influence of the experimental errors on the rate of convergence of this approach, the data listed in Table 2 are corrupted with noise by the equations

Table 3.

Initial Values Used for Obtaining the Particular and Homogeneous Solutions

Variable	Particular Solution	Homogeneous Solutions	
$B_{k+1}(0)$	7.0	0	0
$D_{k+1}(0)$	5.7	0	0
$K_{1,k+1}(0)$	0	1	0
$K_{2,k+1}(0)$	0	0	1

Table 4. Convergence Rates of K_1 and K_2, (Two Parameter Problem)

Iteration	K_1	K_2	K_1	K_2	K_1	K_2
0	0.1000	0.1000	0.5000	0.5000	1.0000	1.0000
1	0.2859	0.7940	0.3306	0.8861	0.3908	0.1005
2	0.3099	1.0136	0.3100	1.0170	0.3095	0.1020
3	0.3100	1.0200	0.3100	1.0200	0.3100	0.1020
4	0.3100	1.0200	0.3100	1.0200	0.3100	0.1020
5	0.3100	1.0200	0.3100	1.0200	0.3100	0.1020

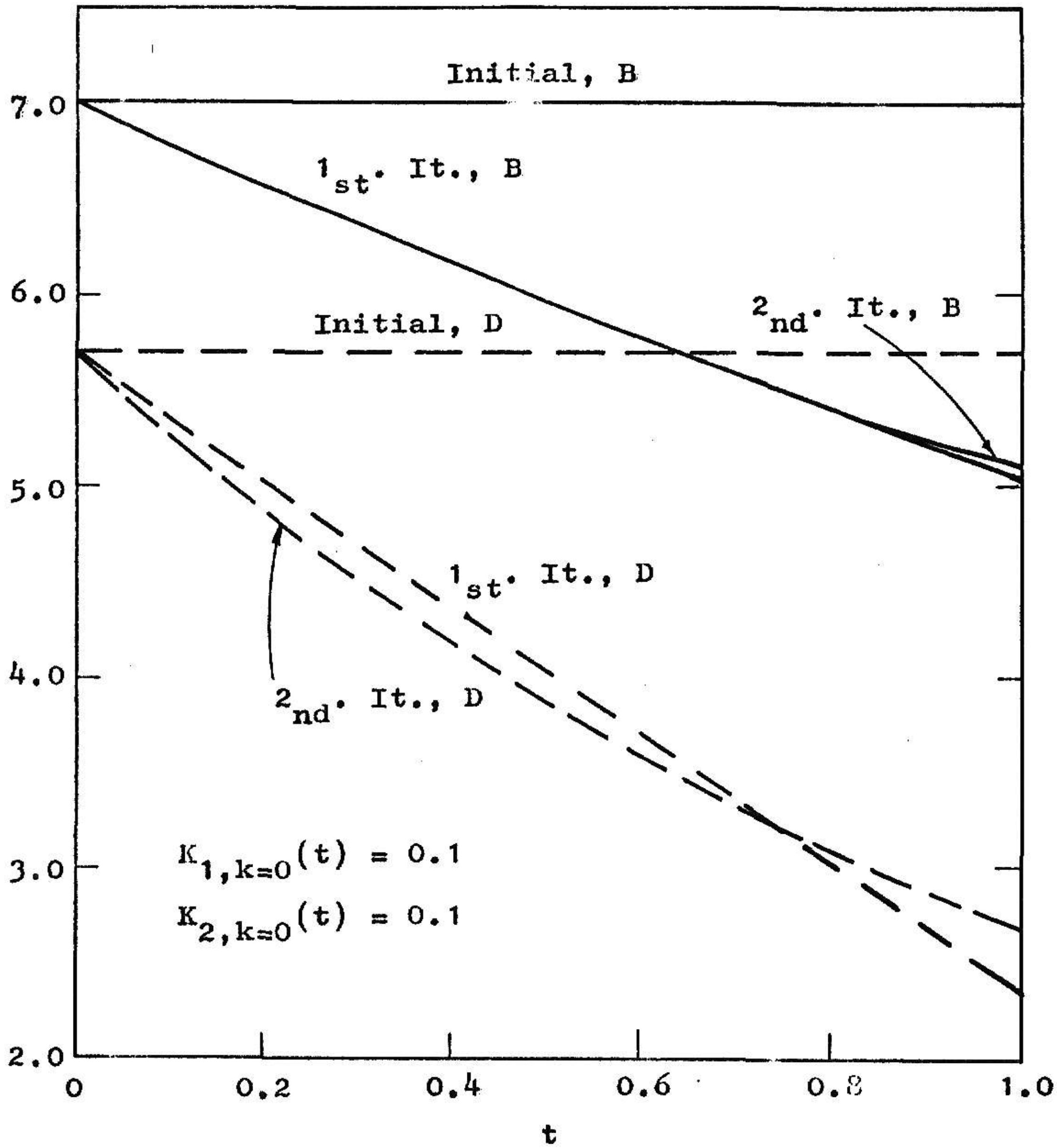

Fig. 3.

Convergence Rates of B and D, Two Parameter Problem

$$b_s^{(noise)} = b_s + R_{bs} \tag{3.49}$$

$$d_s^{(noise)} = d_s + R_{ds} \tag{3.50}$$

where s = 1, 2, ..., S with S = 21. R_{bs} and R_{ds} represent normally distributed random numbers. These random numbers are generated by using the IBM scientific subroutines GAUSS and RANDU. The means for these normally distributed random numbers are zeros and the standard deviations are 0.35 and 0.25 for R_{bs} and R_{ds}, respectively. These standard deviations are approximately five percent of the data listed in Table 2. These noisy data are listed in Table 5.

The problem is solved with the other numerical values remaining the same as that used for the case without noise. The convergence rates for the three sets of initial functions as given in Eq. (3.47) are shown in Table 6. It can be seen that the presence of experimental errors does not slow the convergence rates. However, due to the presence of noise, the values of K_1 and K_2 obtained are not the same as the original given values. It is expected that as the number of the noisy data increases, the estimated values for K_1 and K_2 should approach the original given values. This problem has also been solved with 101 data points for both B and D and with all other numerical values remaining the same. The convergence rates for this 101 data points problem are approximately the same as that shown in Table 6. However, the estimated values are improved to $K_1 = 0.3147$ and $K_2 = 1.0347$

Table 5. Numerical Values Used as Noisy Experimental Data

t_s	s	$B^{(exp)}(t_s) = b_s^{(noise)}$	$D^{(exp)}(t_s) = d_s^{(noise)}$
0.00	1	6.6533	5.8645
0.05	2	6.8742	5.8692
0.10	3	6.5075	5.0755
0.15	4	6.7591	4.8416
0.20	5	6.6911	5.0409
0.25	6	6.7217	4.5628
0.30	7	6.5256	4.5621
0.35	8	6.4335	4.2095
0.40	9	6.0326	4.1910
0.45	10	5.9162	3.9586
0.50	11	5.2339	3.9796
0.55	12	5.8915	3.7372
0.60	13	5.9010	3.2301
0.65	14	6.0309	3.2228
0.70	15	5.9557	3.2451
0.75	16	5.3062	3.0929
0.80	17	5.4196	3.0774
0.85	18	5.4891	2.7755
0.90	19	6.0634	2.7798
0.95	20	5.2012	2.9485
1.00	21	4.7616	2.4054

Table 6.

Convergence Rates of K_1, and K_2
With Noisy Experimental Data
(Two Parameter Problem)

Iteration	K_1	K_2	K_1	K_2	K_1	K_2
0	0.1000	0.1000	0.5000	0.5000	1.0000	1.0000
1	0.2748	0.8026	0.3179	0.8984	0.3762	1.0227
2	0.2967	1.0366	0.2968	1.0405	0.2964	1.0436
3	0.2968	1.0438	0.2968	1.0438	0.2968	1.0439
4	0.2968	1.0439	0.2968	1.0439	0.2968	1.0439

which are fairly close to the original given values for K_1 and K_2.

3.4.3 Estimation of Three Parameters

Now consider K_1, K_2, and K_3 as unknowns. The problem is to estimate these three unknown rate constants in Eqs. (3.4) and (3.5) by using the given initial conditions, Eq. (3.44), and the given numerical values, Eq. (3.45). The values listed in Table 2 are again used as experimental data.

By the use of the initial values as given by Eqs. (3.28) and (3.34), this problem is solved by using the following three different sets of initially assumed functions and the computational procedure listed earlier

$$\begin{aligned}
&(1)\quad K_{1,k=0}(t) = 0.5,\quad K_{2,k=0}(t) = 0.5,\quad K_{3,k=0}(t) = 0.5\\
&\qquad B_{k=0}(t) = 7.0,\quad D_{k=0}(t) = 5.7\\
&(2)\quad K_{1,k=0}(t) = 0.1,\quad K_{2,k=0}(t) = 0.1,\quad K_{3,k=0}(t) = 0.1\\
&\qquad B_{k=0}(t) = 6.1,\quad D_{k=0}(t) = 3.1\\
&(3)\quad K_{1,k=0}(t) = 0.08,\quad K_{2,k=0}(t) = 0.08,\quad K_{3,k=0}(t) = 0.35\\
&\qquad B_{k=0}(t) = 5.0,\quad D_{k=0}(t) = 5.0
\end{aligned}\tag{3.51}$$

for $0 \leq t \leq t_f = 1$. The Runge-Kutta integration scheme with step size $\Delta t = 0.01$ is used again. The convergence rates with the three different sets of initial functions are shown in Table 7. The convergence rates for B and D with $K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 0.5$, $B_{k=0}(t) = 7.0$, and $D_{k=0}(t) = 5.7$ given in (3.51) are shown in Figure 4. The convergence rates for the other two sets of initial functions are approximately the same as those shown in Figure 4.

3.5.4 Estimation With Experimental Errors - Three Parameters

Again, to test the influence of the experimental errors on the rate of convergence for the three parameter problem, the noisy data listed in Table 5 are used once again to estimate the three unknown rate constants K_1, K_2, and K_3.

With the numerical values in (3.44), (3.45) remaining the same, this problem is solved by using the following two different sets of initial functions for B and D:

$$\begin{aligned} &(1) \quad B_{k=0}(t) = 7.0, \quad D_{k=0}(t) = 5.7 \\ &(2) \quad B_{k=0}(t) = 5.0, \quad D_{k=0}(t) = 5.0. \end{aligned} \tag{3.52}$$

The three sets of initial functions used for K_1, K_2, and K_3 are

$$\begin{aligned} &(1) \quad K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 0.1 \\ &(2) \quad K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 0.5 \\ &(3) \quad K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 1.0 \end{aligned} \tag{3.53}$$

for $0 \leq t \leq t_f = 1$. The convergence rates with these different

Table 7A. Convergence Rates of K_1, K_2 and K_3
(Three Parameter problem)

Iteration	$B_0(t) = 7.0$, $D_0(t) = 5.7$		
	K_1	K_2	K_3
0	0.5	0.5	0.5
1	-0.1016	0.3125	0.6367
2	0.4262	1.1268	-0.0956
3	0.3110	1.0215	0.0290
4	0.3100	1.0200	0.0300
5	0.3100	1.0200	0.0300

Table 7B. Convergence Rates of K_1, K_2 and K_3 (Three Parameter Problem)

Iteration	$B_0(t) = 6.1$, $D_0(t) = 3.1$		
	K_1	K_2	K_3
0	0.1	0.1	0.1
1	-1.8891	-3.0000	2.2500
2	0.5601	1.2169	-0.2200
3	0.3180	1.0326	0.0220
4	0.3100	1.0200	0.0300
5	0.3100	1.0200	0.0300

Table 7C. Convergence Rates of K_1, K_2 and K_3
(Three Parameter Problem)

Iteration	$B_0(t) = 5$,	$D_0(t) = 5$	
	K_1	K_2	K_3
0	0.08	0.08	0.35
1	4.2375	4.7500	-3.9688
2	0.8192	1.7918	-0.4800
3	0.2862	0.9865	0.0538
4	0.3100	1.0199	0.0300
5	0.3100	1.0200	0.0300

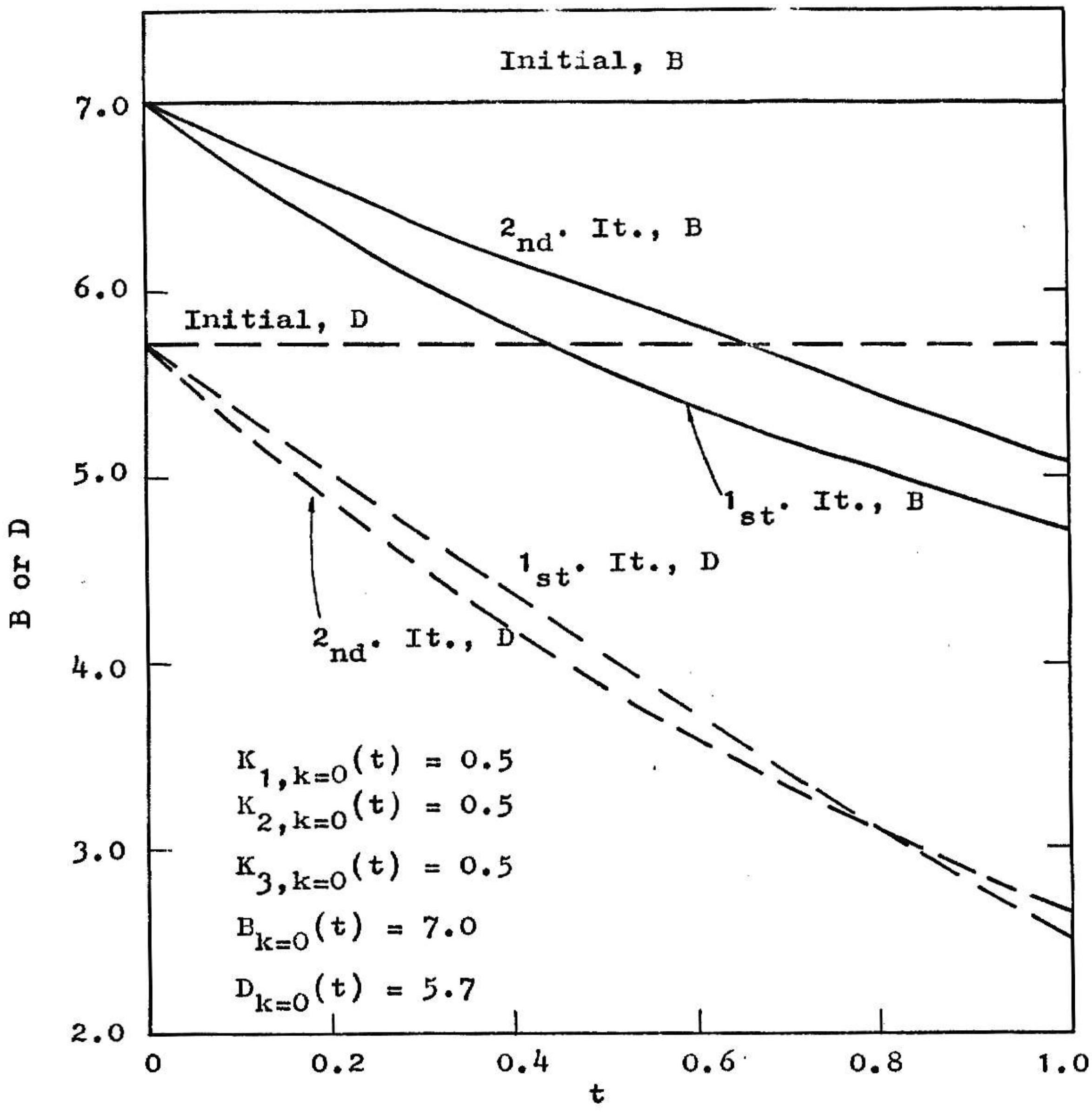

Fig. 4.

Convergence Rates of B and D, Three Parameter Problem sets of initial functions are shown in Table 8. It can be seen that the convergence rates of K_1, K_2, and K_3 remain very rapid. However, due to the presence of noise, the estimated values of K_1, K_2, and K_3 are not the same as the original given values (see Table 8). Especially the value of K_3 obtained, K_3 =-0.0148, is far from that of the original given value, K_3 = 0.03. It can be interpreted that this unstability is caused by three facts: First, the expermental data used are just a partial representation of the complete "oxygen sag" curve. Second, the original given value of K_3 = 0.03 is rather small as compared with the values of K_1 = 0.31, K_2 = 1.02, and those values of experimental data. Third, random noises are imposed. It is expected that the results of this estimation should be improved as a complete "oxygen sag" curve is used as the esperimental data, and a longer duration of the process is used.

In order to further investigate the convergence and other computational aspects of this problem, the following numerical values are used:

$$B^0 = 30.0, \quad D^0 = 1.0, \quad t_f = 5. \tag{3.54}$$

The other values in (3.45) and (3.46) remain the same. Again, Eqs. (3.4) and (3.5) are integrated numerically with the Runge-Kutta integration scheme. The step size used in this integration is increased to Δt = 0.05. Part of the result

Table 8A. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem)

Iteration	$B_0(t) = 7.0$, $D_0(t) = 5.7$		
	K_1	K_2	K_3
0	0.1000	0.1000	0.1000
1	-0.3993	-0.0625	0.7878
2	0.5241	1.2511	-0.1903
3	0.3527	1.0832	-0.0176
4	0.3499	1.0787	-0.0148
5	0.3499	1.0787	-0.0148

Table 8B. Convergence Rates of K_1, K_2, and K_3
With Noisy Experimental Data
(Three Parameter Problem)

Iteration	$B_0(t) = 7.0$, $D_0(t) = 5.7$		
	K_1	K_2	K_3
0	0.5000	0.5000	0.5000
1	2.8500	4.0000	-2.3750
2	0.4950	1.4100	-0.1634
3	0.3389	1.0632	-0.0039
4	0.3498	1.0786	-0.0148
5	0.3499	1.0787	-0.0148
6	0.3499	1.0787	-0.0148

Table 8C. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem)

Iteration	$B_0(t) = 7.0,\ D_0(t) = 5.7$		
	K_1	K_2	K_3
0	1.0000	1.0000	1.0000
1	-1.0093	-0.6875	1.4141
2	0.0196	0.6166	0.3169
3	0.3407	1.0636	-0.0057
4	0.3498	1.0786	-0.0148
5	0.3499	1.0787	-0.0148
6	0.3499	1.0787	-0.0148

Table 8D. Convergence Rates of K_1, K_2, and K_3
With Noisy Experimental Data
(Three Parameter Problem)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$		
	K_1	K_2	K_3
0	0.1000	0.1000	0.1000
1	1.0000	1.5625	-0.8438
2	0.5763	1.3724	-0.2524
3	0.3493	1.0780	-0.0143
4	0.3499	1.0787	-0.0148
5	0.3499	1.0787	-0.0148

Table 8E. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$		
	K_1	K_2	K_3
0	0.5000	0.5000	0.5000
1	-0.0625	0.6250	0.2188
2	0.2964	0.9936	0.0386
3	0.3491	1.0773	-0.0140
4	0.3499	1.0787	-0.0148
5	0.3499	1.0787	-0.0148

Table 8F. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$		
	K_1	K_2	K_3
0	1.0000	1.0000	1.0000
1	2.2375	3.1875	-2.2186
2	0.7523	1.6864	-0.4089
3	0.3384	1.0627	-0.0033
4	0.3498	1.0786	-0.0148
5	0.3499	1.0787	-0.0148
6	0.3499	1.0787	-0.0148

are listed in Table 9. Instead of the equations given in (3.49) and (3.50), the data listed in Table 9 are corrupted with noise by the following equations

$$b_s^{(noise)} = b_s(1 + 0.1\ R_{bs}) \tag{3.55}$$

$$d_s^{(noise)} = d_s(1 + 0.1\ R_{ds}) \tag{3.56}$$

with s = 1, 2, ..., 21. The means for these normally distributed random numbers are remained to be zeros, but the standard deviations now used are 0.50 and 0.10 for R_{bs} and R_{ds}, respectively. By using Eqs. (3.55) and (3.56), the measurement errors are approximately five percent proportional to the true values of B and D listed in Table 9. The noisy data for this problem are shown in Table 10. The data in Table 9 and noisy data in Table 10 are plotted in Figure 5. It is seen that there is a "sag" curve in Figure 5.

For the present case, the initial values given in (3.28) and (3.34) are once again used except that the values for B^0 and D^0 are changed to $B^0 = 30.0$ and $D^0 = 1.0$, respectively. The initial functions used for K_1, K_2, and K_3 are the same as those given in (3.53). The two sets of initial functions for B and D are:

$$\begin{aligned} B_{k=0}(t) &= 30.0, \quad D_{k=0}(t) = 1.0 \\ B_{k=0}(t) &= 5.0, \quad D_{k=0}(t) = 5.0 \end{aligned} \tag{3.57}$$

Table 9. Numerical Values Used as Experimental Data (Complete Oxygen Sag Curve)

t_s	s	$B^{(exp)}(t_s) = b_s$	$D^{(exp)}(t_s) = d_s$
0.00	1	30.0000	1.0000
0.25	2	27.5913	2.5525
0.50	3	25.3789	3.5979
0.75	4	23.3468	4.2632
1.00	5	21.4803	4.6457
1.25	6	19.7658	4.8199
1.50	7	18.1911	4.8427
1.75	8	16.7447	4.7573
2.00	9	15.4162	4.5964
2.25	10	14.1959	4.3847
2.50	11	13.0751	4.1408
2.75	12	12.0456	3.8785
3.00	13	11.0999	3.6077
3.25	14	10.2314	3.3361
3.50	15	9.4336	3.0687
3.75	16	8.7008	2.8092
4.00	17	8.0278	2.5602
4.25	18	7.4096	2.3232
4.50	19	6.8417	2.0991
4.75	20	6.3202	1.8882
5.00	21	5.8411	1.6907

Table 10. Numerical Values Used as Noisy Experimental Data (Complete Oxygen Sag Curve)

t_s	s	$B^{(exp)}(t_s) = b_s^{(noise)}$	$D^{(exp)}(t_s) = d_s^{(noise)}$
0.00	1	30.0086	1.0055
0.25	2	28.1118	2.5871
0.50	3	26.7720	3.5265
0.75	4	21.8259	4.2490
1.00	5	19.7630	4.6455
1.25	6	21.9842	4.8275
1.50	7	17.6209	4.8916
1.75	8	16.3512	4.6931
2.00	9	16.7522	4.6554
2.25	10	14.2938	4.2695
2.50	11	13.7861	4.1462
2.75	12	11.6554	3.9292
3.00	13	10.8524	3.5828
3.25	14	9.6077	3.3559
3.50	15	8.6727	3.0510
3.75	16	8.2575	2.8061
4.00	17	8.2696	2.5929
4.25	18	7.8113	2.3636
4.50	19	7.3904	2.0625
4.75	20	6.4533	1.8874
5.00	21	5.7843	1.7026

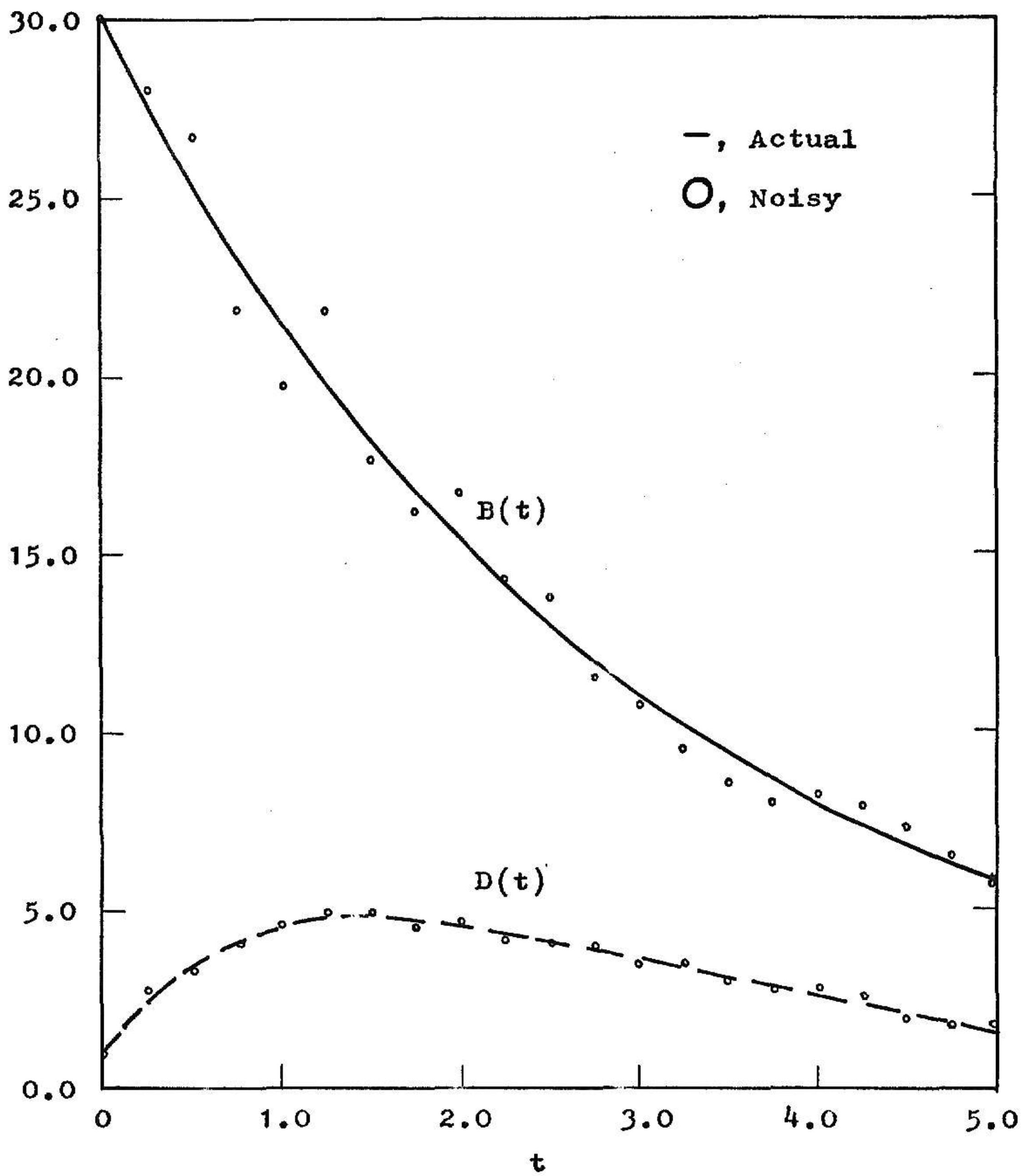

Fig. 5.

Actual and Noisy Experimental Data for B and D
(Complete Oxygen Sag Curve)

Based on the noisy experimental data listed in Table 10, this problem is solved with $\Delta t = 0.05$. The convergence rates for these different sets of initial functions are listed in Table 11. As can be seen in Table 11, the obtained values $K_1 = 0.3086$, $K_2 = 1.0161$, and $K_3 = 0.0307$ are fairly close to the original given values.

3.5.5 Estimation of Five Parameters

It is recognized that methods for measuring some of the rate constants, namely K_3, A, and R, have not been perfected and in most cases are unavailable. However, these rate constants still can be estimated from the stream quality model if the experimental data on B and D along the stream are available.

Now consider K_1, K_2, K_3, A, and R as unknown parameters. The problem can be solved essentially in the same way as that for the three parameter problem. By using Table 2 as the experimental data and with the other numerical values remaining the same, the problem is solved by using the following three different sets of initial functions:

(1) $B_{k=0}(t) = 7.0, \quad D_{k=0}(t) = 5.7,$

$$K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 1.0$$

(2) $B_{k=0}(t) = 5.0, \quad D_{k=0}(t) = 5.0,$

$$K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 0.1 \tag{3.58}$$

Table 11A. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem With Complete Oxygen Sag Curve)

Iteration	$B_0(t) = 30.0$, $D_0(t) = 1.0$ ($\Delta t = 0.05$, $t_f = 5$)		
	K_1	K_2	K_3
0	0.1000	0.1000	0.1000
1	1.0625	2.3125	-0.0625
2	1.0446	2.3051	0.1184
3	0.1137	1.9917	-0.3970
4	0.2862	0.9253	0.0433
5	0.3069	1.0050	0.0330
6	0.3085	1.0157	0.0309
7	0.3086	1.0161	0.0307
8	0.3086	1.0161	0.0307

Table 11B. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem With Complete Oxygen Sag Curve)

Iteration	$B_0(t) = 30.0$, $D_0(t) = 1.0$ ($\Delta t = 0.05$, $t_f = 5$)		
	K_1	K_2	K_3
0	0.5000	0.5000	0.5000
1	0.4625	0.3750	0.4375
2	0.2327	0.9151	-0.2291
3	0.2944	0.9394	0.0360
4	0.3081	1.0136	0.0313
5	0.3086	1.0160	0.0307
6	0.3086	1.0161	0.0307
7	0.3086	1.0161	0.0307

Table 11C. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem With Complete Oxygen Sag Curve)

Iteration	$B_0(t) = 30.0$, $D_0(t) = 1.0$ ($\Delta t = 0.05$, $t_f = 5$)		
	K_1	K_2	K_3
0	1.0000	1.0000	1.0000
1	0.4000	2.2500	0.3125
2	0.5477	1.9378	-0.1195
3	0.2244	0.6987	0.1106
4	0.3058	1.0080	0.0335
5	0.3085	1.0159	0.0308
6	0.3086	1.0161	0.0307
7	0.3086	1.0161	0.0307

Table 11D. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem With Complete Oxygen Sag Curve)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$ ($\Delta t = 0.05$, $t_f = 5$)		
	K_1	K_2	K_3
0	0.1000	0.1000	0.1000
1	3.5875	4.0000	-2.9063
2	0.9958	4.1670	-0.6572
3	0.0385	-0.2514	0.2999
4	0.3558	1.2857	-0.0164
5	0.3099	1.0193	0.0294
6	0.3086	1.0161	0.0307
7	0.3086	1.0161	0.0307

Table 11E. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem With Complete Oxygen Sag Curve)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$ ($\Delta t = 0.05$, $t_f = 5$)		
	K_1	K_2	K_3
0	0.5000	0.5000	0.5000
1	-4.9125	-4.0625	3.9063
2	0.0750	1.0625	-0.1563
3	0.0817	1.0625	-0.1306
4	0.2241	1.2996	-0.0415
5	0.3137	1.0260	0.0116
6	0.3091	1.0182	0.0301
7	0.3086	1.0162	0.0307
8	0.3086	1.0161	0.0307
9	0.3086	1.0161	0.0307

Table 11F. Convergence Rates of K_1, K_2, and K_3 With Noisy Experimental Data (Three Parameter Problem With Complete Oxygen Sag Curve)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$ ($\Delta t = 0.05$, $t_f = 5$)		
	K_1	K_2	K_3
0	1.0000	1.0000	1.0000
1	28.0250	30.0000	-30.6875
2	1.1492	22.7500	-0.5664
3	6.5048	28.9919	-5.9920
4	-1.0027	4.7889	1.2529
5	0.0168	-0.4656	0.3207
6	0.3250	1.1242	0.0142
7	0.3122	1.0305	0.0271
8	0.3087	1.0165	0.0306
9	0.3086	1.0161	0.0307
10	0.3086	1.0161	0.0307

(3) $B_{k=0}(t) = 3.0$, $D_{k=0}(t) = 3.0$,

$K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 0.1$.

The convergence rates for the five constant parameters are shown in Table 12. It can be seen that in spite of the large number of parameters to be estimated, the convergence rates of the problem remain very rapid. Only five iterations are needed to obtain a four digit accuracy. Note that the initially assumed functions as given by Eq. (3.58) are very approximate. With sets (2) and (3) of (3.58) as the initially assumed functions, fairly large oscillations are obtained during the first three iterations (see Table 12). However, the convergence rates have not been reduced in spite of the large oscillations involved. The convergence rates of B and D with $K_{1,k=0}(t) = K_{2,k=0}(t) = K_{3,k=0}(t) = 1.0$, $B_{k=0}(t) = 7.0$, and $D_{k=0}(t) = 5.7$ are shown in Figure 6.

3.6 DISCUSSION

The numerical examples that have been shown above, indicate that the quasilinearization technique is a very useful tool for solving nonlinear boundary-value problems or for estimating the unknown system parameters. In general, it can be said that as long as the initial approximations are reasonable and within the convex region of convergence, the technique converges rapidly- usually within seven iterations.

Table 12A. Convergence Rates of K_1, K_2, K_3, A and R (Five Parameter Problem)

Iteration	$B_0(t) = 7.0$, $D_0(t) = 5.7$				
	K_1	K_2	K_3	A	R
0	1.0000	1.0000	1.0000	-	-
1	-1.2766	-0.7500	0.9961	0.0625	-0.1750
2	-0.4866	-0.0592	-1.2693	1.4366	-14.6611
3	0.2943	1.0014	0.0663	0.8215	0.2948
4	0.2944	1.0196	0.0307	0.8479	0.1500
5	0.3100	1.0200	0.0300	0.8500	0.1500
6	0.3100	1.0200	0.0300	0.8500	0.1500

Table 12B. Convergence Rates of K_1, K_2, K_3, A and R (Five Parameter Problem)

Iteration	$B_0(t) = 5.0$, $D_0(t) = 5.0$				
	K_1	K_2	K_3	A	R
0	0.1000	0.1000	0.1000	-	-
1	3.7033	3.9375	-3.6357	1.9375	-1.1125
2	22.4543	13.9128	-22.0784	82.4427	0.4091
3	0.0352	0.8720	0.3049	-0.2299	0.1503
4	0.3097	1.0195	0.0303	0.8507	0.1500
5	0.3100	1.0200	0.0300	0.8500	0.1500
6	0.3100	1.0200	0.0300	0.8500	0.1500

Table 12C. Convergence Rates of K_1, K_2, K_3, A and R (Five Parameter Problem)

Iteration	$B_0(t) = 3.0$, $D_0(t) = 3.0$				
	K_1	K_2	K_3	A	R
0	0.1000	0.1000	0.1000	-	-
1	26.5531	11.8750	8.2891	56.8750	9.8030
2	26.7191	13.7742	7.3718	112.5150	235.1970
3	0.9036	1.4436	-0.6148	2.6631	-0.5017
4	0.4095	1.0843	-0.0693	1.1923	0.1520
5	0.3101	1.0203	0.0299	0.8499	0.1500
6	0.3100	1.0200	0.0300	0.8500	0.1500
7	0.3100	1.0200	0.0300	0.8500	0.1500

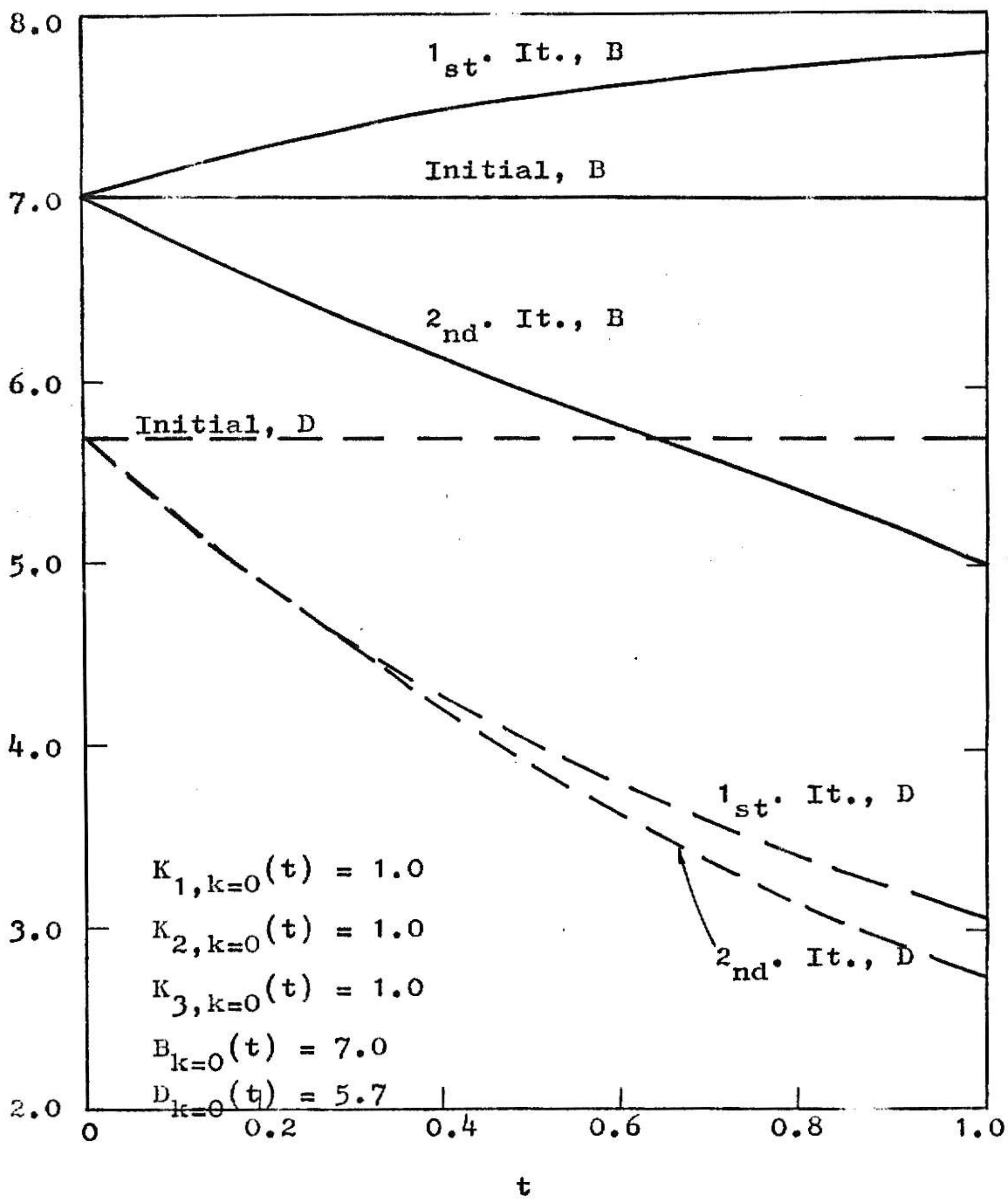

Fig. 6.

Convergence Rates of B and D, Five Parameter Problem

The advantage of this approach is that the parameters and the solution of the differential equations representing the system are obtained simultaneously. Furthermore, any known information about the parameters can also be utilized in estimating the initial approximations or starting values for the parameters.

In order to illustrate the effectiveness of this technique, both the exact solutions and noisy data of B and D have been used as the experimental data. Furthermore, based on two simple differential equations (3.4) and (3.5) which represent the widely used pollution model, different numbers of parameters from two, three, and five have been estimated. It is shown that with very approximate initial guesses for the unknown parameters, only three to seven iterations are needed to obtain a four to five digit accuracy.

CHAPTER 4

INVARIANT IMBEDDING

4.1 INTRODUCTION

In previous chapters, the quasilinearization technique has been introduced to solve nonlinear boundary-value problems arising from stream quality modeling. In this chapter, a completely different approach, known as "invariant imbedding", will be introduced for solving boundary-value problems.

The invariant imbedding principle has its origin in the theory of semigroups. Ambarzumian [1] seems to have been the first one to introduce this principle in any significant fashion. Chandrasekhar [11] generalized the results of Ambarzumain and used this principle elegantly in treating the theory of radiative transfer. This principle has been studied estensively by Bellman, Kalaba, Wing, and co-workers [4, 6, 9]. Recently, Lee has further extended the invariant imbedding applications successfully to various boundary-value problems in chemical engineering [20, 24, 25].

Strictly speaking, the invariant imbedding is only a concept; it is not a technique or method. This concept involves a completely different approach to formulating the problem. Instead of only considering a single problem with a fixed duration or length of the independent variable, the invariant imbedding approach is to consider a family of problems with durations ranging from zero to the duration of the original problem. By imbedding these problems, the particular original problem can be solved. For this reason, this concept can be applied to a variety of different problems.

It should be emphasized that because this concept is completely different from the usual concept, it frequently gives some different insights to the same problem which has been treated previously by the usual method. Furthermore, these new formulations often have distinct advantages over the original formulation, both computationally and theoretically. The dynamic programming [3-4, 7, 20, 26] is a good example. The functional equation of dynamic programming is essentially the invariant imbedding equation with the addition of maximization or minimization.

In this chapter, emphasis will be placed on the use of the basic concept of invariant imbedding as a computational tool. More elegant formulations and the theoretical or analytical applications of the invariant imbedding concept will not be discussed.

4.2 NONLINEAR FILTERING AND ESTIMATION

The invariant imbedding concept has been applied to various two-point boundary-value problems. This concept can also be used to derive some useful results in nonlinear filtering and estimation theory. In this section, application of the invariant imbedding concept to the simultaneous estimation of state and parameter from differential equations will be discussed.

Since the invariant imbedding approach is completely different from the usual classical approach, two main advantages can be obtained. First, it can be applied to a great variety of nonlinear problems. Second, a sequential estimation scheme is obtained. By the use of this sequential scheme, only current data are needed to estimate the current or future values of the parameters. No statistical assumptions are needed concerning the noise or experimental disturbances of the data. The generally used least squares criterion can be used to obtain the optimal estimates. If the information concerning the disturbances are known, better criteria than the classical least squares may be employed.

To illustrate the approach, consider a system whose dynamic behavior can be represented by the following simple nonlinear differential equation:

$$\frac{dx}{dt} = f(x, P, t), \tag{4.1}$$

where f is a known function. The problem is to estimate the values of the state x and the constant parameter P from the measured data on x. Generally, there are two kinds of noise or disturbances involved in the experimental measurements. The first kind is the unknown disturbance on the input. Owing to the presence of this disturbace, the process must be represented by

$$\frac{dx}{dt} = f(x, p, t) + g(x, p, t)\, u(t), \tag{4.2}$$

where g is a known function, and $u(t)$ represents the unknown disturbance on the input. The second kind of disturbance is then the measurement error. Thus, the measured value of $x(t)$ is

$$z(t) = x(t) + (\text{measurement errors}). \tag{4.3}$$

In practical situations, $x(t)$ generally cannot be measured directly, and only a certain function of x can be measured. Let this measurable function be $h(x, t)$; then

$$z(t) = h(x, t) + (\text{measurement errors}), \tag{4.4}$$

where h is a known function of x and t.

Note that the state $x(t)$ and the parameter P are to be estimated simultaneously. Consider P as a dependent variable and as a function of t, the differential equation can be established:

$$\frac{dP}{dt} = 0 \tag{4.5}$$

Notice here that the state of this system is now represented by $x(t)$ and $P(t)$.

By using the classical least squares criterion, this estimation problem can be stated as: Based on the measurement $z(t)$ at various positions of t, $0 = t_0 \leq t \leq t_f$, estimate the unknown state x and the parameter P at the time $t = t_f$ for the system (4.4) such that the following integral expression is minimized:

$$J = \int_0^{t_f} [h(x, t) - z(t)]^2 \, dt \tag{4.6}$$

Where $z(t)$ is the observed function. The function $x(t)$ is determined on the interval $0 \leq t \leq t_f$ by Eq. (4.1). Note that the problem is minimized with respect to the measurement errors only. The minimization on the other kind of input disturbance is not shown here.

The above results can also be generalized to systems with dynamics represented by n differential equations. The equations corresponding to Eqs. (4.1), (4.3), and (4.6) are

$$\frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{f}(\underset{\sim}{x}, t) \tag{4.7}$$

$$\underset{\sim}{z}(t) = \underset{\sim}{h}(\underset{\sim}{x}, t) + (\text{measurement errors}), \tag{4.8}$$

and

$$J = \int_0^{t_f} \sum_{j=1}^{m} [h_j(\underset{\sim}{x}, t) - z_j(t)]^2 \, dt, \tag{4.9}$$

respectively. The vectors $\underset{\sim}{x}$ and $\underset{\sim}{f}$ are n-dimensional, $\underset{\sim}{z}$ and $\underset{\sim}{h}$

are m-dimensional. The functions h_j, $j = 1, 2, \ldots, m$, are evaluated by using the values $\underset{\sim}{x}$ obtained from Eq. (4.7) and z_j, $j = 1, 2, \ldots, m$, are the observed functions as determined by (4.8). The number m represents the number of measurable quantities and $m \leq n$.

Using invariant imbedding and calculus of variations, the following sequential estimator equations are obtained:

$$\frac{d\underset{\sim}{e}}{da} = \underset{\sim}{f}(\underset{\sim}{e}, a) + \underset{\sim}{q}(a)[\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)]^T [\underset{\sim}{z}(a) - \underset{\sim}{h}(\underset{\sim}{e}, a)] \tag{4.10}$$

$$\begin{aligned} \frac{d\underset{\sim}{q}}{da} &= \underset{\sim}{f}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\, \underset{\sim}{q}(a) + \underset{\sim}{q}(a)[\underset{\sim}{f}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)]^T \\ &+ \underset{\sim}{q}(a)\{\underset{\sim}{h}_{\underset{\sim}{e}\underset{\sim}{e}}(\underset{\sim}{e}, a)[\underset{\sim}{z}(a) - \underset{\sim}{h}(\underset{\sim}{e}, a)]\}\, \underset{\sim}{q}(a) \\ &- \underset{\sim}{q}(a)[\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)]^T\, \underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\, \underset{\sim}{q}(a), \end{aligned} \tag{4.11}$$

where $\underset{\sim}{e}$ represents the values of $\underset{\sim}{x}$, and $\underset{\sim}{q}$ is the weighting function. It should be noted that Eq. (4.10) represents n differential equations and (4.11) represents n^2 differential equations of the initial value type.

The above estimator equations were originally obtained by Bellman and co-workers [9], and by Detchmendy and Sridhar [12]. The derivation of these equations can be found in Lee [20].

4.5 DISCUSSION

Since invariant imbedding is a concept, the invariant imbedding equations can be obtained by various different formulations or derivations. It has been shown that this approach is very useful in treating a wide variety of problems such as boundary-value problems, eigenvalue problems, non-linear filtering theory, etc.

In conclusion, the invariant imbedding approach appears to be a powerful tool for both numerical and theoretical study of various problems involved in engineering and science. The distinct advantage of this approach is its completely different concept from the usual formulation of the problem. Thus, many new insights and formulations can be obtained for various problems. However, the invariant imbedding approach also has its disadvantages. Instead of solving the original problem, a family of problems must be solved. Thus, more computer storage and more computation time is generally needed to obtain the solution. Obviously, it is the price that has to be paid to avoid the boundary-value difficulties.

A more detailed discussion of the advantages and dis-advantages of invariant imbedding is to be found in [20].

CHAPTER 5

DYNAMIC MODELING OF STREAM QUALITY BY INVARIANT IMBEDDING

5.1 INTRODUCTION

In Chapter 3, the quasilinearization technique has been used extensively to identify or to estimate the unknown system parameters in stream quality models. The estimation problem was treated as a two-point or multipoint boundary-value problem. In this chapter, a completely different approach, invariant imbedding, is used to estimate the dynamic response of stream pollution action.

A water quality model of a stream or estuary must represent the complex blending of biological, chemical, and physical factors. It is not simple and must be represented by complicated differential equations. Furthermore, due to the constant fluctuation of pollutants with time and space, complicated partial differential equations sometimes are needed. In order to establish these equations, the reaction and diffusion constants must be estimated from actual experimental data. Note that these constants generally cannot be measured directly, they must be calculated from the measured concentrations. Due to the complicacy of the partial or ordinary differential equations and the constantly fluctuating concentrations, it is not easy to estimate these constants.

By the use of the invariant imbedding approach, a sequential estimation scheme is obtained. This scheme provides a distinct advantage in that only current data are needed for the estimation process. Thus, not only the parameters but also the future concentrations of the pollutants can be estimated. This approach forms an effective on-line up-dating scheme for the computer modeling and control. Consquently, a large amount of computer memory and computer time can be saved.

Based on the stream quality model developed by Camp and Dobbins, serveral estimation problems are solved. It is shown that this approach forms an effective tool for the dynamic modeling and adaptive forecasting of stream or estuary quality.

5.2 ESTIMATION OF STATE AND PARAMETERS

To illustrate the approach, the simple representation of stream quality by Camp and Dobbins is considered

$$\frac{dB}{dt} = -(K_1 + K_3)B + R \tag{5.1}$$

$$\frac{dD}{dt} = K_1 B - K_2 D - A, \tag{5.2}$$

where B represents the BOD concentration, D is the DO deficit, R is the BOD addition rate due to runoff and scour, A is the oxygen production rate due to plant photosynthesis; K_1, K_2, and K_3 are the rate constants for deoxygenation, reaeration, and sedimentation, respectively.

To estimate the rate constants, K_1, K_2, and K_3, let

$$\frac{dK_1}{dt} = 0 \tag{5.3}$$

$$\frac{dK_2}{dt} = 0 \tag{5.4}$$

$$\frac{dK_3}{dt} = 0. \tag{5.5}$$

The system of equations (5.1)-(5.5) can be represented symbolically by Eq. (4.7) with n = 5.

The estimation of state B, D, and parameters K_1, K_2, and K_3 can now be approached by the nonlinear filtering theory of invariant imbedding which has been presented previously in Section 4.2.

5.3 NUMERICAL EXAMPLES

To test the effectiveness of this approach, the state and the rate constants in Eqs. (5.1) and (5.2), are to be estimated from the noisy measurements on the concentration of BOD and the DO deficit. The noisy measurements are obtained numerically in two steps. First, the differential equations (5.1) and (5.2) are integrated by the Runge-Kutta integration scheme using the following numerical values

$$B(0) = 7.0, \; D(0) = 5.7,$$

$$R = 0.15, \quad A = 0.85, \quad \Delta t = 0.02, \quad t_f = 2, \tag{5.7}$$

$$K_1 = 0.31, \quad K_2 = 1.02, \quad K_3 = 0.03,$$

where Δt is the integration step size. Second, the result obtained from this integration are corrupted with noise by the equations

$$Bz(t_i) = B(t_i) + R_b(t_i) \tag{5.8a}$$

$$Dz(t_i) = D(t_i) + R_b(t_i), \tag{5.8b}$$

with $i = 0, 1, 2, \ldots, N$, $t_0 = 0$, $t_n = t_f$, and $t_{i+1} - t_i = \Delta t$. The R_b's and R_d's represent the measurement errors and are random numbers with Gaussian distributions. The means of these distributions are zeros and the stardard deviations are 0.35 and 0.25 for R_b's and R_d's, respectively. These measurement errors are approximately five percent of the true values of B and D, respectively. The measured data at every tenth point are given in Table 13, and in Figure 7 and 8.

5.3.1 Estimation of State and One Parameter

First, the case with one parameter ($n = 3$) is considered. The state, BOD concentration B, DO deficit D, and the deoxygenation constant K_1 are to be estimated from the noisy measurements given in Table 13

The system of equations corresponding to Eq. (4.7) is (5.1)-(5.3) with $n = 3$, $m = 2$. By applying the established vector equations (4.10) and (4.11) with

$$\underset{\sim}{e}(a) = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix}, \tag{5.9a}$$

$$\underset{\sim}{f}(\underset{\sim}{e},\ a) = \begin{bmatrix} -(e_3 + K_3)e_1 + R \\ e_3 e_1 - K_2 e_2 - A \\ 0 \end{bmatrix}, \tag{5.9b}$$

$$\underset{\sim}{h}(\underset{\sim}{e},\ a) = \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}, \tag{5.9c}$$

$$\underset{\sim}{z}(a) = \begin{bmatrix} Bz(a) \\ Dz(a) \end{bmatrix}, \tag{5.9d}$$

and

$$\underset{\sim}{q}(a) = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix}, \tag{5.9e}$$

the desired estimator equations are obtained

$$\begin{bmatrix} \dot{e}_1 \\ \dot{e}_2 \\ \dot{e}_3 \end{bmatrix} = \begin{bmatrix} -(e_3 + K_3)e_1 + R \\ e_3 e_1 - K_2 e_2 - A \\ 0 \end{bmatrix}$$

$$+ \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Bz(a) - e_1 \\ Dz(a) - e_2 \end{bmatrix} \qquad (5.10)$$

$$\begin{bmatrix} \dot{q}_{11} & \dot{q}_{12} & \dot{q}_{13} \\ \dot{q}_{21} & \dot{q}_{22} & \dot{q}_{23} \\ \dot{q}_{31} & \dot{q}_{32} & \dot{q}_{33} \end{bmatrix} = \begin{bmatrix} -(e_3 + K_3) & 0 & -e_1 \\ e_3 & -K_2 & e_1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix}$$

$$+ \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \begin{bmatrix} -(e_3 + K_3) & e_3 & 0 \\ 0 & -K_2 & 0 \\ -e_1 & e_1 & 0 \end{bmatrix} + \underset{\sim}{0}$$

$$- \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix}, \qquad (5.11)$$

where $\dot{e}_i$ and $\dot{q}_{ij}$ represent $\frac{de_i}{da}$ and $\frac{dq_{ij}}{da}$ ($i = 1, 2, 3$; $j = 1, 2, 3$), respectively. The functions e_1, e_2, and e_3 are the optimal estimates of B, D, and K_1, respectively. Eqs. (5.10) and (5.11) represent twelve simultaneous estimator equations which can be written as follows:

$$\dot{e}_1 = -(e_3 + K_3)e_1 + R + q_{11}\left[Bz(a) - e_1\right] + q_{12}\left[Dz(a) - e_2\right] \tag{5.12a}$$

$$\dot{e}_2 = e_3 e_1 - K_2 e_2 - A + q_{21}\left[Bz(a) - e_1\right] + q_{22}\left[Dz(a) - e_2\right] \tag{5.12b}$$

$$\dot{e}_3 = q_{31}\left[Bz(a) - e_1\right] + q_{32}\left[Dz(a) - e_2\right] \tag{5.12c}$$

$$\dot{q}_{11} = -2\, q_{11}(e_3 + K_3) - (q_{31} + q_{13})e_1 - q_{11}^2 - q_{12}q_{21} \tag{5.13a}$$

$$\dot{q}_{12} = -q_{12}(e_3 + K_3) + q_{11}e_3 - (q_{32} - q_{13})e_1 - q_{12}K_2 - q_{11}q_{12} - q_{12}q_{22} \tag{5.13b}$$

$$\dot{q}_{13} = -q_{13}(e_3 + K_3) - q_{33}e_1 - q_{11}q_{13} - q_{12}q_{23} \tag{5.13c}$$

$$\dot{q}_{21} = (q_{31} - q_{23})e_1 - q_{21}K_2 - q_{21}(e_3 + K_3) + q_{11}e_3 - q_{21}q_{11} - q_{22}q_{21} \tag{5.13d}$$

$$\dot{q}_{22} = (q_{12} + q_{21})e_3 + (q_{32} + q_{23})e_1 - 2\, q_{22}K_2 - q_{21}q_{12} - q_{22}^2 \tag{5.13e}$$

$$\dot{q}_{23} = q_{13}e_3 + q_{33}e_1 - q_{23}K_2 - q_{21}q_{13} - q_{22}q_{23} \tag{5.13f}$$

$$\dot{q}_{31} = -q_{31}(e_3 + K_3) - q_{33}e_1 - q_{31}q_{11} - q_{32}q_{21} \tag{5.13g}$$

$$\dot{q}_{32} = q_{31}e_3 + q_{33}e_1 - q_{32}K_2 - q_{31}q_{12} - q_{32}q_{22} \tag{5.13h}$$

$$\dot{q}_{33} = -q_{31}q_{13} - q_{32}q_{23} \tag{5.13i}$$

The Runge-Kutaa integration scheme is used with the step size $\Delta t = 0.02$. The problem is solved with various sets of assumed initial values. A few have been selected for illustrations. One selected set of initial values is

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ 0 \end{bmatrix} \tag{5.14a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & q_{33}(0) \end{bmatrix}, \tag{5.14b}$$

where values for $q_{33}(0)$ are 1, 5, 10, 20, and 50, respectively. The estimated values for the deoxygenation rate constant K_1 are shown in Figure 9. The true value of this estimated parameter is obtained rapidly by time $t = 1.2$. It is seen that the estimated values of K_1 approach the true value more rapidly as the assumed value of $q_{33}(0)$ increases. However, if the value of $q_{33}(0)$ becomes too large, such as $q_{33}(0) = 50$, it results in a slight overestimation of the value of K_1 or the e_3 trajectory.

Another set of chosen initial values is

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ e_3(0) \end{bmatrix} \tag{5.15a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 5 \end{bmatrix}, \tag{5.15b}$$

where $e_3(0)$ represents the various initial values for K_1. These values are 0.01, 0.1, 0.31, 0.5, and 1, respectively. The results are shown in Figure 10. In spite of the very approximate initial guesses for the unknown parameter K_1, the true value is obtained by time $t = 0.8$.

In order to estimate the state B, D, and the parameter K_1 simultaneously, the following set of initial values is used

$$e(0) = \begin{bmatrix} e_1(0) \\ e_2(0) \\ 0.1 \end{bmatrix} \tag{5.16a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 50 & 1 & 1 \\ 1 & 50 & 1 \\ 1 & 1 & 50 \end{bmatrix}, \qquad (5.16b)$$

where the vector $\begin{vmatrix} e_1(0) \\ e_2(0) \end{vmatrix}$ represents a few sets of initial values for state B and D. They are

$$\begin{bmatrix} e_1(0) \\ e_2(0) \end{bmatrix} = \begin{bmatrix} 7.0 \\ 5.7 \end{bmatrix}, \begin{bmatrix} 6 \\ 7 \end{bmatrix}, \begin{bmatrix} 8 \\ 6 \end{bmatrix}, \begin{bmatrix} 5 \\ 4 \end{bmatrix}, \qquad (5.17)$$

and

$$\begin{bmatrix} 10 \\ 5 \end{bmatrix},$$

respectively. Satisfactory results for the estimated values for B, D and K_1 are obtained and shown in Figure 11, 12, and 13, respectively. Notice that in Figure 13, in spite of the large oscillations of K_1 or the e_3 trajectory between time $t = 0$ and $t = 0.8$, the true value is obtained by time $t = 1.6$.

Instead of using the value $q_{ij}(0) = 50$, $i = j = 1, 2, 3$, for the diagonal terms of $q(0)$ in Eq. (5.16b), the value

$q_{ij}(0) = 10$, $i = j = 1, 2, 3$, is also used. Only the estimated values of the state B are plotted in Figure 14. It is seen in the figure, the results are not very good.

It should be emphasized that in actual calculations, not only the values of $\underset{\sim}{e}(0)$, but also the values of $\underset{\sim}{q}(0)$ are very important. If the assumed values for $\underset{\sim}{e}(0)$ and $\underset{\sim}{q}(0)$ are reasonable, fairly satisfactory estimated results should be obtained in most cases. However, one must keep in mind that the filtering action of the estimation process depends greatly upon the values assumed for the diagonal terms of matrix $\underset{\sim}{q}(0)$. In general, for most practical problems, a rough idea about these values can be obtained either by experience and intuition or by the trial-and-error method.

5.3.2 <u>Estimation of State and Two Parameters</u>

Now consider both the rate constants K_1 (deoxygention) and K_2 (reaeration) as unknowns. The problem of this simultaneous estimation of the state B, D and the parameters K_1 and K_2 is solved.

The equations corresponding to Eq. (4.7) are now Eqs. (5.1)-(5.4) with $n = 4$, $m = 2$. Using Eqs. (4.10) and (4.11) with $\underset{\sim}{h}(\underset{\sim}{e}, a)$ and $\underset{\sim}{z}(a)$ remaining the same as in (5.9c) and (5,9d), but with $\underset{\sim}{e}(a)$, $\underset{\sim}{f}(\underset{\sim}{e}, a)$ and $\underset{\sim}{q}(a)$ changed to

$$\underset{\sim}{e}(a) = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix}. \tag{5.18a}$$

$$\underset{\sim}{f}(\underset{\sim}{e}, a) = \begin{bmatrix} -(e_3 + K_3)e_1 + R \\ e_3 e_1 - e_4 e_2 - A \\ 0 \\ 0 \end{bmatrix}, \tag{5.18b}$$

and

$$\underset{\sim}{q}(a) = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} \\ q_{21} & q_{22} & q_{23} & q_{24} \\ q_{31} & q_{32} & q_{33} & q_{34} \\ q_{41} & q_{42} & q_{43} & q_{44} \end{bmatrix}, \tag{5,18c}$$

twenty simultaneous estimator equations are obtained:

$$\dot{e}_1 = -(e_3 + K_3)e_1 + R + q_{11}[Bz(a) - e_1] + q_{22}[Dz(a) - e_2] \tag{5.19a}$$

$$\dot{e}_2 = e_3 e_1 - e_4 e_2 - A + q_{21}[Bz(a) - e_1] + q_{22}[Dz(a) - e_2] \tag{5.19b}$$

$$\dot{e}_3 = q_{31}[Bz(a) - e_1] + q_{32}[Dz(a) - e_2] \tag{5.19c}$$

$$\dot{e}_4 = q_{41}[Bz(a) - e_1] + q_{42}[Dz(a) - e_2] \tag{5.19d}$$

$$\begin{aligned}\dot{q}_{11} = &-2\, q_{11}(e_3 + K_3) - (q_{31} + q_{13})e_1 \\ &- q_{11}{}^2 - q_{12}q_{21}\end{aligned} \tag{5.20a}$$

$$\begin{aligned}\dot{q}_{12} = &-q_{12}(e_3 + K_3) + q_{11}e_3 - (q_{32} - q_{13})e_1 \\ &- q_{12}e_4 - q_{14}e_2 - q_{11}q_{12} - q_{12}q_{22}\end{aligned} \tag{5.20b}$$

$$\begin{aligned}\dot{q}_{13} = &-q_{13}(e_3 + K_3) - q_{33}e_1 - q_{11}q_{13} \\ &- q_{12}q_{23}\end{aligned} \tag{5.20c}$$

$$\begin{aligned}\dot{q}_{14} = &-q_{14}(e_3 + K_3) - q_{34}e_1 - q_{11}q_{14} \\ &- q_{12}q_{24}\end{aligned} \tag{5.20d}$$

$$\begin{aligned}\dot{q}_{21} = &\ (q_{31} - q_{23})e_1 - q_{21}e_4 - q_{21}(e_3 + K_3) \\ &+ q_{11}e_3 - q_{41}e_2 - q_{21}q_{11} - q_{22}q_{21}\end{aligned} \tag{5.20e}$$

$$\begin{aligned}\dot{q}_{22} = &\ (q_{12} + q_{21})e_3 + (q_{32} + q_{23})e_1 - 2\, q_{22}e_4 \\ &- (q_{42} + q_{24})e_2 - q_{21}q_{12} - q_{22}{}^2\end{aligned} \tag{5.20f}$$

$$\begin{aligned}\dot{q}_{23} = &\ q_{13}e_3 + q_{33}e_1 - q_{23}e_4 - q_{43}e_2 \\ &- q_{21}q_{13} - q_{22}q_{23}\end{aligned} \tag{5.20g}$$

$$\dot{q}_{24} = q_{14}e_3 + q_{34}e_1 - q_{24}e_4 - q_{44}e_2$$
$$- q_{21}q_{14} - q_{22}q_{24} \qquad (5.20h)$$

$$\dot{q}_{31} = -q_{31}(e_3 + K_3) - q_{33}e_1 - q_{31}q_{11}$$
$$- q_{32}q_{21} \qquad (5.20i)$$

$$\dot{q}_{32} = q_{31}e_3 + q_{33}e_1 - q_{32}e_4 - q_{34}e_2$$
$$- q_{31}q_{12} - q_{32}q_{22} \qquad (5.20j)$$

$$\dot{q}_{33} = -q_{31}q_{13} - q_{32}q_{23} \qquad (5.20k)$$

$$\dot{q}_{34} = -q_{31}q_{14} - q_{32}q_{24} \qquad (5.20l)$$

$$\dot{q}_{41} = -q_{41}(e_3 + K_3) - q_{43}e_1 - q_{41}q_{11}$$
$$- q_{42}q_{21} \qquad (5.20m)$$

$$\dot{q}_{42} = q_{41}e_3 + q_{43}e_1 - q_{42}e_4 - q_{44}e_2$$
$$- q_{41}q_{12} - q_{42}q_{22} \qquad (5.20n)$$

$$\dot{q}_{43} = -q_{41}q_{13} - q_{42}q_{23} \qquad (5.20o)$$

$$\dot{q}_{44} = -q_{41}q_{14} - q_{42}q_{24} \qquad (5.20p)$$

Where the functions e_1, e_2 and e_3 are defined the same as in the one parameter problem, e_4 represents the optimal estimate of K_2 for the present case.

Using the following two sets of initial conditions, Eqs. (5.19) and (5.20) are solved:

1)

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ e_3(0) \\ e_4(0) \end{bmatrix} \tag{5.21a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 5 & 1 \\ 1 & 1 & 1 & 5 \end{bmatrix}, \tag{5.21b}$$

2)

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ e_3(0) \\ e_4(0) \end{bmatrix} \tag{5.22a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 50 & 1 & 1 & 1 \\ 1 & 50 & 1 & 1 \\ 1 & 1 & 50 & 1 \\ 1 & 1 & 1 & 50 \end{bmatrix}, \tag{5.22b}$$

where $\begin{bmatrix} e_3(0) \\ e_4(0) \end{bmatrix}$ represents several different sets of initial values assumed for the estimation of K_1 and K_2. They are

$$\begin{bmatrix} e_3(0) \\ e_4(0) \end{bmatrix} = \begin{bmatrix} 0.1 \\ 0.5 \end{bmatrix}, \quad \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix}, \quad \begin{bmatrix} 0.31 \\ 1.02 \end{bmatrix}, \quad \begin{bmatrix} 0.5 \\ 2 \end{bmatrix}, \tag{5.23}$$

and

$$\begin{bmatrix} 1 \\ 5 \end{bmatrix},$$

respectively. The results shown in Figures 15-18 are obtained by using the Runge-Kutta integration scheme with the integration step size $\Delta t = 0.02$. Only the estimated values for the parameters K_1 and K_2 are presented in these figures. It is clearly shown that in Figures 15 and 16 the true values for K_1 and K_2 are obtained at approximately $t = 1.2$, except when the set of initial values in which $\begin{bmatrix} e_3(0) \\ e_4(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$ is used. The reason for this is simply because the values chosen for $e_3(0) = 1$ and $e_4(0) = 5$ are far from the true values of K_1 and K_2. However, when the values of the diagonal terms in the weighting function $\underset{\sim}{q}(0)$ are increased from 5 to 50, as shown in (5.22b), the results are much improved (see Figure 17, 18).

To estimate extensively the state B, D, and the parameters K_1, and K_2, the following initial values are used

$$\underset{\sim}{e}(0) = \begin{bmatrix} e_1(0) \\ e_2(0) \\ 0.1 \\ 0.5 \end{bmatrix} \tag{5.24a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 50 & 1 & 1 & 1 \\ 1 & 50 & 1 & 1 \\ 1 & 1 & 50 & 1 \\ 1 & 1 & 1 & 50 \end{bmatrix}, \tag{5.24b}$$

where $\begin{bmatrix} e_1(0) \\ e_2(0) \end{bmatrix}$ represents the initial values as follows:

$$\begin{bmatrix} e_1(0) \\ e_2(0) \end{bmatrix} = \begin{bmatrix} 7.0 \\ 5.7 \end{bmatrix}, \quad \begin{bmatrix} 6 \\ 7 \end{bmatrix}, \quad \begin{bmatrix} 8 \\ 6 \end{bmatrix}, \tag{5.25}$$

and

$$\begin{bmatrix} 10 \\ 5 \end{bmatrix}.$$

The results of the estimated state and parameters are shown in Figures 19-22. The estimates for B and D are very stable, but large oscillations are observed in the K_1 and K_2 trajectories between time $t = 0$ and $t = 0.8$. Nevertheless, the results obtained are still acceptable for practical purposes.

Experiments using $q_{ij}(0) = 10$ and $q_{ij}(0) = 100$, $i = j = 1, 2, \ldots, 4$, for the diagonal terms of the weighting function matrix $q(0)$, have also been performed. The obtained results are very poor. Consquently, the best filtering action is obtained with $q_{ij}(0) = 50$, $i = j = 1, 2, \ldots, 4$, for the present case.

5.3.3 <u>A More General Estimation Problem</u>

Given observed measurements for the BOD concentration B, and the DO deficit D, along the stream and that the stream quality model can be represented by Eqs. (5.1) and (5.2), one obtains the best estimates for the state B, D, and the parameters K_1, K_2 and K_3. This estimation problem can be solved exactly in the same way as previous problems except for the presence of three parameters. The system can be represented by Eqs. (5.1)-(5.5).

Again, with n = 5, m = 2, and using Eqs. (4.10) and (4.11) with

$$\underset{\sim}{e}(a) = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \end{bmatrix}, \qquad (5.26a)$$

$$\underset{\sim}{f}(\underset{\sim}{e}, a) = \begin{bmatrix} -(e_3 + e_5)e_1 + R \\ e_3e_1 - e_4e_2 - A \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{5.26b}$$

$$\underset{\sim}{q}(a) = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} \\ q_{21} & q_{22} & q_{23} & q_{24} & q_{25} \\ q_{31} & q_{32} & q_{33} & q_{34} & q_{35} \\ q_{41} & q_{42} & q_{43} & q_{44} & q_{45} \\ q_{51} & q_{52} & q_{53} & q_{54} & q_{55} \end{bmatrix}, \tag{5.26c}$$

and with $\underset{\sim}{h}(\underset{\sim}{e}, a)$ and $\underset{\sim}{z}(a)$ remaining the same. Thirty simultaneous estimator equations are obtained:

$$\dot{e}_1 = -(e_3 + e_5)e_1 + R + q_{11}[Bz(a) - e_1] + q_{12}[Dz(a) - e_2] \tag{5.27a}$$

$$\dot{e}_2 = e_3e_1 - e_4e_2 - A + q_{21}[Bz(a) - e_1] + q_{22}[Dz(a) - e_2] \tag{5.27b}$$

$$\dot{e}_3 = q_{31}[Bz(a) - e_1] + q_{32}[Dz(a) - e_2] \tag{5.27c}$$

$$\dot{e}_4 = q_{41}[Bz(a) - e_1] + q_{42}[Dz(a) - e_2] \tag{5.27d}$$

$$\dot{e}_5 = q_{51}[Bz(a) - e_1] + q_{52}[Dz(a) - e_2] \tag{5.27e}$$

$$\dot{q}_{11} = -2\,q_{11}(e_3 + e_5) - (q_{31} + q_{13} + q_{51} + q_{15})e_1 - q_{11}^2 - q_{12}q_{21} \tag{5.28a}$$

$$\dot{q}_{12} = -q_{12}(e_3 + e_5) + (q_{13} - q_{32} - q_{52})e_1 - q_{14}e_2 + q_{11}e_3 - q_{12}e_4 - (q_{11} + q_{22})\,q_{12} \tag{5.28b}$$

$$\dot{q}_{13} = -q_{13}(e_3 + e_5) - (q_{33} + q_{53})e_1 - q_{11}q_{13} - q_{12}q_{23} \tag{5.28c}$$

$$\dot{q}_{14} = -q_{14}(e_3 + e_5) - (q_{34} + q_{54})e_1 - q_{11}q_{14} - q_{12}q_{24} \tag{5.28d}$$

$$\dot{q}_{15} = -q_{15}(e_3 + e_5) - (q_{35} + q_{55})e_1 - q_{11}q_{15} - q_{12}q_{25} \tag{5.28e}$$

$$\dot{q}_{21} = -q_{21}(e_3 + e_5) + (q_{31} - q_{23} - q_{25})e_1 - q_{41}e_2 + q_{11}e_3 - q_{21}e_4 - q_{21}(q_{11} + q_{22}) \tag{5.28f}$$

$$\dot{q}_{22} = (q_{32} + q_{23})e_1 - (q_{42} + q_{24})e_2 + (q_{12} + q_{21})e_3 - 2\,q_{22}e_4 - q_{21}q_{12} - q_{22}^2 \tag{5.28g}$$

$$\dot{q}_{23} = q_{33}e_1 - q_{43}e_2 + q_{13}e_3 - q_{23}e_4$$
$$- q_{21}q_{13} - q_{22}q_{23} \qquad (5.28h)$$

$$\dot{q}_{24} = q_{34}e_1 - q_{44}e_2 + q_{14}e_3 - q_{24}e_4$$
$$- q_{21}q_{14} - q_{22}q_{24} \qquad (5.28i)$$

$$\dot{q}_{25} = q_{35}e_1 - q_{45}e_2 + q_{15}e_3 - q_{25}e_4$$
$$- q_{21}q_{15} - q_{22}q_{25} \qquad (5.28j)$$

$$\dot{q}_{31} = -q_{31}(e_3 + e_5) - (q_{33} + q_{35})e_1$$
$$- q_{31}q_{11} - q_{32}q_{21} \qquad (5.28k)$$

$$\dot{q}_{32} = q_{33}e_1 - q_{34}e_2 + q_{31}e_3 - q_{32}e_4$$
$$- q_{31}q_{12} - q_{32}q_{22} \qquad (5.28l)$$

$$\dot{q}_{33} = -q_{31}q_{13} - q_{32}q_{23} \qquad (5.28m)$$

$$\dot{q}_{34} = -q_{31}q_{14} - q_{32}q_{24} \qquad (5.28n)$$

$$\dot{q}_{35} = -q_{31}q_{15} - q_{32}q_{25} \qquad (5.28o)$$

$$\dot{q}_{41} = -q_{41}(e_3 + e_5) - (q_{43} + q_{45})e_1$$
$$- q_{41}q_{11} - q_{42}q_{21} \qquad (5.28p)$$

$$\dot{q}_{42} = q_{43}e_1 - q_{44}e_2 + q_{41}e_3 - q_{42}e_4$$
$$- q_{41}q_{12} - q_{42}q_{22} \qquad (5.28q)$$

$$\dot{q}_{43} = -q_{41}q_{13} - q_{42}q_{23} \qquad (5.28r)$$

$$\dot{q}_{44} = -q_{41}q_{14} - q_{42}q_{24} \qquad (5.28s)$$

$$\dot{q}_{45} = -q_{41}q_{15} - q_{42}q_{25} \qquad (5.28t)$$

$$\dot{q}_{51} = -q_{51}(e_3 + e_5) - (q_{53} + q_{55})e_1$$
$$- q_{51}q_{11} - q_{52}q_{21} \qquad (5.28u)$$

$$\dot{q}_{52} = q_{53}e_1 - q_{54}e_2 + q_{51}e_3 - q_{52}e_4$$
$$- q_{51}q_{12} - q_{52}q_{22} \qquad (5.28v)$$

$$\dot{q}_{53} = -q_{51}q_{13} - q_{52}q_{23} \qquad (5.28w)$$

$$\dot{q}_{54} = -q_{51}q_{14} - q_{52}q_{24} \qquad (5.28x)$$

$$\dot{q}_{55} = -q_{51}q_{15} - q_{52}q_{25} \qquad (5.28y)$$

Where the functions e_1, e_2, e_3, and e_4 remaining the same. The function e_5 represents the optimal estimate for the additional parameter K_3.

Different sets of initial values have been used to solve this three parameter problem. These sets are :

1)

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ 0.31 \\ 1.02 \\ 0.03 \end{bmatrix}, \tag{5.29a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & q_{33}(0) & 1 & 1 \\ 1 & 1 & 1 & q_{44}(0) & 1 \\ 1 & 1 & 1 & 1 & q_{55}(0) \end{bmatrix} \tag{5.29b}$$

where $q_{33}(0) = q_{44}(0) = q_{55}(0) = 5$, 20, and 100, respectively.

2)

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ e_3(0) \\ e_4(0) \\ e_5(0) \end{bmatrix}, \tag{5.30a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} q_{11}(0) & 1 & 1 & 1 & 1 \\ 1 & q_{22}(0) & 1 & 1 & 1 \\ 1 & 1 & q_{33}(0) & 1 & 1 \\ 1 & 1 & 1 & q_{44}(0) & 1 \\ 1 & 1 & 1 & 1 & q_{55}(0) \end{bmatrix} \tag{5.30b}$$

where $\begin{bmatrix} e_3(0) \\ e_4(0) \\ e_5(0) \end{bmatrix}$ represents the initial values

$$\begin{bmatrix} e_3(0) \\ e_4(0) \\ e_5(0) \end{bmatrix} = \begin{bmatrix} 0.31 \\ 1.02 \\ 0.03 \end{bmatrix}, \quad \begin{bmatrix} 0.1 \\ 0.5 \\ 0.01 \end{bmatrix}, \quad \begin{bmatrix} 0.5 \\ 0.8 \\ 0.05 \end{bmatrix}, \tag{5.31}$$

and

$$\begin{bmatrix} 1.0 \\ 2.0 \\ 0.05 \end{bmatrix},$$

respectively. The values selected for $q_{ij}(0)$, $i = j = 1, 2, \ldots, 5$, are 5 and 50. Note that the Runge-Kutta integration scheme is again used with $\Delta t = 0.02$.

The estimated results for this problem are very poor and they will not be shown. Among the above various sets of initial values, only the set with values

$$\underset{\sim}{e}(0) = \begin{bmatrix} 7.0 \\ 5.7 \\ 0.31 \\ 1.02 \\ 0.03 \end{bmatrix}, \tag{5.32a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} 50 & 1 & 1 & 1 & 1 \\ 1 & 50 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \tag{5.32b}$$

shows fair estimates for the state B, D and the parameters K_1, K_2, and K_3. Some minus values and unreasonable estimates are obtained for the other sets of initial values used. Consquently, the true values of this estimation problem for both state and parameters are not obtained satisfactorily.

It is understood that the poor estimates may be caused by two reasons. First, the true value of $K_3 = 0.03$ is relatively small compared with the true values of $K_1 = 0.31$, $K_2 = 1.02$, and B, D profiles. Second, the problem becomes more complicated and unstable when thirty simultaneous differential equations are involved.

5.4 DISCUSSION

The invariant imbedding approach has been used to solve the estimation problem for both state and parameters simultaneously. Three numerical examples in dynamic stream quality modeling are solved. The results of the optimal estimates for problems with one parameter and two parameters are very good. However, unsatisfactory results for the third problem with three parameters are obtained. Thus, in spite of this approach appears to be an effective tool for solving nonlinear estimation problems, much more research and computational experiments are needed.

It should be emphasized that in actual calculations the number of estimator equations increases rapidly as the number of parameters increases. However, if the estimator equations are not too complicated, and since the original problem has been converted into initial-value type, no iterative procedure is needed. Consquently, a lot of computer memory and computer time can be saved.

Table 13. Numerical Values Used as Noisy Measurements

t_i	$Bz(t_i)$	$Dz(t_i)$
0.0	7.0020	5.8369
0.1	7.5664	5.3087
0.2	6.9495	4.9066
0.3	6.0073	4.4836
0.4	6.0980	4.3540
0.5	6.4141	3.3631
0.6	6.4561	3.6594
0.7	5.2465	3.1703
0.8	5.3337	3.2807
0.9	5.4875	2.7151
1.0	4.8351	2.6218
1.1	5.1369	2.1120
1.2	4.9037	1.7501
1.3	4.2546	1.9986
1.4	5.4648	1.8651
1.5	3.9549	2.0035
1.6	4.3701	1.7669
1.7	4.0002	1.7151
1.8	4.4408	1.0743
1.9	3.8943	1.1499
2.0	3.7120	1.4434

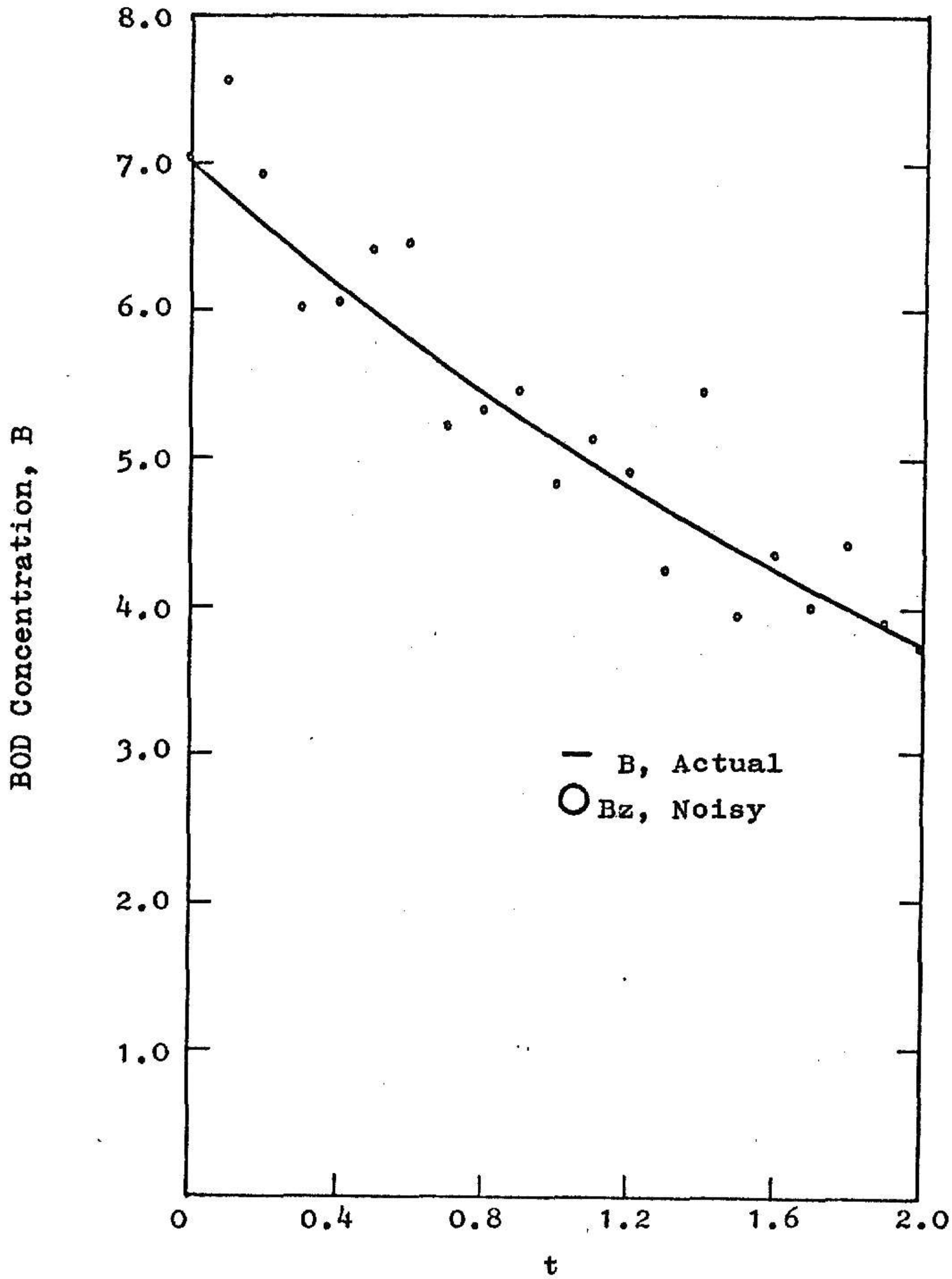

Fig. 7.

Actual and Noisy Measurements of BOD Concentration

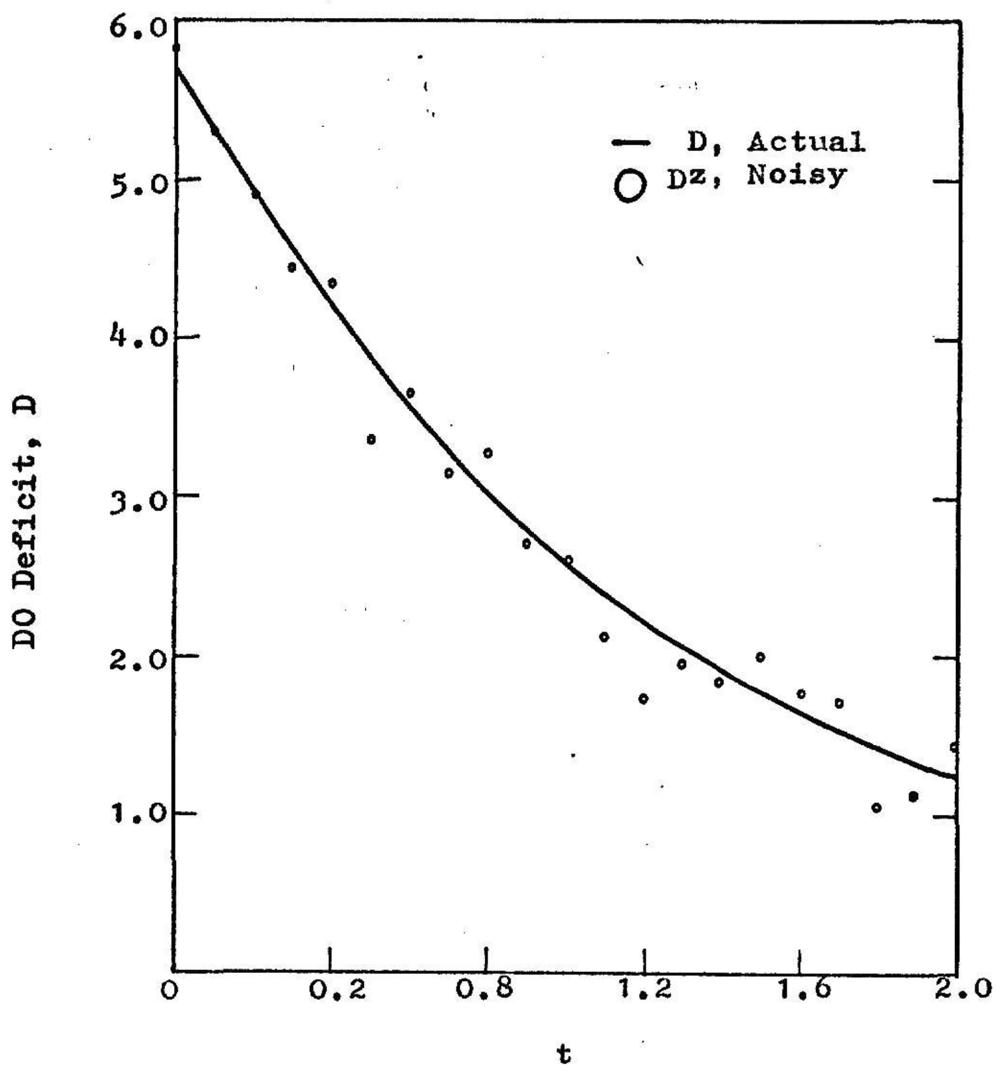

Fig. 8.

Actual and Noisy Measurements of DO Deficit

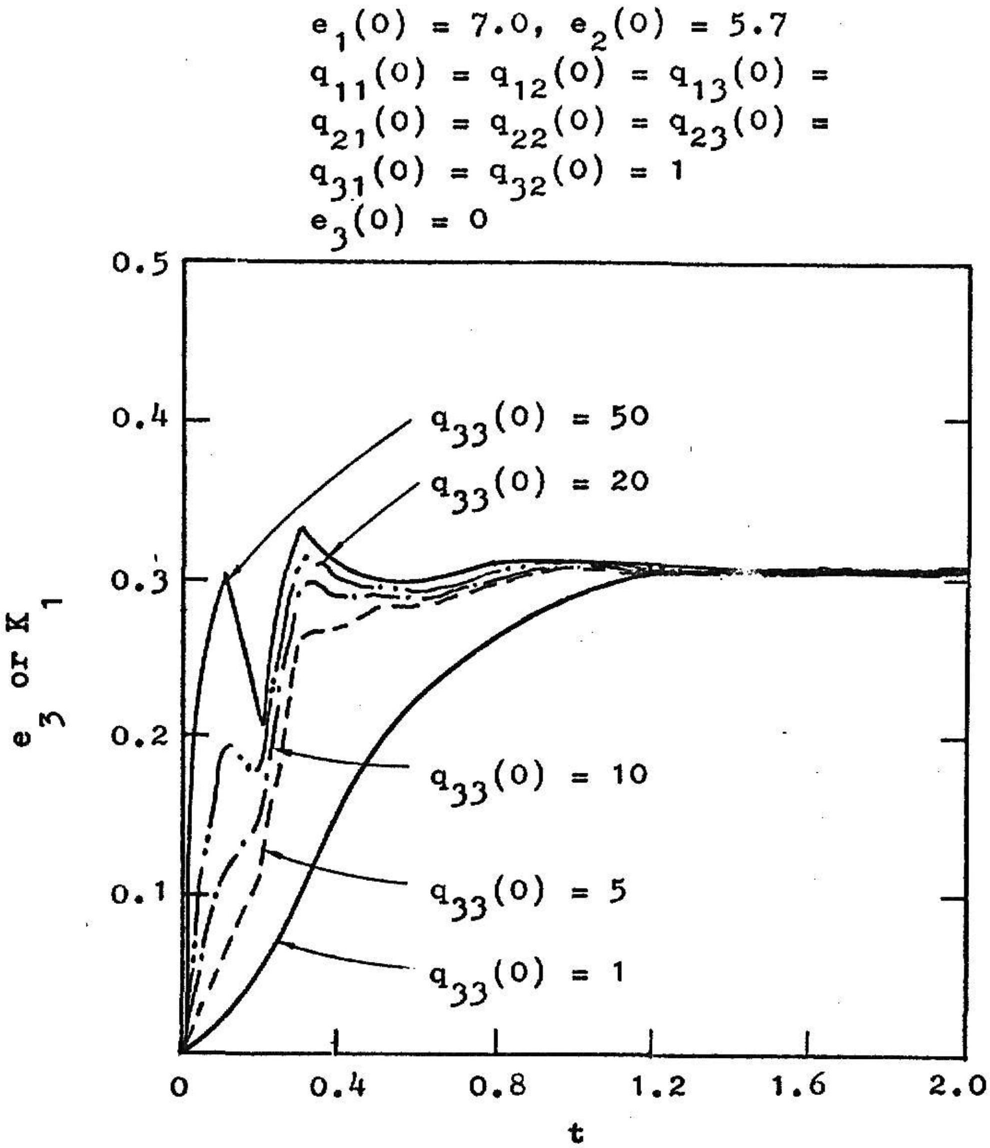

Fig. 9.

Estimated Parameter K_1 as A Function of $q_{33}(0)$

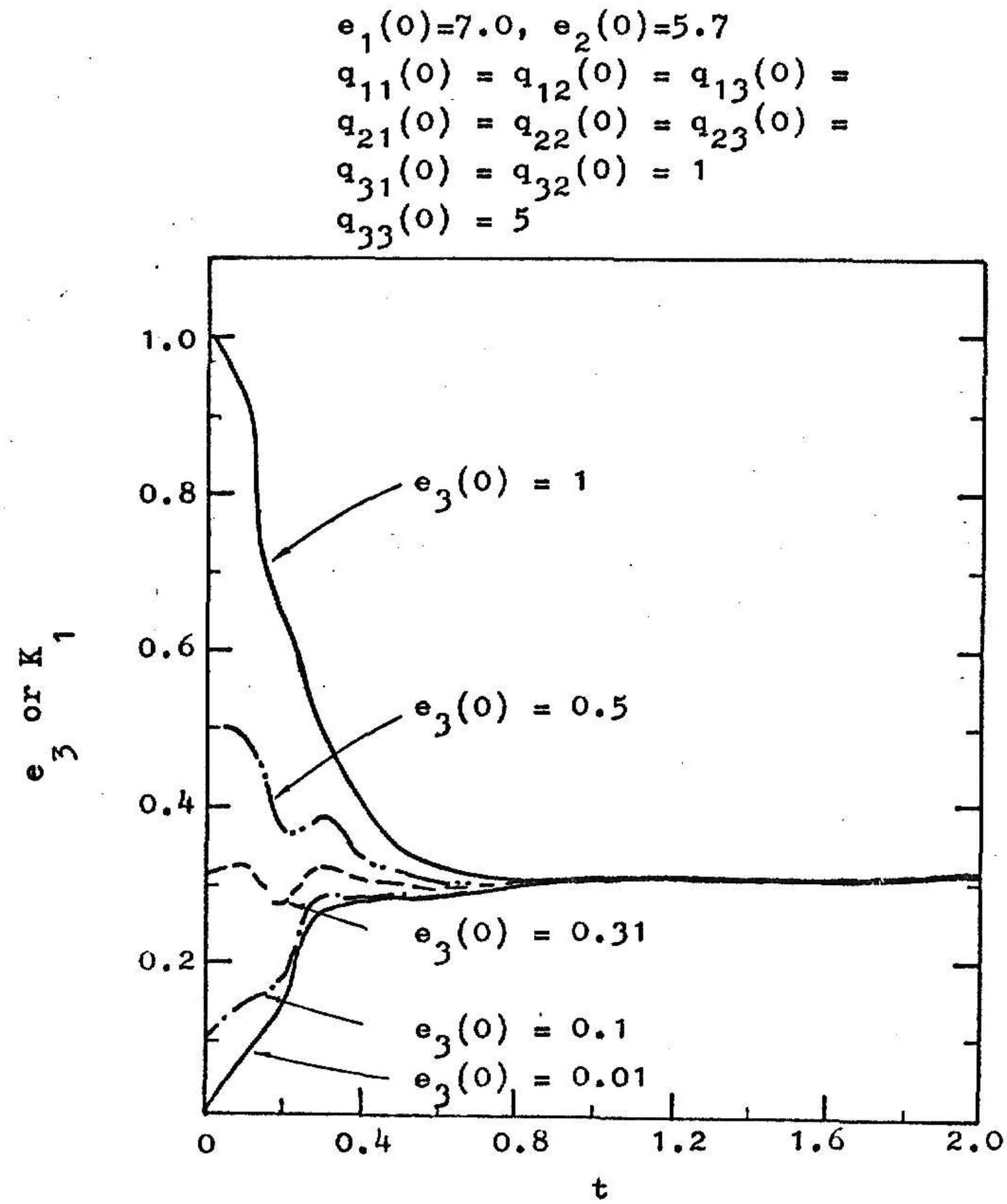

Fig. 10.

Estimated Parameter K_1 as A Function of $e_3(0)$

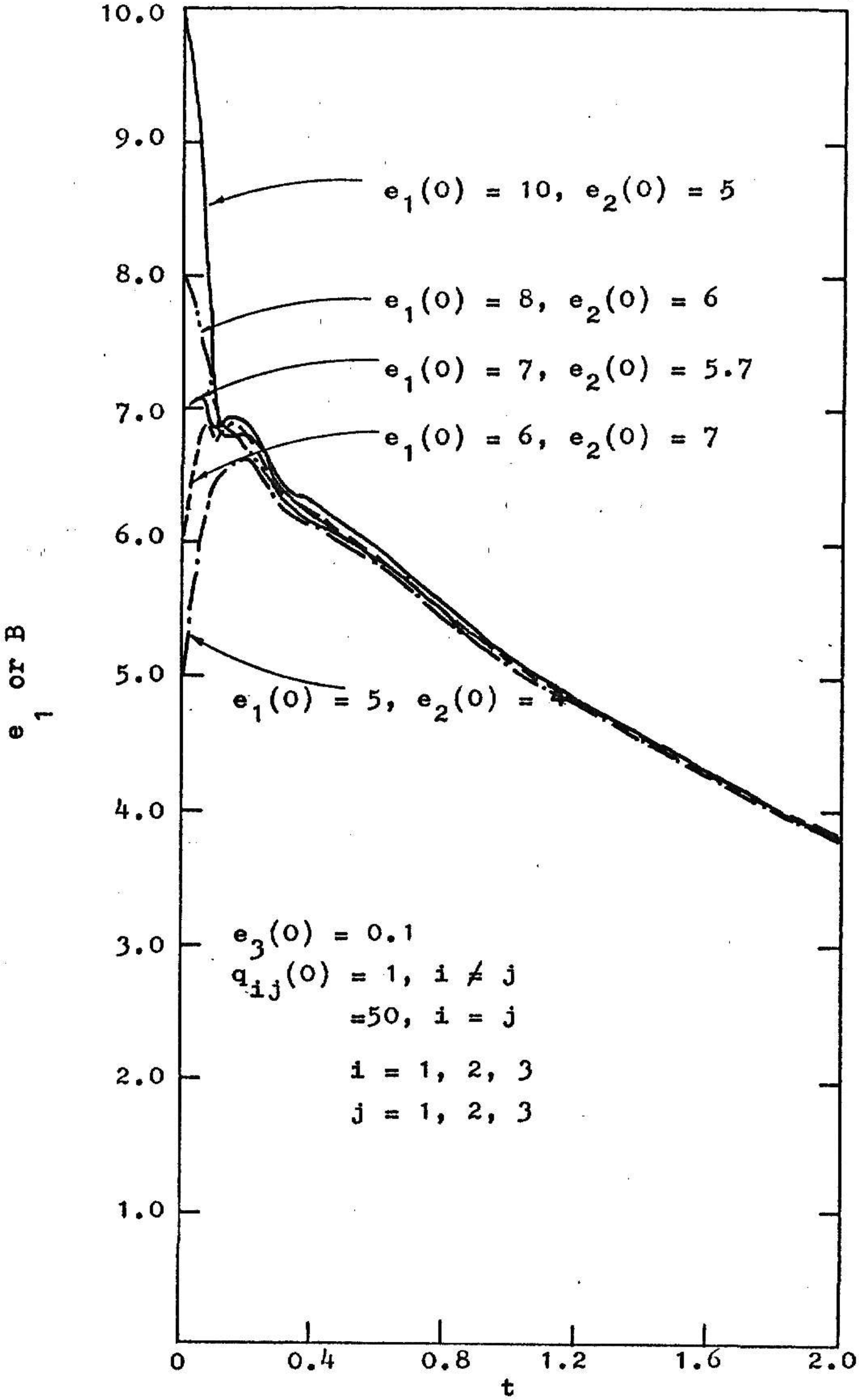

Fig. 11.

Estimated State B as A Function of $e_1(0)$, $e_2(0)$

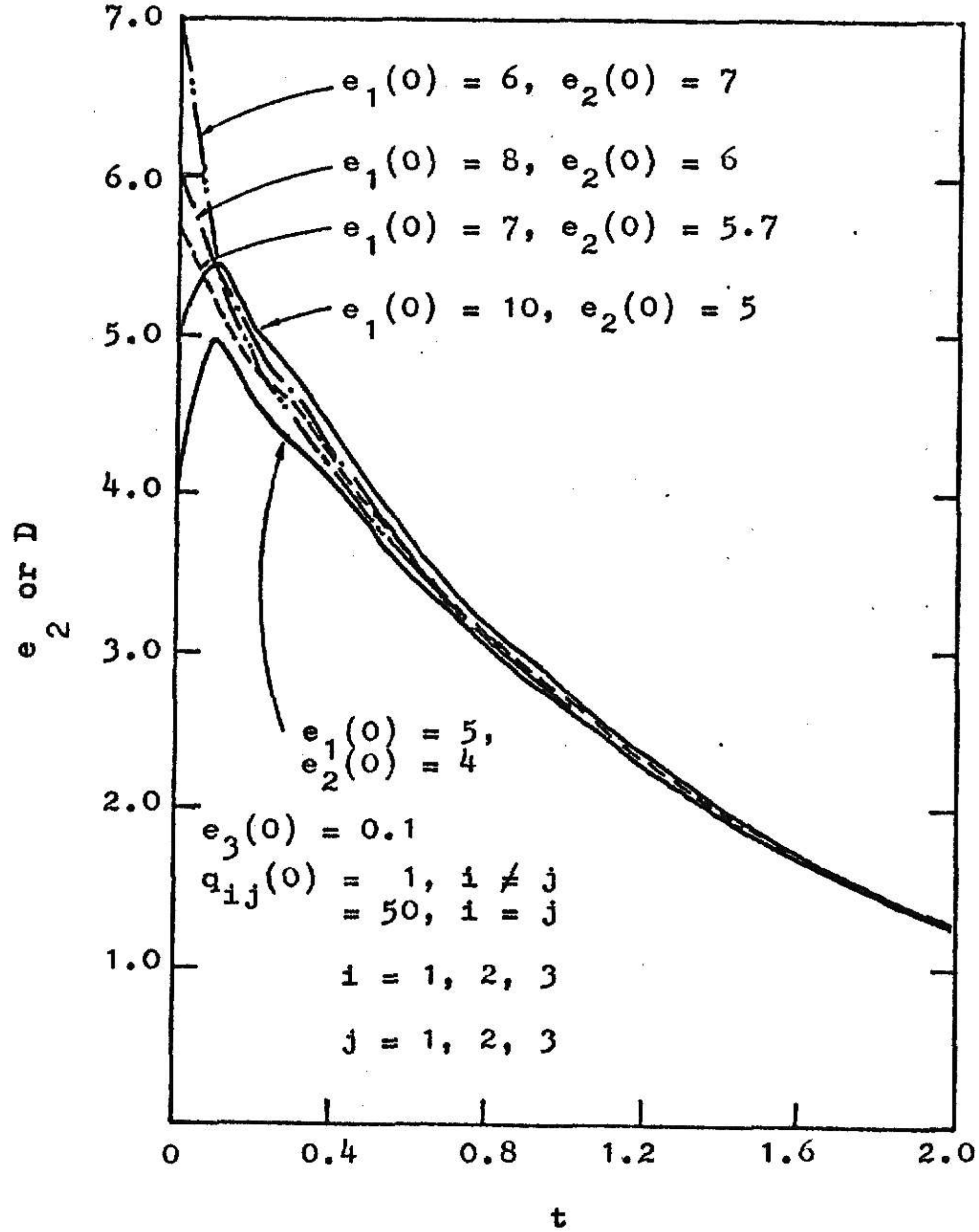

Fig. 12.

Estimated State D as A Function of $e_1(0)$, $e_2(0)$

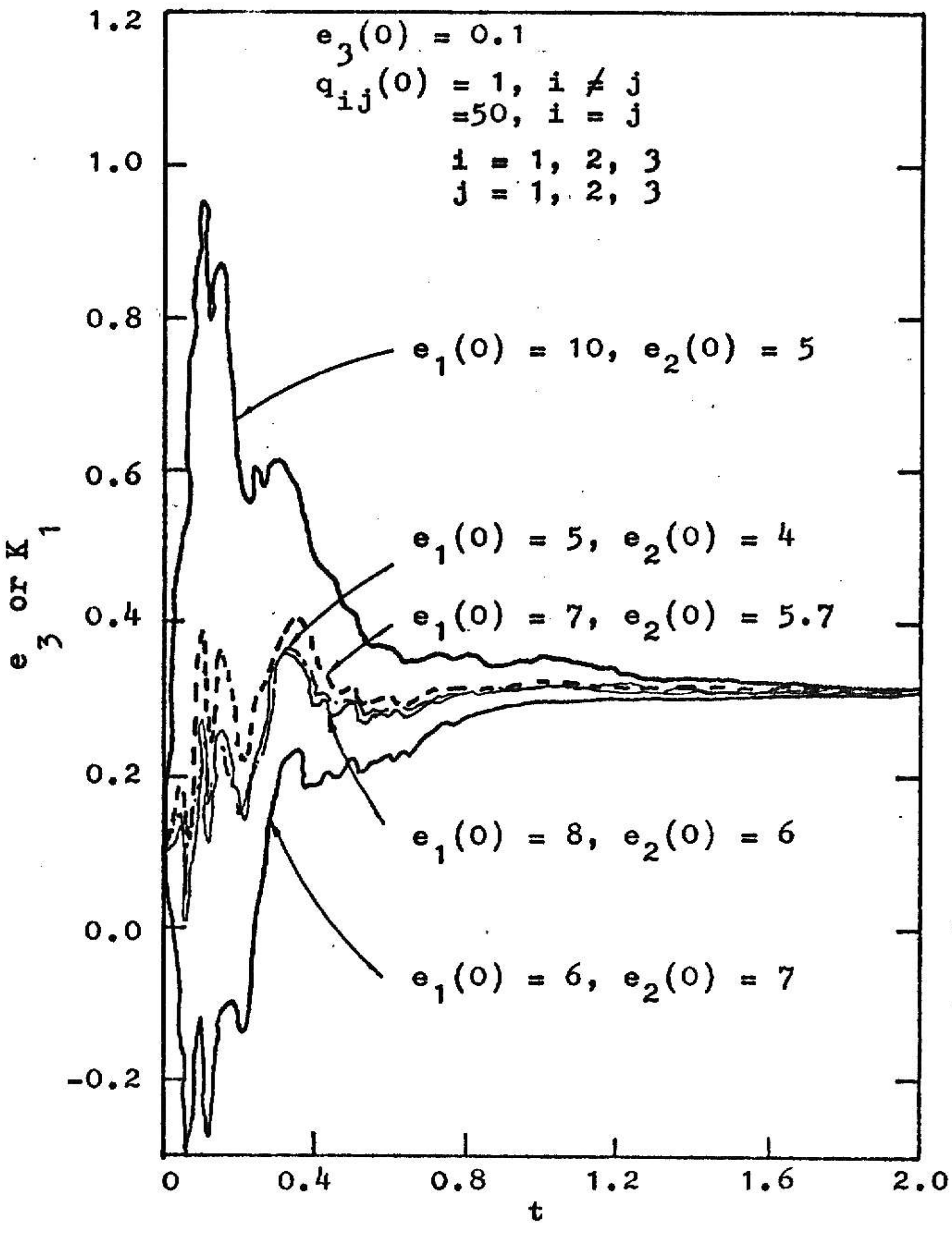

Fig. 13.

Estimated Parameter K_1 as A Function of $e_1(0)$, $e_2(0)$

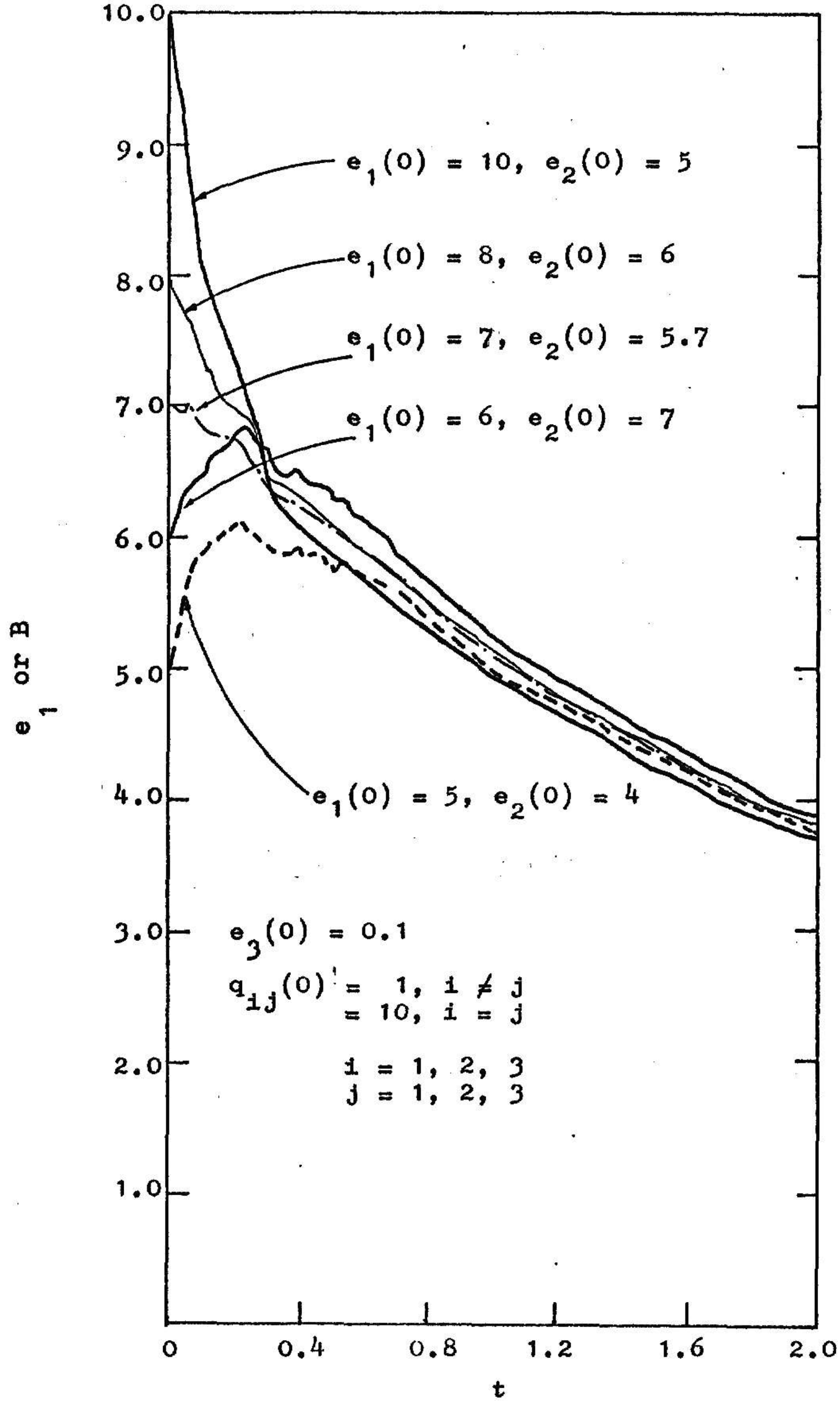

Fig. 14.

Estimated State B as A Function of $e_1(0)$, $e_2(0)$

$e_1(0) = 7.0,\ e_2(0) = 5.7$
$q_{11}(0) = q_{12}(0) = q_{13}(0) = q_{14}(0) =$
$q_{21}(0) = q_{22}(0) = q_{23}(0) = q_{24}(0) =$
$q_{31}(0) = q_{32}(0) = q_{34}(0) = q_{41}(0) =$
$q_{42}(0) = q_{43}(0) = 1$
$q_{33}(0) = q_{44}(0) = 5$

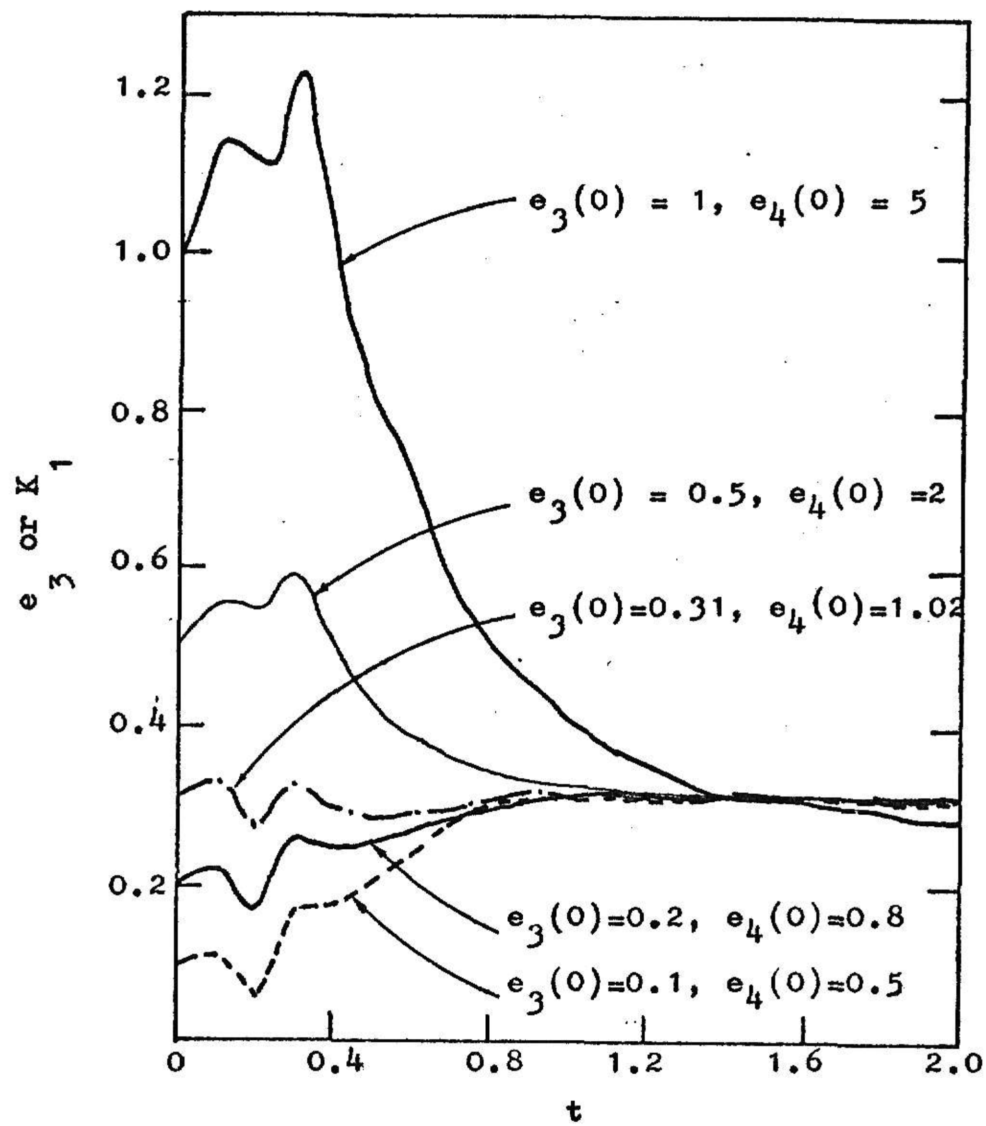

Fig. 15.

Estimated Parameter K_1 as A Function of $e_3(0)$, $e_4(0)$

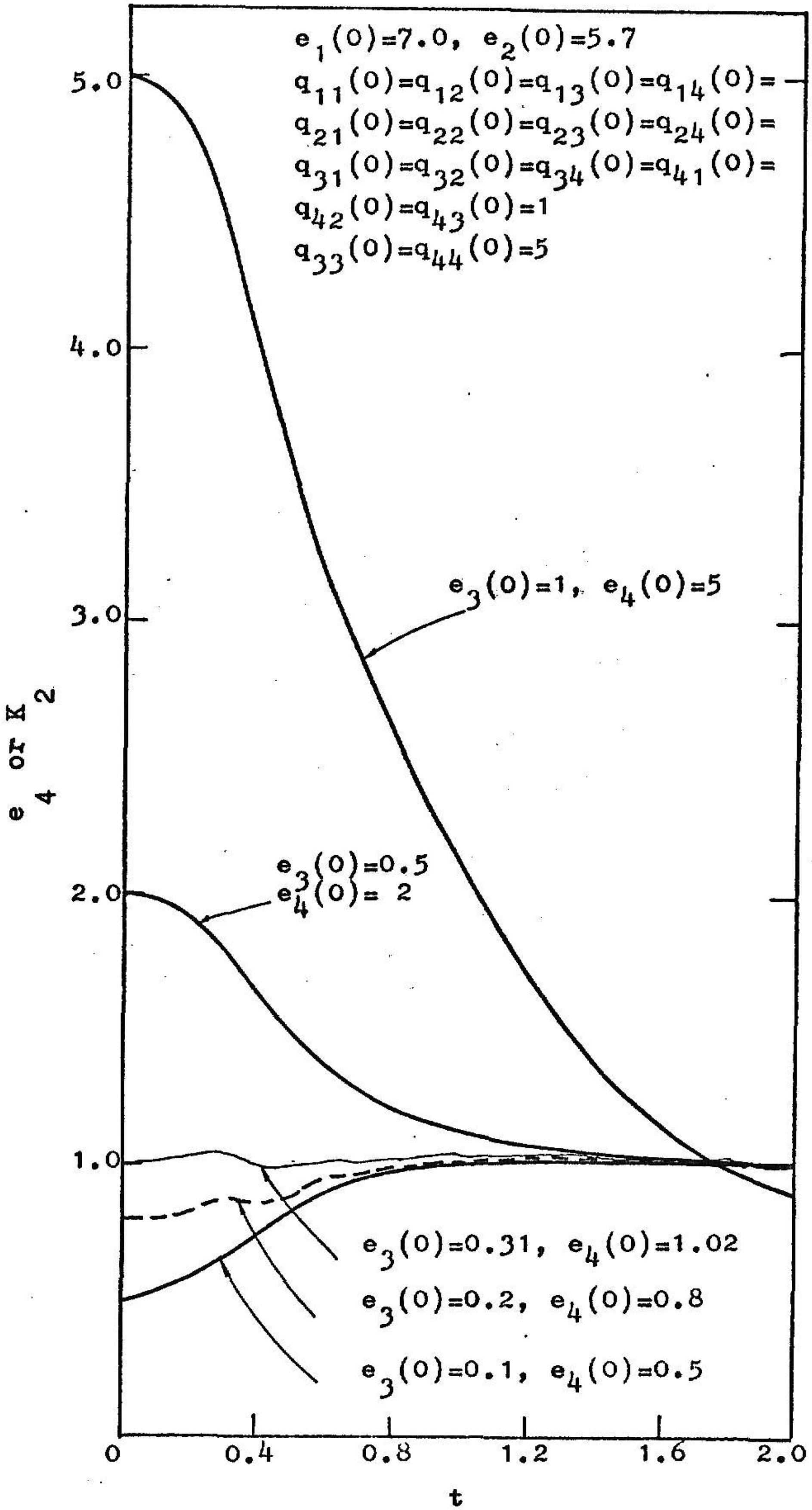

Fig. 16.

Estimated Parameter K_2 as A Function of $e_3(0)$, $e_4(0)$

$e_1(0)=70.$, $e_2(0)=5.7$

$q_{ij}(0)=1$, $i \neq j$

$=50$, $i=j$

$i=1, 2, \ldots, 4$

$j=1, 2, \ldots, 4$

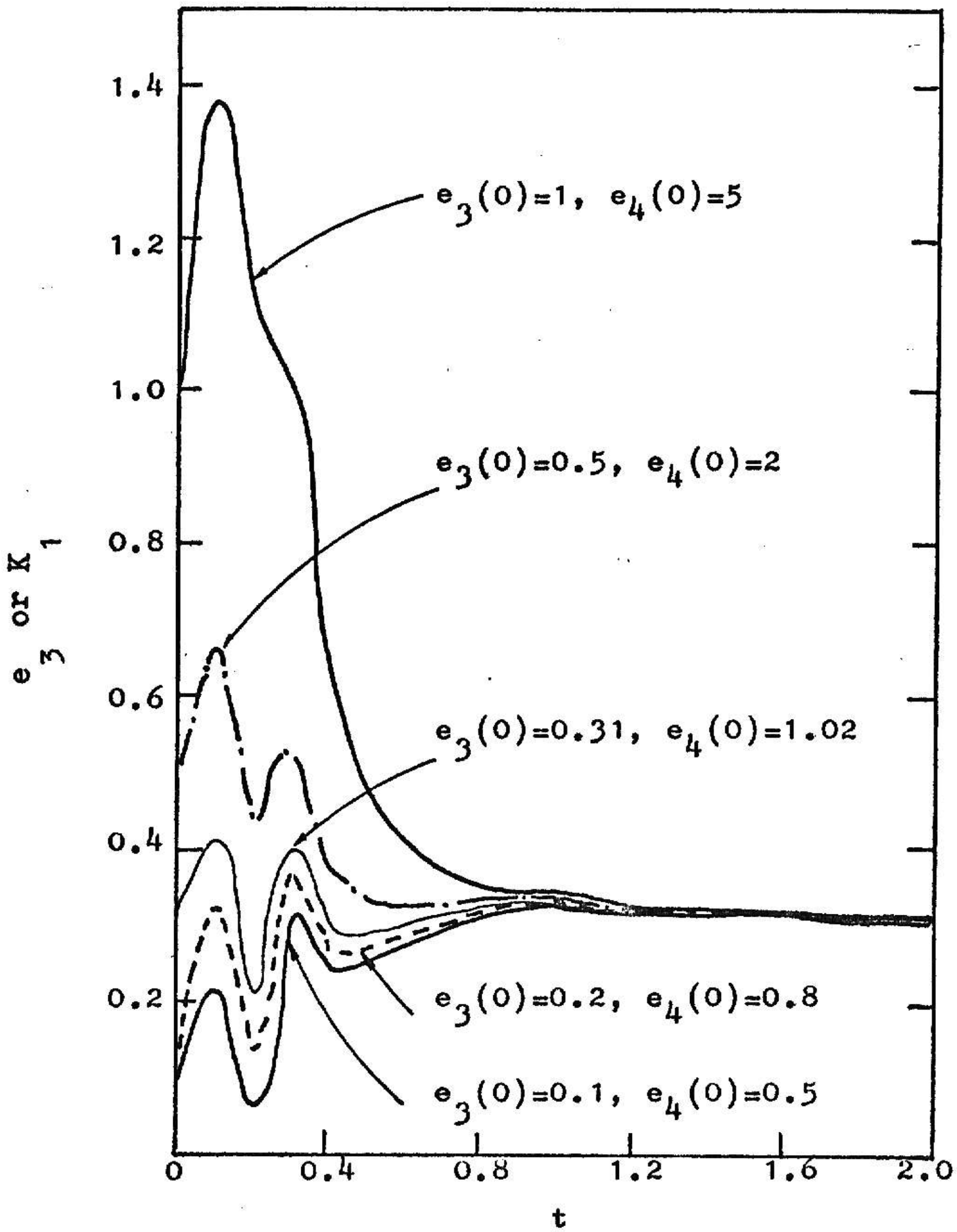

Fig. 17.

Estimated Parameter K_1 as A Function of $e_3(0)$, $e_4(0)$

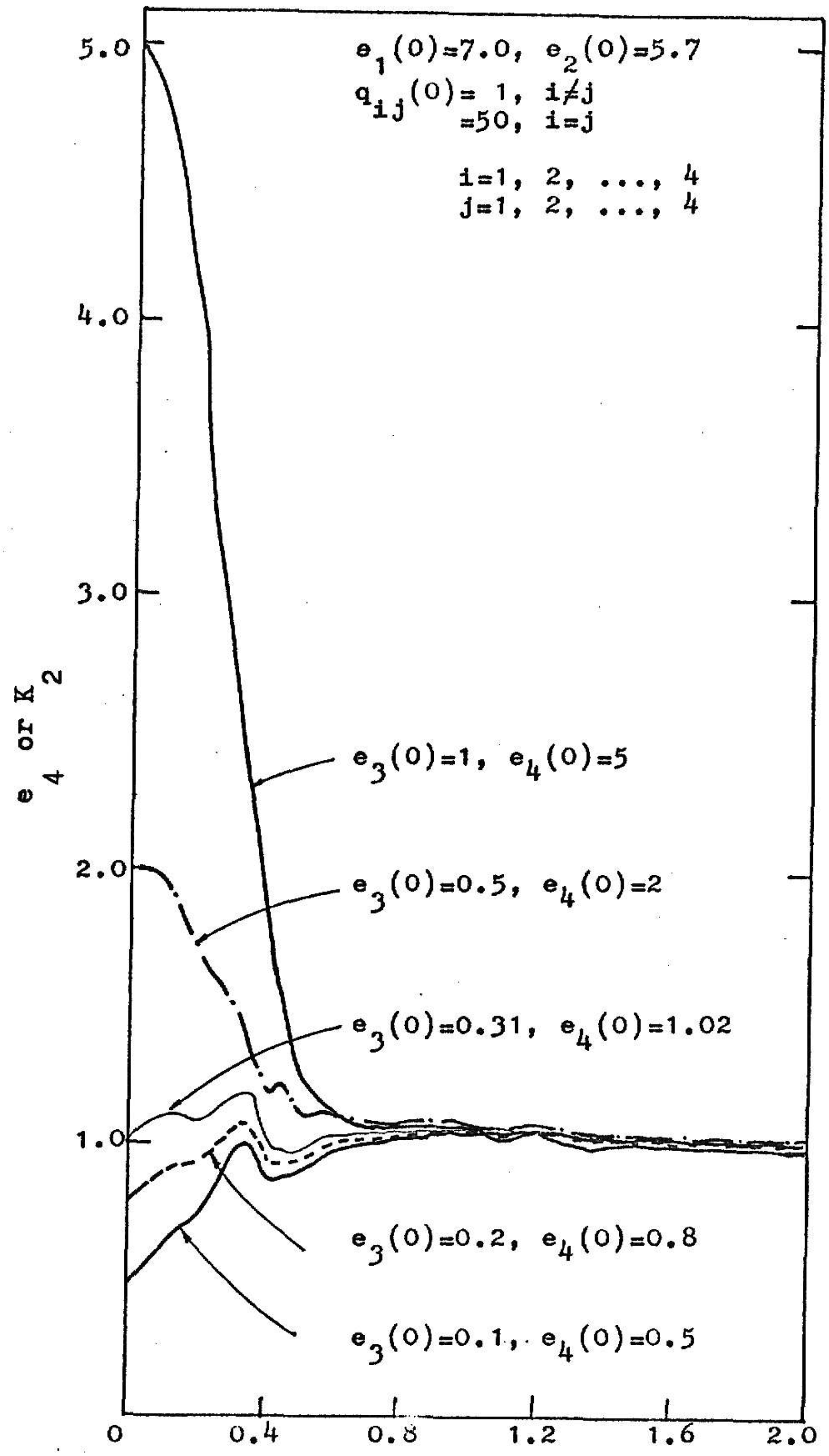

Fig. 18.

Estimated Parameter K_2 as A Function of $e_3(0)$, $e_4(0)$

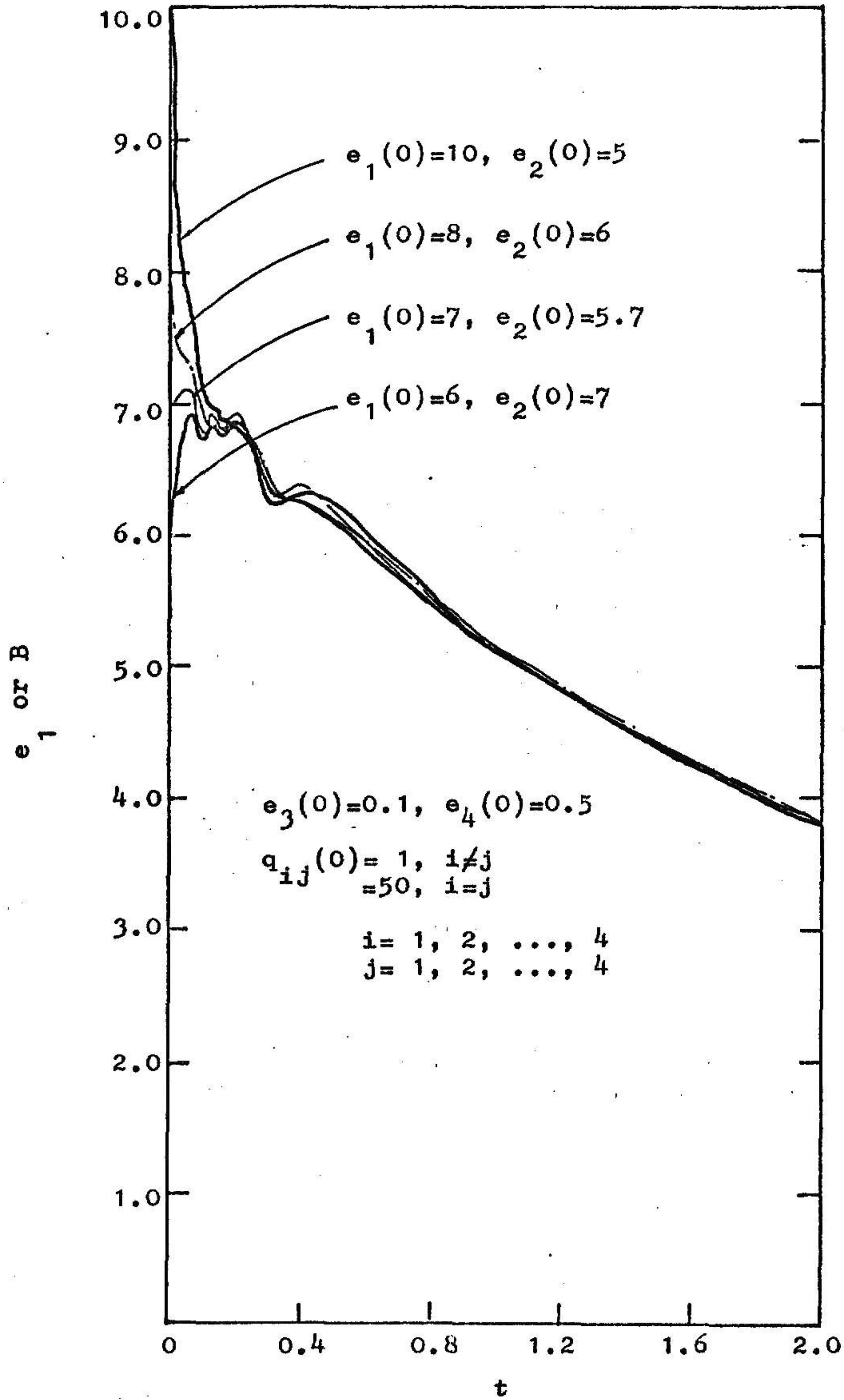

Fig. 19.

Estimated State B as A Function of $e_1(0)$, $e_2(0)$

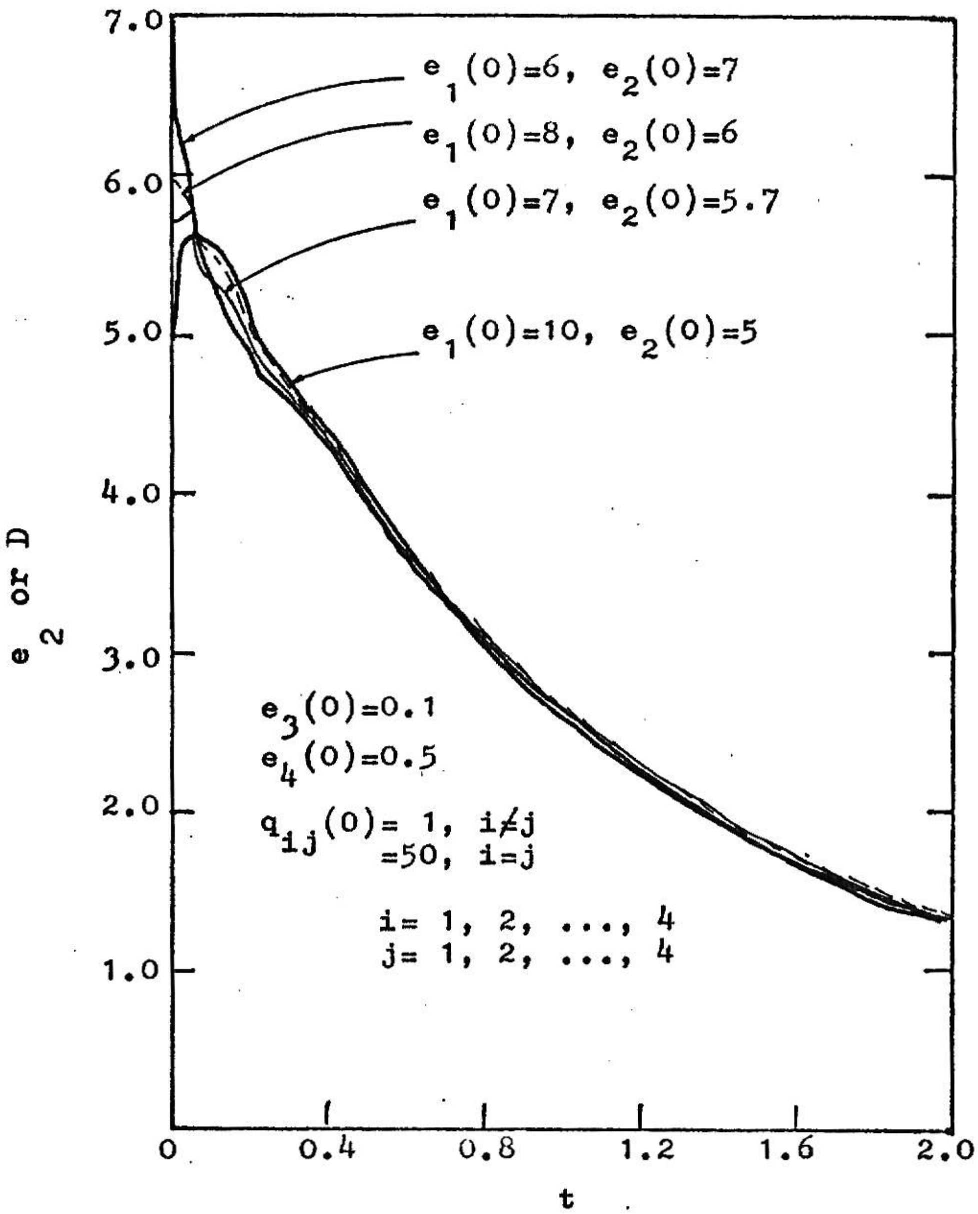

Fig. 20.

Estimated State D as A Function of $e_1(0)$, $e_2(0)$

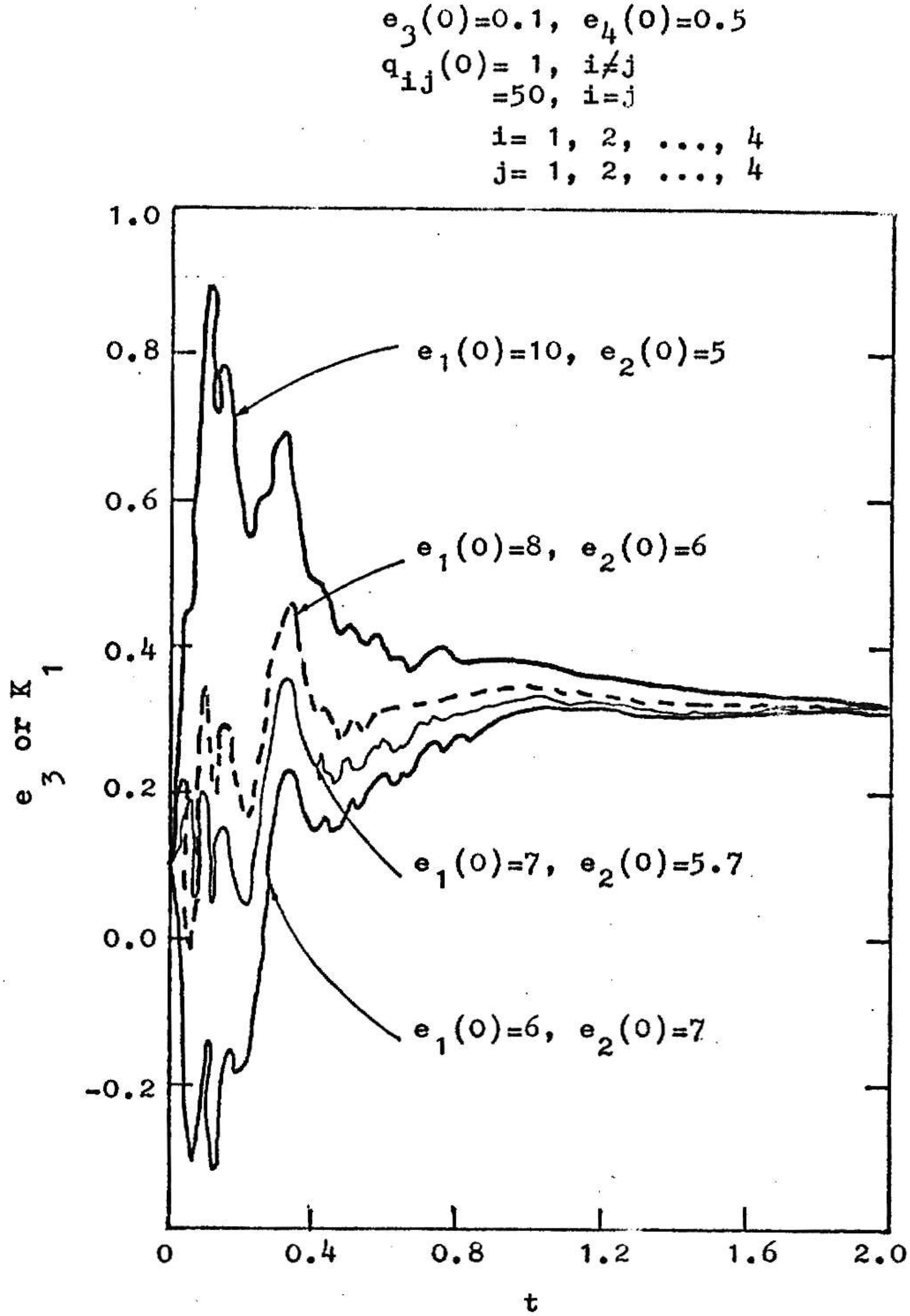

Fig. 21.

Estimated Parameter K_1 as A Function of $e_1(0)$, $e_2(0)$

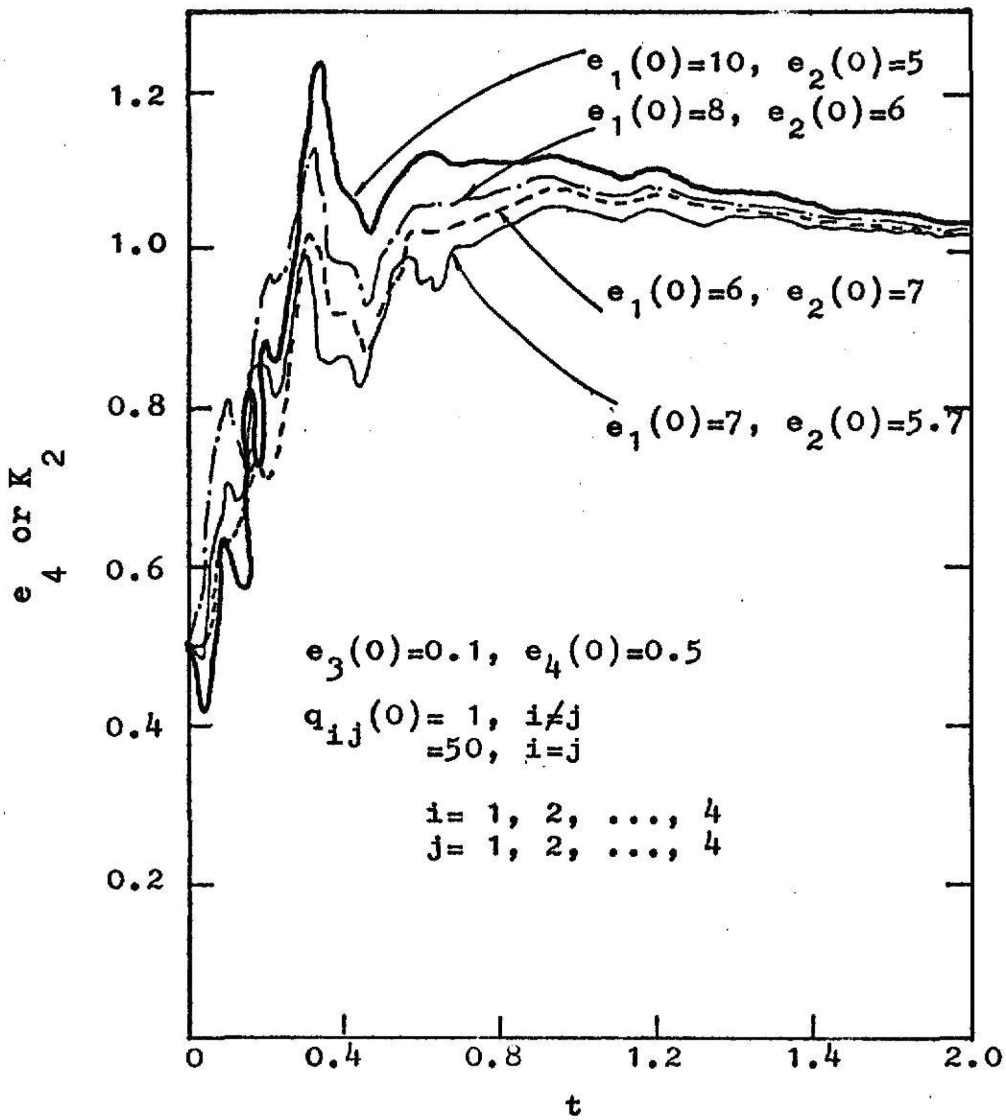

Fig. 22.

Estimated Parameter K_2 as A Function of $e_1(0)$, $e_2(0)$

CHAPTER 6

CONCLUSION

The nonlinear system estimation problem represents a major hinderance to the synthesis as well as to the analysis of accurate dynamic water-resource system models. The reasons are: 1) absence of explicit analytical solutions to the nonlinear models which represent the systems; 2) difficulties of numerical solutions obtained from the nonlinear models of the boundary-value type on digital computers. Quasilinearization and invariant imbedding represent two powerful computational tools for overcoming these difficulties.

As has been shown in the numerical examples presented in this work, the parameter estimation problems are effectively solved by quasilinearization and invariant imbedding. It has been proven that these two numerical techniques are very promising for the dynamic modeling and adaptive forecasting of stream or estuary quality.

The most attractive nature of the quasilinearization technique lies in its gereral applicability to a large class of complicated nonlinear models and its rapid convergence property. Solutions to the examples in this study reveal:

1. Accurate initial conditions are not required. Only reasonable approximations are needed.
2. Convergence rates of state and parameters to the optimal values are fairly rapid (within seven iterations).
3. Convergence rates are not reduced in the presence of

noise or experimental errors (five percent noise level is imposed on the data).

4. Fairly high accuracy is obtained (four to five digit accuracy).
5. In general, if convergence does not occur in five to seven iterations, convergence will not result.

Since the above estimation problem is essentially a two-point or multipoint boundary-value problem, it can also be solved by the invariant imbedding approach. By using this approach, expressions for the missing boundary conditions can be obtained by a sequential estimation scheme. The optimal sequential estimator equations are a system of ordinary differential equations of initial value type, which can be solved very easily on digital or analog computers. Thus, the invariant imbedding approach is ideally suited for solving this estimation problem. However, along with these advantages, the drawbacks are also noted:

1. The estimated results are less accurate than those obtained by quasilinearization. However, these results are still accurate enough for practical purposes.
2. It is subtle in choosing the intial values for the weighting functions. In general, they must be obtained by experience or the trial-and-error method, or the best filtering action for the estimation process cannot be obtained.

3. Experiences indicate that reasonable accurate values of the optimal estimates cannot be obtained for problems with a large number of complicated equations.

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APPENDICES

Computer Programs

APPENDIX 1.

COMPUTER PROGRAM FOR THE PROBLEM OF ESTIMATION OF THREE PARAMETERS WITH EXPERIMENTAL ERRORS BY QUASILINEARIZATION

```
C     ****************************************************************
C
C     STREAM QUALITY MODELING AND ESTIMATION BY QUASILINEARIZATION--
C     ESTIMATION OF THREE PARAMETERS WITH EXPERIMENTAL ERRORS
C
C     THE CAMP-DOBBINS STREAM QUALITY MODEL
C
C     DB/DT=-(K1+K3)*B + R
C     DD/DT=K1*B - K2*D - A
C
C     NOTATION
C
C     B---- BOD CONCENTRATION
C     D---- DISSOLVED OXYGEN DEFICIT
C     A---- OXYGEN PRODUCTION OR REDUCTION DUE TO PLANTS AND BOTTOM
C           DEPOSITS
C     R---- BOD ADDITION RATE
C     K1--- DEOXYGENATION RATE CONSTANT
C     K2--- REAERATION RATE CONSTANT
C     K3--- SEDIMENTATION AND ABSORPTION RATE CONSTANT
C
C     THIS PROBLEM IS TO ESTIMATE THE RATE CONSTANTS K1, K2, AND
C     K3 BASED UPON THE ABOVE CAMP-DOBBINS STREAM QUALITY MODEL
C
C     THIS PROGRAM WAS WRITTEN BY IRVING K. HWANG, DEPARTMENT OF
C     INDUSTRIAL ENGINEERING, KANSAS STATE UNIVERSITY, MANHATTAN,
C     KANSAS, MAY, 1969.
C
C     ****************************************************************
C
C     NOTE:  DOUBLE PRECISION IS USED IN THIS PROGRAM.
C
C     THE MAIN PROGRAM.
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION B(101),D(101),BN(101),DN(101),BS(101),DS(101),BZ(101),
     1DZ(101),BP(101),DP(101),BH1(101),BH2(101),BH3(101),DH1(101),
     2DH2(101),DH3(101),Q(3,3),BB(3),X(3)
      COMMON G1N,G2N,G3N,A,R,BN,DN,K
C
C     1.  PRINT OUT THE PROGRAM TITLE.
C
      READ (1,51) ND
   51 FORMAT(I3)
      WRITE(3,11) ND
   11 FORMAT(//5X'NO. OF DATA SETS:  ND=' I5//)
      DO 1000 IM=1,ND
      WRITE(3,1)
    1 FORMAT(//5X,'STREAM QUALITY MODELING AND ESTIMATION BY ',
     1'QUASILINEARIZATION-'//3X,'ESTIMATION OF PARAMETERS K1, K2, ',
```

```
      2'AND K3 WITH EXPERIMENTAL ERRORS'//)

C     2.  READ IN AND PRINT OUT DATA.

      WRITE(3,2)
    2 FORMAT(/1X6(1H*)/1X'*DATA*'/1X6(1H*)/)
      READ(1,50) C1,C2,G1,G2,G3,G1N,G2N,G3N,A,R,DT,S1,S2,B1,B2,B3,B4,N,
     1NO,MN
   50 FORMAT(10F5.2/7F5.2/3I3)
      WRITE(3,3) C1,C2,G1,G2,G3,G1N,G2N,G3N,A,R,DT,S1,S2,B1,B2,B3,B4,N,
     1NO,MN
    3 FORMAT(/4X'   C1='F5.2,'   C2='F5.2,'   G1='F5.2,'   G2='F5.2,
     1'   G3='F5.2/4X' G1N='F5.2,' G2N='F5.2,' G3N='F5.2,'    A='F5.2,
     2'    R='F5.2/4X'   DT='F5.2,'   S1='F5.2,'   S2='F5.2/4X'   B1='F5.2,
     3'   B2='F5.2,'   B3='F5.2,'   B4='F5.2/4X'    N='I5,'   NO='I5,
     4'   MN='I5/)

C     3.  SOLVE THE CAMP-DOBBINS DIFFERENTIAL EQUATIONS AS
C         EXPERIMENTAL DATA.

      BS(1)=C1
      DS(1)=C2
      CALL RUGKU1(BS,DS,G1,G2,G3,A,R,DT,N)

C     4.  CORRUPT THE EXPERIMENTAL DATA WITH GAUSSIAN DISTRIBUTED
C         RANDOM NOISE.

      II=1
      IX=53471
      AM=B1
      S=S1
   55 DO 22 I=1,N,5
      AA=0.
      DO 23 K=1,12
      CALL RANDU(IX,IY,YFL)
      PX=IY
      AA=AA+YFL
   23 IX=PX
      V=(AA-6.)*S+AM
      IF(II .NE. 1) GO TO 45
      BZ(I)=BS(I)*(1.+0.10*V)
      GO TO 22
   45 DZ(I)=DS(I)*(1.+0.10*V)
   22 CONTINUE
      IF(II .GE. 2) GO TO 111
      IX=31353
      AM=B1
      S=S2
      II=II+1
      GO TO 55
```

```
111 WRITE(3,4)
  4 FORMAT(/10X'EXPERIMENTAL DATA VS. NOISY EXPERIMENTAL DATA:'/)
    DO 100 I=1,N,5
100 WRITE(3,5) I,BS(I),I,DS(I),I,BZ(I),I,DZ(I)
  5 FORMAT(5X'BS(',I3')='D14.6,5X'DS(',I3')='D14.6,5X'BZ(',I3')='D14.6
   1,5X'DZ(',I3')='D14.6)

    5.  ESTIMATE PARAMETERS K1, K2, AND K3 BY QUASILINEARIZATION.

    QUASILINEARIZATION LOOP STARTS HERE.

    L=1

    5.1  ASSUME INITIAL FUNCTIONS FOR B AND D.

    DO 200 I=1,N
    BN(I)=C1
200 DN(I)=C2
555 K=1
    WRITE(3,6) L
  6 FORMAT(///1X25(1H*)/1X17H*    ITERATION   I3,4X1H*/1X25(1H*)/)

    5.2  ASSUME INITIAL VALUES AND SOLVE FOR THE ONE SET OF
         PARTICULAR SOLUTIONS.

    BP(1)=C1
    DP(1)=C2
    G1P=B1
    G2P=B1
    G3P=B1
    CALL RUGKU2(BP,DP,G1P,G2P,G3P,DT,N)

    5.3  ASSUME INITIAL VALUES AND SOLVE FOR THE THREE SETS OF
         HOMOGENEOUS SOLUTIONS.

    K=2
    BH1(1)=B1
    DH1(1)=B1
    G1H1=B4
    G2H1=B1
    G3H1=B3
    CALL RUGKU2(BH1,DH1,G1H1,G2H1,G3H1,DT,N)
    BH2(1)=B1
    DH2(1)=B1
    G1H2=B4
    G2H2=B4
    G3H2=B1
    CALL RUGKU2(BH2,DH2,G1H2,G2H2,G3H2,DT,N)
    BH3(1)=B1
    DH3(1)=B1
```

```
      G1H3=B2
      G2H3=B1
      G3H3=B4
      CALL RUGKU2(BH3,DH3,G1H3,G2H3,G3H3,DT,N)

      5.4  SOLVE FOR THE INTEGRATION CONSTANTS A1, A2, AND A3.

      DO 300 I=1,MN
      DO 400 J=1,MN
  400 Q(I,J)=B1
  300 BB(I)=B1
      DO 500 I=1,N,5
      Q(1,1)=Q(1,1)+BH1(I)*BH1(I)+DH1(I)*DH1(I)
      Q(1,2)=Q(1,2)+BH1(I)*BH2(I)+DH1(I)*DH2(I)
      Q(1,3)=Q(1,3)+BH1(I)*BH3(I)+DH1(I)*DH3(I)
      Q(2,1)=Q(2,1)+BH2(I)*BH1(I)+DH2(I)*DH1(I)
      Q(2,2)=Q(2,2)+BH2(I)*BH2(I)+DH2(I)*DH2(I)
      Q(2,3)=Q(2,3)+BH2(I)*BH3(I)+DH2(I)*DH3(I)
      Q(3,1)=Q(3,1)+BH3(I)*BH1(I)+DH3(I)*DH1(I)
      Q(3,2)=Q(3,2)+BH3(I)*BH2(I)+DH3(I)*DH2(I)
      Q(3,3)=Q(3,3)+BH3(I)*BH3(I)+DH3(I)*DH3(I)
      BB(1)=BB(1)+BZ(I)*BH1(I)-BH1(I)*BP(I)+DZ(I)*DH1(I)-DH1(I)*DP(I)
      BB(2)=BB(2)+BZ(I)*BH2(I)-BH2(I)*BP(I)+DZ(I)*DH2(I)-DH2(I)*DP(I)
      BB(3)=BB(3)+BZ(I)*BH3(I)-BH3(I)*BP(I)+DZ(I)*DH3(I)-DH3(I)*DP(I)
  500 CONTINUE
      CALL GJRM(Q,BB,X,MN)
      A1=X(1)
      A2=X(2)
      A3=X(3)
      WRITE(3,7) A1,A2,A3
    7 FORMAT(//1X'THE INTEGRATION CONSTANTS ARE OBTAINED:  A1='D14.6,
     13X'A2='D14.6,3X'A3='D14.6//)

      5.5  ONCE THE INTEGRATION CONSTANTS ARE KNOWN, THE
           GENERAL SOLUTIONS ARE OBTAINED.

      WRITE(3,8)
    8 FORMAT(/5X'##### THE GENERAL SOLUTIONS #####'//)
      DO 600 I=1,N
      B(I)=BP(I)+A1*BH1(I)+A2*BH2(I)+A3*BH3(I)
  600 D(I)=DP(I)+A1*DH1(I)+A2*DH2(I)+A3*DH3(I)
      DO 700 I=1,N,5
  700 WRITE(3,9) I,B(I),I,D(I)
    9 FORMAT(5X'B(',I3')='D14.6,5X'D(',I3')='D14.6)

      5.6  THE ESTIMATED PARAMETERS K1, K2, AND K3 ARE OBTAINED.

      G1=A1+A2+B2*A3
      G2=A2
      G3=B3*A1+A3
```

```
      WRITE(3,10) G1,G2,G3
   10 FORMAT(//5X'***** THE ESTIMATED PARAMETERS ARE OBTAINED *****'///
     110X'K1='D14.6,10X'K2='D14.6,10X'K3='D14.6///)

      5.7  REPEAT THE ITERATIVE PROCEDURE UNTIL THE PROCESS
           CONVERGES AND THE DESIRED VALUES ARE OBTAINED.

      G1N=G1
      G2N=G2
      G3N=G3
      DO 800 I=1,N
      BN(I)=B(I)
  800 DN(I)=D(I)
      L=L+1
      IF(L .LE. NO) GO TO 555

      QUASILINEARIZATION LOOP ENDS HERE.

 1000 CONTINUE
      STOP
      END
```

```
      SUBROUTINE RUGKU1(B,D,G1,G2,G3,A,R,DT,N)

      RUNGE-KUTTA INTEGRATION SUBROUTINE FOR SOLVING
      THE CAMP AND DOBBINS DIFFERENTIAL EQUATIONS

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION B(1),D(1)
      NN=N-1
      P1=-(G1+G3)
      DO 10 I=1,NN
      A1=(P1*B(I)+R)*DT
      B1=(G1*B(I)-G2*D(I)-A)*DT
      A2=(P1*(B(I)+A1/2.)+R)*DT
      B2=(G1*(B(I)+A1/2.)-G2*(D(I)+B1/2.)-A)*DT
      A3=(P1*(B(I)+A2/2.)+R)*DT
      B3=(G1*(B(I)+A2/2.)-G2*(D(I)+B2/2.)-A)*DT
      A4=(P1*(B(I)+A3)+R)*DT
      B4=(G1*(B(I)+A3)-G2*(D(I)+B3)-A)*DT
      B(I+1)=B(I)+(A1+2.*A2+2.*A3+A4)/6.
      D(I+1)=D(I)+(B1+2.*B2+2.*B3+B4)/6.
   10 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE RANDU(IX,IY,YFL)

      SUBROUTINE COMPUTES UNIFORMLY DISTRIBUTED RANDOM REAL NUMBERS
      BETWEEN 0 AND 1.0, AND RANDOM INTEGERS BETWEEN 0 AND 2**31.

      IMPLICIT REAL*8(A-H,O-Z)
      IY=IX*65539
      IF(IY .GE. 0) GO TO 10
      IY=IY+2147483647+1
   10 YFL=IY
      YFL=YFL*.4656613D-9
      RETURN
      END
```

```
      SUBROUTINE RUGKU2(B,D,G1,G2,G3,DT,N)

      RUNGE-KUTTA INTEGRATION SUBROUTINE FOR SOLVING
      THE PARTICULAR AND HOMOGENEOUS SETS OF SOLUTIONS

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION B(1),D(1),BN(101),DN(101)
      COMMON G1N,G2N,G3N,A,R,BN,DN,K
      NN=N-1
      P1=-(G1N+G3N)
      DO 10 I=1,NN
      P2=-BN(I)*(G1+G3)
      P3=BN(I)*G1-DN(I)*G2
      IF(K .NE. 1) GO TO 20
      P4=-P1*BN(I)+R
      P5=-G1N*BN(I)+G2N*DN(I)-A
      GO TO 30
   20 P4=0.
      P5=0.
   30 A1=(P1*B(I)+P2+P4)*DT
      B1=(G1N*B(I)-G2N*D(I)+P3+P5)*DT
      A2=(P1*(B(I)+A1/2.)+P2+P4)*DT
      B2=(G1N*(B(I)+A1/2.)-G2N*(D(I)+B1/2.)+P3+P5)*DT
      A3=(P1*(B(I)+A2/2.)+P2+P4)*DT
      B3=(G1N*(B(I)+A2/2.)-G2N*(D(I)+B2/2.)+P3+P5)*DT
      A4=(P1*(B(I)+A3)+P2+P4)*DT
      B4=(G1N*(B(I)+A3)-G2N*(D(I)+B3)+P3+P5)*DT
      B(I+1)=B(I)+(A1+2.*A2+2.*A3+A4)/6.
      D(I+1)=D(I)+(B1+2.*B2+2.*B3+B4)/6.
   10 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE GJRM(Q,BB,X,MN)

      SUBROUTINE FOR SOLVING SUSTEM OF ALGEBRAIC EQUATIONS BY THE
      GAUSS-JORDAN REDUCTION METHOD

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION P(4,4),Q(1,1),T(4,4),U(4,4),X(1),BB(1)
      DO 400 I=1,MN
      DO 400 J=1,MN
      IF(I-J)410,420,410
  410 P(I,J)=0.
      GO TO 400
  420 P(I,J)=1.
  400 CONTINUE
      DO 500 K=1,MN
      IF(Q(K,K))510,520,510
  520 IF(K-MN)530,540,530
  530 NI=K+1
      DO 600 I=NI,MN
      IF(Q(I,K))610,600,610
  600 CONTINUE
  540 WRITE(3,120)
  120 FORMAT(30X15(1H*),' NO SOLUTION ',15(1H*))
      GO TO 2000
  610 DO 700 J=1,MN
      U(K,J)=Q(K,J)
      Q(K,J)=Q(I,J)
      Q(I,J)=U(K,J)
      T(K,J)=P(K,J)
      P(K,J)=P(I,J)
      P(I,J)=T(K,J)
  700 CONTINUE
  510 IF(Q(K,K)-1.)710,720,710
  710 QQ=Q(K,K)
      DO 800 J=1,MN
      Q(K,J)=Q(K,J)/QQ
  800 P(K,J)=P(K,J)/QQ
  720 DO 500 I=1,MN
      IF(I-K)910,500,910
  910 IF(Q(I,K))920,500,920
  920 PP=Q(I,K)
      DO 1000 J=1,MN
      Q(I,J)=Q(I,J)-PP*Q(K,J)
 1000 P(I,J)=P(I,J)-PP*P(K,J)
  500 CONTINUE
      DO 1100 I=1,MN
      X(I)=0.
      DO 1100 J=1,MN
 1100 X(I)=X(I)+P(I,J)*BB(J)
 2000 RETURN
      END
```

APPENDIX 2.

COMPUTER PROGRAM FOR THE PROBLEM OF SIMULTANEOUS ESTIMATION OF STATE AND TWO PARAMETERS BY INVARIANT IMBEDDING

```
*****************************************************************

DYNAMIC MODELING OF STREAM QUALITY BY INVARIANT IMBEDDING--
SIMULTANEOUS ESTIMATION OF STATE AND TWO PARAMETERS.

THE CAMP-DOBBINS STREAM QUALITY MODEL

DB/DT=-(K1+K3)*B+R
DD/DT=K1*B-K2*D-A

NOTATION

B      BOD CONCENTRATION
D      DISSOLVED OXYGEN DEFICIT
A      OXYGEN PRODUCTION OR REDUCTION DUE TO PLANTS AND BOTTOM
       DEPOSITS
R      BOD ADDITION RATE
K1     DEOXYGENATION RATE CONSTANT
K2     REAERATION RATE CONSTANT
K3     SEDIMENTATION AND ABSORPTION RATE CONSTANT

THIS PROBLEM IS TO ESTIMATE THE STATE B, D, AND THE
RATE CONSTANTS K1, K2 SIMULTANEOUSLY BASED UPON THE
ABOVE CAMP-DOBBINS STREAM QUALITY MODEL.

THIS PROGRAM WAS WRITTEN BY IRVING K. HWANG, DEPARTMENT OF
INDUSTRIAL ENGINEERING, KANSAS STATE UNIVERSITY, MANHATTAN,
KANSAS, FEB. 1970.

*****************************************************************

NOTE:  DOUBLE PRECISION IS USED IN THIS PROGRAM.

THE MAIN PROGRAM.

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION B(101),D(101),BZ(101),DZ(101),E1(101),E2(101),
1E3(101),E4(101),Q11(101),Q12(101),Q13(101),Q14(101),
2Q21(101),Q22(101),Q23(101),Q24(101),Q31(101),Q32(101),
3Q33(101),Q34(101),Q41(101),Q42(101),Q43(101),Q44(101)

1.  PRINT OUT THE PROGRAM TITLE.

WRITE(3,1)
1 FORMAT(//5X,'DYNAMIC MODELING OF STREAM QUALITY BY',
 1' INVARIANT IMBEDDING-'//3X,'SIMULTANEOUS ESTIMATION OF',
 2' STATE B, D, AND PARAMETERS K1, K2'//)

2.  READ IN AND PRINT OUT DATA.
```

```
      READ (1,30) M
   30 FORMAT(I3)
      WRITE(3,12) M
   12 FORMAT(//'  NO. OF DATA SETS:  M='I3)
      K=1
      READ (1,10) G1,G2,G3,A,R,DEL,C1,C2,AM,S1,S2,N
   10 FORMAT(11F5.2,I4)
      WRITE(3,3) G1,G2,G3,A,R,DEL,C1,C2,AM,S1,S2,N
    3 FORMAT(/5X,'  G1='F5.2,'  G2='F5.2,'  G3='F5.2,'   A='F5.2,'   R='
     1F5.2,' DEL='F5.2//5X,'  C1='F5.2,'  C2='F5.2,'  AM='F5.2,'  S1='
     2F5.2,'  S2='F5.2,'   N='I5)
 1000 WRITE(3,2) K
    2 FORMAT(//5X,5(1H*),'DATA SET NO.',I3,5(1H*)//)
      READ(1,20) A1,A2,A3,A4,A5,A6,A7
   20 FORMAT(F5.1,6F5.2)
      WRITE(3,4) A1,A2,A3,A4,A5,A6,A7
    4 FORMAT(/5X,'  A1='F5.1,'  A2='F5.2,'  A3='F5.2,'  A4='F5.2,'  A5='
     1F5.2,'  A6='F5.2,'  A7='F5.2/)
      IF(K .GE. 2) GO TO 2000

      3. SOLVE THE CAMP-DOBBINS DIFFERENTIAL EQUATIONS.

      WRITE(3,5)
    5 FORMAT(/4X1HI,6X'B(I)',10X'D(I)',9X'BZ(I)',9X'DZ(I)')
      WRITE(3,6)
    6 FORMAT(61(1H*))
      B(1)=C1
      D(1)=C2
      CALL RUKUT1(B,D,G1,G2,G3,A,R,DEL,N)

      4.  CORRUPT THE CAMP-DOBBINS SOLUTION WITH GAUSSIAN
          DISTRIBUTED RANDOM NOISE AND USE THE RESULTS AS THE
          EXPERIMENTAL DATA.

      I1=1
      IX=53471
      S=S1
  400 DO 100 I=1,N
      AA=0.0
      DO 200 II=1,12
      CALL RANDU(IX,IY,YFL)
      PX=IY
      AA=AA+YFL
  200 IX=PX
      V=(AA-6.0)*S+AM
      IF(I1 .GT. 1) GO TO 300
      BZ(I)=B(I)+V
      GO TO 100
  300 DZ(I)=D(I)+V
  100 CONTINUE
```

```
      IF(I1 .GE. 2) GO TO 500
      IX=31353
      S=S2
      I1=I1+1
      GO TO 400
  500 DO 600 I=1,N
  600 WRITE(3,7) I,B(I),D(I),BZ(I),DZ(I)
    7 FORMAT(I5,4(D14.6))
      WRITE(3,6)

      5.  SOLVE THE SEQUENTIAL OPTIMAL DIFFERENTIAL ESTIMATOR
          EQUATIONS.

 2000 WRITE(3,8)
    8 FORMAT(//4X1HI,6X'E1-B',10X'E2-D',9X'E3-K1',9X'E4-K2')
      WRITE(3,9)
    9 FORMAT(61(1H*))

      5.1  ASSUME INITIAL VALUES FOR THE ESTIMATOR EQUATIONS.

      E1(1)=A2
      E2(1)=A3
      E3(1)=A5
      E4(1)=A6
      Q11(1)=A1
      Q12(1)=A4
      Q13(1)=A4
      Q14(1)=A4
      Q21(1)=A4
      Q22(1)=A1
      Q23(1)=A4
      Q24(1)=A4
      Q31(1)=A4
      Q32(1)=A4
      Q33(1)=A1
      Q34(1)=A4
      Q41(1)=A4
      Q42(1)=A4
      Q43(1)=A4
      Q44(1)=A1

      5.2  CALL THE RUNGE-KUTTA INTEGRATION SUBROUTINE(RUKUT2)
           TO SOLVE THE ESTIMATOR EQUATIONS.

      CALL RUKUT2(E1,E2,E3,E4,Q11,Q12,Q13,Q14,Q21,Q22,Q23,Q24,Q31,Q32,
     1Q33,Q34,Q41,Q42,Q43,Q44,BZ,DZ,A,R,G3,DEL,N)

      6.  PRINT OUT THE OPTIMAL ESTIMATES OF THE STATE AND
          THE PARAMETERS.
```

```
      DO 700 I=1,N
  700 WRITE(3,11) I,E1(I),E2(I),E3(I),E4(I)
   11 FORMAT(I5,4(D14.6))
      WRITE(3,9)

      7.  PRINT OUT THE OPTIMAL ESTIMATES OF THE WEIGHTING
          FUNCTIONS.

      WRITE(3,13)
   13 FORMAT(//4X1HI,7X'Q11',11X'Q12',11X'Q13',11X'Q14',11X'Q21',11X
     1'Q22',11X'Q23',11X'Q24')
      WRITE(3,14)
   14 FORMAT(1X,116(1H*))
      DO 800 I=1,N,5
  800 WRITE(3,15) I,Q11(I),Q12(I),Q13(I),Q14(I),Q21(I),Q22(I),Q23(I),
     1Q24(I)
   15 FORMAT(I5,8(D14.6))
      WRITE(3,14)
      WRITE(3,16)
   16 FORMAT(//4X1HI,7X'Q31',11X'Q32',11X'Q33',11X'Q34',11X'Q41',11X
     1'Q42',11X'Q43',11X'Q44')
      WRITE(3,14)
      DO 900 I=1,N,5
  900 WRITE(3,15) I,Q31(I),Q32(I),Q33(I),Q34(I),Q41(I),Q42(I),Q43(I),
     1Q44(I)
      WRITE(3,14)
      K=K+1
      IF(K .LE. M) GO TO 1000
      STOP
      END
```

```
      SUBROUTINE RUKUT1(B,D,G1,G2,G3,A,R,DEL,N)

      RUNGE-KUTTA INTEGRATION SUBROUTINE FOR SOLVING THE
      CAMP AND DOBBINS DIFFERENTIAL EQUATIONS

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION B(1),D(1)
      NN=N-1
      DO 10 I=1,NN
      A1=(-(G1+G3)*B(I)+R)*DEL
      B1=(G1*B(I)-G2*D(I)-A)*DEL
      A2=(-(G1+G3)*(B(I)+A1/2.)+R)*DEL
      B2=(G1*(B(I)+A1/2.)-G2*(D(I)+B1/2.)-A)*DEL
      A3=(-(G1+G3)*(B(I)+A2/2.)+R)*DEL
      B3=(G1*(B(I)+A2/2.)-G2*(D(I)+B2/2.)-A)*DEL
      A4=(-(G1+G3)*(B(I)+A3)+R)*DEL
      B4=(G1*(B(I)+A3)-G2*(D(I)+B3)-A)*DEL
      B(I+1)=B(I)+(A1+2.*A2+2.*A3+A4)/6.
      D(I+1)=D(I)+(B1+2.*B2+2.*B3+B4)/6.
   10 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE RANDU(IX,IY,YFL)

      SUBROUTINE COMPUTES UNIFORMLY DISTRIBUTED RANDOM REAL NUMBERS
      BETWEEN 0 AND 1.0 AND RANDOM INTEGERS BETWEEN 0 AND 2**31.

      IMPLICIT REAL*8(A-H,O-Z)
      IY=IX*65539
      IF(IY .GE. 0) GO TO 10
      IY=IY+2147483647+1
   10 YFL=IY
      YFL=YFL*.4656613D-9
      RETURN
      END
```

```
 SUBROUTINE RUKUT2(E1,E2,E3,E4,Q11,Q12,Q13,Q14,Q21,Q22,Q23,Q24,Q31,
1Q32,Q33,Q34,Q41,Q42,Q43,Q44,BZ,DZ,A,R,G3,DEL,N)

 RUNGE-KUTTA INTEGRATION SUBROUTINE FOR SOLVING THE SIMULTANEOUS
 DIFFERENTIAL ESTIMATOR EQUATIONS

 IMPLICIT REAL*8(A-H,O-Z)
 DIMENSION E1(1),E2(1),E3(1),E4(1),Q11(1),Q12(1),Q13(1),Q14(1),
1Q21(1),Q22(1),Q23(1),Q24(1),Q31(1),Q32(1),Q33(1),Q34(1),Q41(1),
2Q42(1),Q43(1),Q44(1),BZ(1),DZ(1)
 NN=N-1
 DO 10 I=1,NN
 A1=(-(E3(I)+G3)*E1(I)+R+Q11(I)*(BZ(I)-E1(I))+Q12(I)*(DZ(I)-E2(I)))
1*DEL
 B1=(E3(I)*E1(I)-E4(I)*E2(I)-A+Q21(I)*(BZ(I)-E1(I))+Q22(I)*(DZ(I)-
1E2(I)))*DEL
 C1=(Q31(I)*(BZ(I)-E1(I))+Q32(I)*(DZ(I)-E2(I)))*DEL
 D1=(Q41(I)*(BZ(I)-E1(I))+Q42(I)*(DZ(I)-E2(I)))*DEL
 F1=(-2.*Q11(I)*(E3(I)+G3)-(Q31(I)+Q13(I))*E1(I)-Q11(I)**2-Q12(I)*
1Q21(I))*DEL
 H1=(-Q12(I)*(E3(I)+G3)+Q11(I)*E3(I)-(Q32(I)-Q13(I))*E1(I)-Q12(I)*
1E4(I)-Q14(I)*E2(I)-Q11(I)*Q12(I)-Q12(I)*Q22(I))*DEL
 O1=(-Q13(I)*(E3(I)+G3)-Q33(I)*E1(I)-Q11(I)*Q13(I)-Q12(I)*Q23(I))*
1DEL
 P1=(-Q14(I)*(E3(I)+G3)-Q34(I)*E1(I)-Q11(I)*Q14(I)-Q12(I)*Q24(I))*
1DEL
 Q1=((Q31(I)-Q23(I))*E1(I)-Q21(I)*E4(I)-Q21(I)*(E3(I)+G3)+Q11(I)*E3
1(I)-Q41(I)*E2(I)-Q21(I)*Q11(I)-Q22(I)*Q21(I))*DEL
 R1=((Q12(I)+Q21(I))*E3(I)+(Q32(I)+Q23(I))*E1(I)-2.*Q22(I)*E4(I)-
1(Q42(I)+Q24(I))*E2(I)-Q21(I)*Q12(I)-Q22(I)**2)*DEL
 S1=(Q13(I)*E3(I)+Q33(I)*E1(I)-Q23(I)*E4(I)-Q43(I)*E2(I)-Q21(I)*Q13
1(I)-Q22(I)*Q23(I))*DEL
 T1=(Q14(I)*E3(I)+Q34(I)*E1(I)-Q24(I)*E4(I)-Q44(I)*E2(I)-Q21(I)*
1Q14(I)-Q22(I)*Q24(I))*DEL
 U1=(-Q31(I)*(E3(I)+G3)-Q33(I)*E1(I)-Q31(I)*Q11(I)-Q32(I)*Q21(I))*
1DEL
 V1=(Q31(I)*E3(I)+Q33(I)*E1(I)-Q32(I)*E4(I)-Q34(I)*E2(I)-Q31(I)*
1Q12(I)-Q32(I)*Q22(I))*DEL
 W1=(-Q31(I)*Q13(I)-Q32(I)*Q23(I))*DEL
 X1=(-Q31(I)*Q14(I)-Q32(I)*Q24(I))*DEL
 Y1=(-Q41(I)*(E3(I)+G3)-Q43(I)*E1(I)-Q41(I)*Q11(I)-Q42(I)*Q21(I))*
1DEL
 Z1=(Q41(I)*E3(I)+Q43(I)*E1(I)-Q42(I)*E4(I)-Q44(I)*E2(I)-Q41(I)*
1Q12(I)-Q42(I)*Q22(I))*DEL
 AA1=(-Q41(I)*Q13(I)-Q42(I)*Q23(I))*DEL
 BB1=(-Q41(I)*Q14(I)-Q42(I)*Q24(I))*DEL
 A2=(-((E3(I)+C1/2.)+G3)*(E1(I)+A1/2.)+R+(Q11(I)+F1/2.)*(BZ(I)-(
1E1(I)+A1/2.))+(Q12(I)+H1/2.)*(DZ(I)-(E2(I)+B1/2.)))*DEL
 B2=((E3(I)+C1/2.)*(E1(I)+A1/2.)-(E4(I)+D1/2.)*(E2(I)+B1/2.)-A+(
1Q21(I)+Q1/2.)*(BZ(I)-(E1(I)+A1/2.))+(Q22(I)+R1/2.)*(DZ(I)-(E2(I)+
```

```
2B1/2.)))*DEL
 C2=((Q31(I)+U1/2.)*(BZ(I)-(E1(I)+A1/2.))+(Q32(I)+V1/2.)*(DZ(I)-(
1E2(I)+B1/2.)))*DEL
 D2=((Q41(I)+Y1/2.)*(BZ(I)-(E1(I)+A1/2.))+(Q42(I)+Z1/2.)*(DZ(I)-(
1E2(I)+B1/2.)))*DEL
 F2=(-2.*(Q11(I)+F1/2.)*((E3(I)+C1/2.)+G3)-((Q31(I)+U1/2.)+(Q13(I)+
1O1/2.))*(E1(I)+A1/2.)-(Q11(I)+F1/2.)**2-(Q12(I)+H1/2.)*(Q21(I)+Q1/
22.))*DEL
 H2=(-(Q12(I)+H1/2.)*((E3(I)+C1/2.)+G3)+(Q11(I)+F1/2.)*(E3(I)+C1/2.
1)-((Q32(I)+V1/2.)-(Q13(I)+O1/2.))*(E1(I)+A1/2.)-(Q12(I)+H1/2.)*(
2E4(I)+D1/2.)-(Q14(I)+P1/2.)*(E2(I)+B1/2.)-(Q11(I)+F1/2.)*(Q12(I)+
3H1/2.)-(Q12(I)+H1/2.)*(Q22(I)+R1/2.))*DEL
 O2=(-(Q13(I)+O1/2.)*((E3(I)+C1/2.)+G3)-(Q33(I)+W1/2.)*(E1(I)+A1/2.
1)-(Q11(I)+F1/2.)*(Q13(I)+O1/2.)-(Q12(I)+H1/2.)*(Q23(I)+S1/2.))*DEL
 P2=(-(Q14(I)+P1/2.)*((E3(I)+C1/2.)+G3)-(Q34(I)+X1/2.)*(E1(I)+A1/2.
1)-(Q11(I)+F1/2.)*(Q14(I)+P1/2.)-(Q12(I)+H1/2.)*(Q24(I)+T1/2.))*DEL
 Q2=(((Q31(I)+U1/2.)-(Q23(I)+S1/2.))*(E1(I)+A1/2.)-(Q21(I)+Q1/2.)*
1(E4(I)+D1/2.)-(Q21(I)+Q1/2.)*((E3(I)+C1/2.)+G3)+(Q11(I)+F1/2.)*(
2E3(I)+C1/2.)-(Q41(I)+Y1/2.)*(E2(I)+B1/2.)-(Q21(I)+Q1/2.)*(Q11(I)+
3F1/2.)-(Q22(I)+R1/2.)*(Q21(I)+Q1/2.))*DEL
 R2=(((Q12(I)+H1/2.)+(Q21(I)+Q1/2.))*(E3(I)+C1/2.)+((Q32(I)+V1/2.)+
1(Q23(I)+S1/2.))*(E1(I)+A1/2.)-2.*(Q22(I)+R1/2.)*(E4(I)+D1/2.)-
2((Q42(I)+Z1/2.)+(Q24(I)+T1/2.))*(E2(I)+B1/2.)-(Q21(I)+Q1/2.)*(
3Q12(I)+H1/2.)-(Q22(I)+R1/2.)**2)*DEL
 S2=((Q13(I)+O1/2.)*(E3(I)+C1/2.)+(Q33(I)+W1/2.)*(E1(I)+A1/2.)-(
1Q23(I)+S1/2.)*(E4(I)+D1/2.)-(Q43(I)+AA1/2.)*(E2(I)+B1/2.)-(Q21(I)+
2Q1/2.)*(Q13(I)+O1/2.)-(Q22(I)+R1/2.)*(Q23(I)+S1/2.))*DEL
 T2=((Q14(I)+P1/2.)*(E3(I)+C1/2.)+(Q34(I)+X1/2.)*(E1(I)+A1/2.)-(
1Q24(I)+T1/2.)*(E4(I)+D1/2.)-(Q44(I)+BB1/2.)*(E2(I)+B1/2.)-(Q21(I)+
1Q1/2.)*(Q14(I)+P1/2.)-(Q22(I)+R1/2.)*(Q24(I)+T1/2.))*DEL
 U2=(-(Q31(I)+U1/2.)*((E3(I)+C1/2.)+G3)-(Q33(I)+W1/2.)*(E1(I)+A1/2.
1)-(Q31(I)+U1/2.)*(Q11(I)+F1/2.)-(Q32(I)+V1/2.)*(Q21(I)+Q1/2.))*DEL
 V2=((Q31(I)+U1/2.)*(E3(I)+C1/2.)+(Q33(I)+W1/2.)*(E1(I)+A1/2.)-(
1Q32(I)+V1/2.)*(E4(I)+D1/2.)-(Q34(I)+X1/2.)*(E2(I)+B1/2.)-(Q31(I)+
2U1/2.)*(Q12(I)+H1/2.)-(Q32(I)+V1/2.)*(Q22(I)+R1/2.))*DEL
 W2=(-(Q31(I)+U1/2.)*(Q13(I)+O1/2.)-(Q32(I)+V1/2.)*(Q23(I)+S1/2.))*
1DEL
 X2=(-(Q31(I)+U1/2.)*(Q14(I)+P1/2.)-(Q32(I)+V1/2.)*(Q24(I)+T1/2.))*
1DEL
 Y2=(-(Q41(I)+Y1/2.)*((E3(I)+C1/2.)+G3)-(Q43(I)+AA1/2.)*(E1(I)+A1/
12.)-(Q41(I)+Y1/2.)*(Q11(I)+F1/2.)-(Q42(I)+Z1/2.)*(Q21(I)+Q1/2.))*
2DEL
 Z2=((Q41(I)+Y1/2.)*(E3(I)+C1/2.)+(Q43(I)+AA1/2.)*(E1(I)+A1/2.)-(
1Q42(I)+Z1/2.)*(E4(I)+D1/2.)-(Q44(I)+BB1/2.)*(E2(I)+B1/2.)-(Q41(I)+
2Y1/2.)*(Q12(I)+H1/2.)-(Q42(I)+Z1/2.)*(Q22(I)+R1/2.))*DEL
 AA2=(-(Q41(I)+Y1/2.)*(Q13(I)+O1/2.)-(Q42(I)+Z1/2.)*(Q23(I)+S1/2.))
1*DEL
 BB2=(-(Q41(I)+Y1/2.)*(Q14(I)+P1/2.)-(Q42(I)+Z1/2.)*(Q24(I)+T1/2.))
1*DEL
 A3=(-((E3(I)+C2/2.)+G3)*(E1(I)+A2/2.)+R+(Q11(I)+F2/2.)*(BZ(I)-(
```

```
1E1(I)+A2/2.))+(Q12(I)+H2/2.)*(DZ(I)-(E2(I)+B2/2.)))*DEL
 B3=((E3(I)+C2/2.)*(E1(I)+A2/2.)-(E4(I)+D2/2.)*(E2(I)+B2/2.)-A+(
1Q21(I)+Q2/2.)*(BZ(I)-(E1(I)+A2/2.))+(Q22(I)+R2/2.)*(DZ(I)-(E2(I)+
2B2/2.)))*DEL
 C3=((Q31(I)+U2/2.)*(BZ(I)-(E1(I)+A2/2.))+(Q32(I)+V2/2.)*(DZ(I)-(
1E2(I)+B2/2.)))*DEL
 D3=((Q41(I)+Y2/2.)*(BZ(I)-(E1(I)+A2/2.))+(Q42(I)+Z2/2.)*(DZ(I)-(
1E2(I)+B2/2.)))*DEL
 F3=(-2.*(Q11(I)+F2/2.)*((E3(I)+C2/2.)+G3)-((Q31(I)+U2/2.)+(Q13(I)+
1O2/2.))*(E1(I)+A2/2.)-(Q11(I)+F2/2.)**2-(Q12(I)+H2/2.)*(Q21(I)+Q2/
22.))*DEL
 H3=(-(Q12(I)+H2/2.)*((E3(I)+C2/2.)+G3)+(Q11(I)+F2/2.)*(E3(I)+C2/2.
1)-((Q32(I)+V2/2.)-(Q13(I)+O2/2.))*(E1(I)+A2/2.)-(Q12(I)+H2/2.)*(
2E4(I)+D2/2.)-(Q14(I)+P2/2.)*(E2(I)+B2/2.)-(Q11(I)+F2/2.)*(Q12(I)+
3H2/2.)-(Q12(I)+H2/2.)*(Q22(I)+R2/2.))*DEL
 O3=(-(Q13(I)+O2/2.)*((E3(I)+C2/2.)+G3)-(Q33(I)+W2/2.)*(E1(I)+A2/2.
1)-(Q11(I)+F2/2.)*(Q13(I)+O2/2.)-(Q12(I)+H2/2.)*(Q23(I)+S2/2.))*DEL
 P3=(-(Q14(I)+P2/2.)*((E3(I)+C2/2.)+G3)-(Q34(I)+X2/2.)*(E1(I)+A2/2.
1)-(Q11(I)+F2/2.)*(Q14(I)+P2/2.)-(Q12(I)+H2/2.)*(Q24(I)+T2/2.))*DEL
 Q3=(((Q31(I)+U2/2.)-(Q23(I)+S2/2.))*(E1(I)+A2/2.)-(Q21(I)+Q2/2.)*
1(E4(I)+D2/2.)-(Q21(I)+Q2/2.)*((E3(I)+C2/2.)+G3)+(Q11(I)+F2/2.)*(
2E3(I)+C2/2.)-(Q41(I)+Y2/2.)*(E2(I)+B2/2.)-(Q21(I)+Q2/2.)*(Q11(I)+
3F2/2.)-(Q22(I)+R2/2.)*(Q21(I)+Q2/2.))*DEL
 R3=(((Q12(I)+H2/2.)+(Q21(I)+Q2/2.))*(E3(I)+C2/2.)+((Q32(I)+V2/2.)+
1(Q23(I)+S2/2.))*(E1(I)+A2/2.)-2.*(Q22(I)+R2/2.)*(E4(I)+D2/2.)-
2((Q42(I)+Z2/2.)+(Q24(I)+T2/2.))*(E2(I)+B2/2.)-(Q21(I)+Q2/2.)*(
3Q12(I)+H2/2.)-(Q22(I)+R2/2.)**2)*DEL
 S3=((Q13(I)+O2/2.)*(E3(I)+C2/2.)+(Q33(I)+W2/2.)*(E1(I)+A2/2.)-(
1Q23(I)+S2/2.)*(E4(I)+D2/2.)-(Q43(I)+AA2/2.)*(E2(I)+B2/2.)-(Q21(I)+
2Q2/2.)*(Q13(I)+O2/2.)-(Q22(I)+R2/2.)*(Q23(I)+S2/2.))*DEL
 T3=((Q14(I)+P2/2.)*(E3(I)+C2/2.)+(Q34(I)+X2/2.)*(E1(I)+A2/2.)-(
1Q24(I)+T2/2.)*(E4(I)+D2/2.)-(Q44(I)+BB2/2.)*(E2(I)+B2/2.)-(Q21(I)+
1Q2/2.)*(Q14(I)+P2/2.)-(Q22(I)+R2/2.)*(Q24(I)+T2/2.))*DEL
 U3=(-(Q31(I)+U2/2.)*((E3(I)+C2/2.)+G3)-(Q33(I)+W2/2.)*(E1(I)+A2/2.
1)-(Q31(I)+U2/2.)*(Q11(I)+F2/2.)-(Q32(I)+V2/2.)*(Q21(I)+Q2/2.))*DEL
 V3=((Q31(I)+U2/2.)*(E3(I)+C2/2.)+(Q33(I)+W2/2.)*(E1(I)+A2/2.)-(
1Q32(I)+V2/2.)*(E4(I)+D2/2.)-(Q34(I)+X2/2.)*(E2(I)+B2/2.)-(Q31(I)+
2U2/2.)*(Q12(I)+H2/2.)-(Q32(I)+V2/2.)*(Q22(I)+R2/2.))*DEL
 W3=(-(Q31(I)+U2/2.)*(Q13(I)+O2/2.)-(Q32(I)+V2/2.)*(Q23(I)+S2/2.))*
1DEL
 X3=(-(Q31(I)+U2/2.)*(Q14(I)+P2/2.)-(Q32(I)+V2/2.)*(Q24(I)+T2/2.))*
1DEL
 Y3=(-(Q41(I)+Y2/2.)*((E3(I)+C2/2.)+G3)-(Q43(I)+AA2/2.)*(E1(I)+A2/
12.)-(Q41(I)+Y2/2.)*(Q11(I)+F2/2.)-(Q42(I)+Z2/2.)*(Q21(I)+Q2/2.))*
2DEL
 Z3=((Q41(I)+Y2/2.)*(E3(I)+C2/2.)+(Q43(I)+AA2/2.)*(E1(I)+A2/2.)-(
1Q42(I)+Z2/2.)*(E4(I)+D2/2.)-(Q44(I)+BB2/2.)*(E2(I)+B2/2.)-(Q41(I)+
2Y2/2.)*(Q12(I)+H2/2.)-(Q42(I)+Z2/2.)*(Q22(I)+R2/2.))*DEL
 AA3=(-(Q41(I)+Y2/2.)*(Q13(I)+O2/2.)-(Q42(I)+Z2/2.)*(Q23(I)+S2/2.))
1*DEL
```

```
 BB3=(-(Q41(I)+Y2/2.)*(Q14(I)+P2/2.)-(Q42(I)+Z2/2.)*(Q24(I)+T2/2.))
1*DEL
 A4=(-((E3(I)+C3)+G3)*(E1(I)+A3)+R+(Q11(I)+F3)*(BZ(I)-(E1(I)+A3))+(
1Q12(I)+H3)*(DZ(I)-(E2(I)+B3)))*DEL
 B4=((E3(I)+C3)*(E1(I)+A3)-(E4(I)+D3)*(E2(I)+B2)-A+(Q21(I)+Q3)*(
1BZ(I)-(E1(I)+A3))+(Q22(I)+R3)*(DZ(I)-(E2(I)+B3)))*DEL
 C4=((Q31(I)+U3)*(BZ(I)-(E1(I)+A3))+(Q32(I)+V3)*(DZ(I)-(E2(I)+B3)))
1*DEL
 D4=((Q41(I)+Y3)*(BZ(I)-(E1(I)+A3))+(Q42(I)+Z3)*(DZ(I)-(E2(I)+B3)))
1*DEL
 F4=(-2.*(Q11(I)+F3)*((E3(I)+C3)+G3)-((Q31(I)+U3)+(Q13(I)+O3))*(
1E1(I)+A3)-(Q11(I)+F3)**2-(Q12(I)+H3)*(Q21(I)+Q3))*DEL
 H4=(-(Q12(I)+H3)*((E3(I)+C3)+G3)+(Q11(I)+F3)*(E3(I)+C3)-((Q32(I)+
1V3)-(Q13(I)+O3))*(E1(I)+A3)-(Q12(I)+H3)*(E4(I)+D3)-(Q14(I)+P3)*(
2E2(I)+B3)-(Q11(I)+F3)*(Q12(I)+H3)-(Q12(I)+H3)*(Q22(I)+R3))*DEL
 O4=(-(Q13(I)+O3)+((E3(I)+C3)+G3)-(Q33(I)+W3)*(E1(I)+A3)-(Q11(I)+F3
1)*(Q13(I)+O3)-(Q12(I)+H3)*(Q23(I)+S3))*DEL
 P4=(-(Q14(I)+P3)*((E3(I)+C3)+G3)-(Q34(I)+X3)*(E1(I)+A3)-(Q11(I)+
1F3)*(Q14(I)+P3)-(Q12(I)+H3)*(Q24(I)+T3))*DEL
 Q4=(((Q31(I)+U3)-(Q23(I)+S3))*(E1(I)+A3)-(Q21(I)+Q3)*(E4(I)+D3)-
1(Q21(I)+Q3)*((E3(I)+C3)+G3)+(Q11(I)+F3)*(E3(I)+C3)-(Q41(I)+Y3)*(
2E2(I)+B3)-(Q21(I)+Q3)*(Q11(I)+F3)-(Q22(I)+R3)*(Q21(I)+Q3))*DEL
 R4=(((Q12(I)+H3)+(Q21(I)+Q3))*(E3(I)+C3)+((Q32(I)+V3)+(Q23(I)+S3))
1*(E1(I)+A3)-2.*(Q22(I)+R3)*(E4(I)+D3)-((Q42(I)+Z3)+(Q24(I)+T3))*(
2E2(I)+B3)-(Q21(I)+Q3)*(Q12(I)+H3)-(Q22(I)+R3)**2)*DEL
 S4=((Q13(I)+O3)*(E3(I)+C3)+(Q33(I)+W3)*(E1(I)+A3)-(Q23(I)+S3)*(
1E4(I)+D3)-(Q43(I)+AA3)*(E2(I)+B3)-(Q21(I)+Q3)*(Q13(I)+O3)-(Q22(I)+
2R3)*(Q23(I)+S3))*DEL
 T4=((Q14(I)+P3)*(E3(I)+C3)+(Q34(I)+X3)*(E1(I)+A3)-(Q24(I)+T3)*(
1E4(I)+D3)-(Q44(I)+BB3)*(E2(I)+B3)-(Q21(I)+Q3)*(Q14(I)+P3)-(Q22(I)+
2R3)*(Q24(I)+T3))*DEL
 U4=(-(Q31(I)+U3)*((E3(I)+C3)+G3)-(Q33(I)+W3)*(E1(I)+A3)-(Q31(I)+U3
1)*(Q11(I)+F3)-(Q32(I)+V3)*(Q21(I)+Q3))*DEL
 V4=((Q31(I)+U3)*(E3(I)+C3)+(Q33(I)+W3)*(E1(I)+A3)-(Q32(I)+V3)*(
1E4(I)+D3)-(Q34(I)+X3)*(E2(I)+B3)-(Q31(I)+U3)*(Q12(I)+H3)-(Q32(I)+
2V3)*(Q22(I)+R3))*DEL
 W4=(-(Q31(I)+U3)*(Q13(I)+O3)-(Q32(I)+V3)*(Q23(I)+S3))*DEL
 X4=(-(Q31(I)+U3)*(Q14(I)+P3)-(Q32(I)+V3)*(Q24(I)+T3))*DEL
 Y4=(-(Q41(I)+Y3)*((E3(I)+C3)+G3)-(Q43(I)+AA3)*(E1(I)+A3)-(Q41(I)+
1Y3)*(Q11(I)+F3)-(Q42(I)+Z3)*(Q21(I)+Q3))*DEL
 Z4=((Q41(I)+Y3)*(E3(I)+C3)+(Q43(I)+AA3)*(E1(I)+A3)-(Q42(I)+Z3)*(
1E4(I)+D3)-(Q44(I)+BB3)*(E2(I)+B3)-(Q41(I)+Y3)*(Q12(I)+H3)-(Q42(I)+
2Z3)*(Q22(I)+R3))*DEL
 AA4=(-(Q41(I)+Y3)*(Q13(I)+O3)-(Q42(I)+Z3)*(Q23(I)+S3))*DEL
 BB4=(-(Q41(I)+Y3)*(Q14(I)+P3)-(Q42(I)+Z3)*(Q24(I)+T3))*DEL
 E1(I+1)=E1(I)+(A1+2.*A2+2.*A3+A4)/6.
 E2(I+1)=E2(I)+(B1+2.*B2+2.*B3+B4)/6.
 E3(I+1)=E3(I)+(C1+2.*C2+2.*C3+C4)/6.
 E4(I+1)=E4(I)+(D1+2.*D2+2.*D3+D4)/6.
 Q11(I+1)=Q11(I)+(F1+2.*F2+2.*F3+F4)/6.
```

```
      Q12(I+1)=Q12(I)+(H1+2.*H2+2.*H3+H4)/6.
      Q13(I+1)=Q13(I)+(O1+2.*O2+2.*O3+O4)/6.
      Q14(I+1)=Q14(I)+(P1+2.*P2+2.*P3+P4)/6.
      Q21(I+1)=Q21(I)+(Q1+2.*Q2+2.*Q3+Q4)/6.
      Q22(I+1)=Q22(I)+(R1+2.*R2+2.*R3+R4)/6.
      Q23(I+1)=Q23(I)+(S1+2.*S2+2.*S3+S4)/6.
      Q24(I+1)=Q24(I)+(T1+2.*T2+2.*T3+T4)/6.
      Q31(I+1)=Q31(I)+(U1+2.*U2+2.*U3+U4)/6.
      Q32(I+1)=Q32(I)+(V1+2.*V2+2.*V3+V4)/6.
      Q33(I+1)=Q33(I)+(W1+2.*W2+2.*W3+W4)/6.
      Q34(I+1)=Q34(I)+(X1+2.*X2+2.*X3+X4)/6.
      Q41(I+1)=Q41(I)+(Y1+2.*Y2+2.*Y3+Y4)/6.
      Q42(I+1)=Q42(I)+(Z1+2.*Z2+2.*Z3+Z4)/6.
      Q43(I+1)=Q43(I)+(AA1+2.*AA2+2.*AA3+AA4)/6.
      Q44(I+1)=Q44(I)+(BB1+2.*BB2+2.*BB3+BB4)/6.
   10 CONTINUE
      RETURN
      END
```

WATER RESOURCES MODELING BY QUASILINEARIZATION AND INVARIANT IMBEDDING

by

IRVING KEAO HWANG

B.S.(Ind. Mgt.), Cheng Kung University
Tainan, Taiwan, China, 1966

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Manhattan, Kansas

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Quasilinearization and invariant imbedding are two useful techniques for obtaining the numerical solutions of nonlinear boundary-value problems. Furthermore, these techniques have been shown to be very effective for solving various estimation problems. The principle advantages of these approaches are that various estimation criteria such as the least squares criterion can be used and the estimation procedures converge rapidly to the desired value.

The purpose of this work is to investigate the effectiveness of these two recently developed numerical tools for solving various estimation problems involved in water resources modeling.

The quasilinearization technique is used to identify or to estimate the parameters in river or stream pollution. By using this technique, the parameters can be estimated directly from the differential equations representing the pollution model and from the measured data such as BOD and DO. Several numerical examples are solved. It is shown that with very approximate initial guesses for the unknown parameters, only three to seven iterations are needed to obtain a four to five digit accuracy. Due to the rapid convergence property of this approach, it appears to be a powerful technique for the dynamic modeling of stream quality problems.

The invariant imbedding approach is also used to estimate these parameters of dynamic stream quality models. In this approach, a sequential estimation scheme is obtained. By the use of this sequential scheme, only current data are needed to estimate the current or future values of the parameters. The classical least squares criterion is used to obtain the optimal estimates. A few examples are solved to illustrate this approach. It is seen that not only the parameters but also the state or the future concentrations of the pollutants are estimated by this approach. Thus, this approach also forms an effective tool for the modeling and adaptive forecasting of stream or estuary quality.