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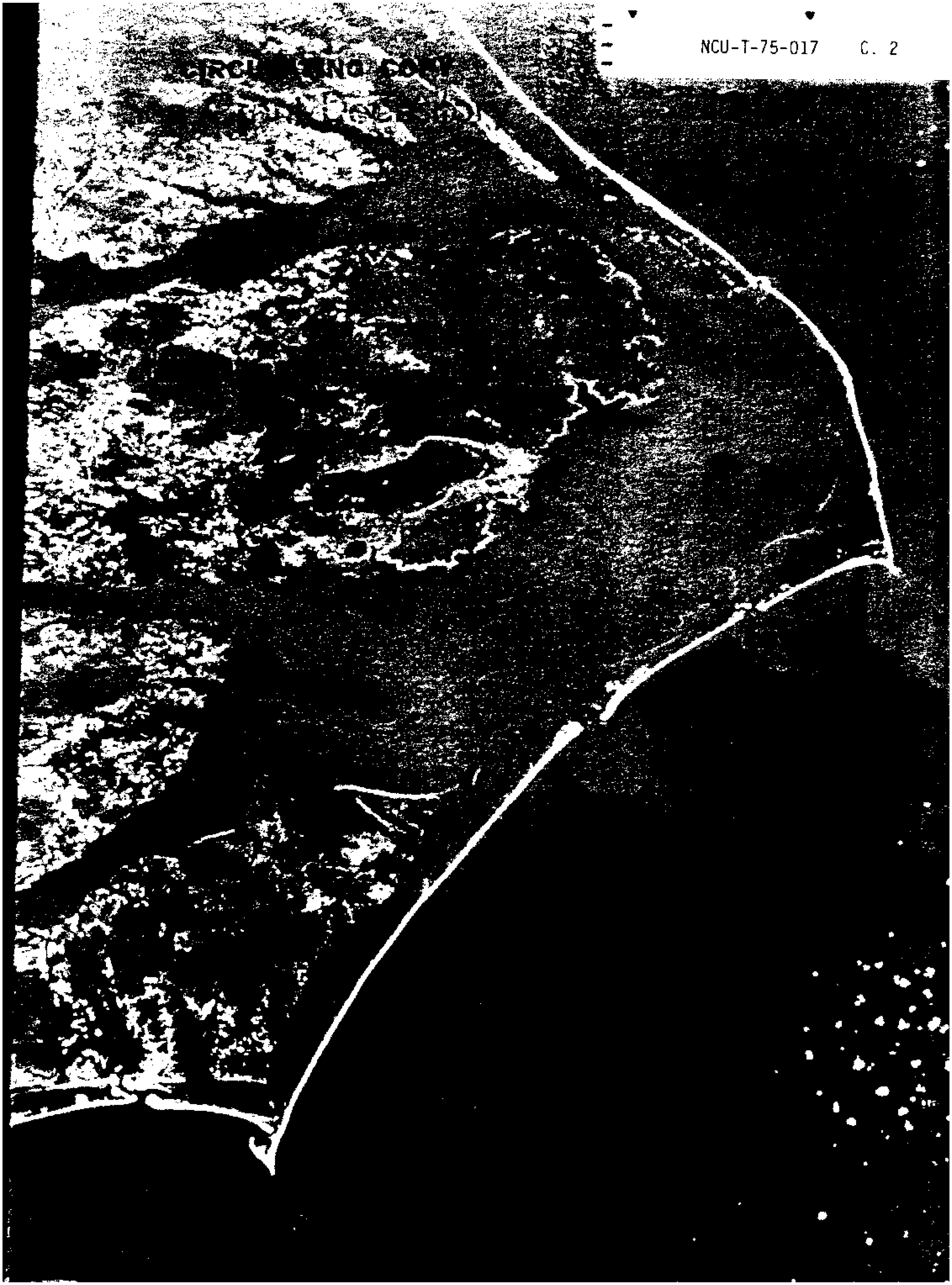

A DYNAMIC WATER QUALITY MODEL FOR THE NEUSE ESTUARY, N. C.

by

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This work was partially supported by Office of Sea Grant, NOAA, U. S. Department of Commerce, under Grant Numbers 2-35178 and 04-3-158-40, and the State of North Carolina, Department of Administration. The U. S. Government is authorized to produce and distribute reprints for governmental purposes notwithstanding any copyright that may appear hereon.

SEA GRANT PUBLICATION UNC-SG-75-28 December, 1975

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CONTENTS

ABSTRACT

The numerical model consists of two parts. The first part employs an implicit method for the solution of the shallow water hydrodynamic equations. The objective of this part of the work is to obtain the values of discharge, velocity and depth in the estuary under the action of fresh-water inflow, surface runoff, winds and tides.

The second part of the model uses an explicit method for the solution of the unsteady mass-balance equation (equation of mass transport). The objective of this part of the work is to obtain values for concentration of materials in the estuary. The process can be steady or unsteady, the material can be conservative or non-conservative.

Applications of the model to the Neuse Estuary are given and the model is tested with field data for ammonia, nitrates and dissolved oxygen.

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I. INTRODUCTION

The Neuse River Estuary is approximately 40 miles long (from New Bern, North Carolina to Pamlico Sound) and the estuary is typical of North Carolina coastal waters. Its depth at the upper portion is 12-14 ft. while in the lower portion the average depth is about 20 ft. Notations on the Coast and Geodetic Survey charts report that the main tidal fluctuation is "less than one half foot" but also points out that there can be a variation in depth as great as four feet at New Bern and as great as two feet at the mouth of the estuary depending on meteorological conditions. Most of the side streams flowing into the estuary contribute little as far as flows are concerned, but may bring considerable wastes to the estuary.

The purposes of this report are: (1) to develop a mathematical numerical model for predicting flow dynamics of an estuary; (2) to develop a mathematical numerical model for predicting interrelated water quality parameters for an estuary; (3) to show the application of the model to the Neuse River, North Carolina, estuary using the available field data; and (4) to identify the type and quantity of data that are needed by the model to provide useful and comprehensive information.

This report contains the application of the model to wind effects and to routing BOD (Biochemical Oxygen Demand), DO (dissolved oxygen), NH_3, NO_2-N and NO_3-N, Algal Nitrogen and organic nitrogen through an estuary system. The model is based on the use of the equations of unsteady flow coupled with the equation of mass transport. The model operates in two stages and employs a different solution technique in each stage for greater efficiency. In the first stage, the flow equations are solved implicitly (Amein and Fang, 1970; Amein and Chu, 1975) to find the values of the velocity, discharge, depth and area. In the second stage, the equation for mass transport is solved explicitly to obtain values for the water quality parameters. The values of the variables determined in the first stage are used as input data for computations in the second stage. The equations of unsteady flow contain a term for the wind stress because of the important role played by wind in estuary dynamics.

II. BASIC EQUATIONS

II. A. Equations of Unsteady Flow

The basic equations describing the movement of water in an estuary are the well-known one-dimensional equations of unsteady flow in open channels. They consist of the equations for the conservation of mass and momentum. The equations are:

$$\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} - q = 0 \qquad (1)$$

$$\frac{\partial Q}{\partial x} + \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) = gAS_o - gAS_f - gA\frac{\partial y}{\partial x} + \frac{\tau_x}{\rho}B \qquad (2)$$

where

- Q = volume flow rate
- A = cross sectional area
- q = lateral inflow rate
- S_o = channel bottom slope
- S_f = friction slope
- y = water depth
- g = acceleration due to gravity
- x = distance along the channel
- t = time
- τ_x = wind stress along the channel
- ρ = density of water
- B = channel top width

Equation (1) is the equation for the conservation of mass (equation of continuity) and equation (2) is the equation for conservation of momentum. The equations are commonly known as the St. Venant equations and as the shallow water equations. Their derivation is given in standard reference works (Chow, 1959; Dronkers, 1964; Henderson, 1966; Stoker, 1957). It should be noted that the equations used in this report include a term for shear stress due to the wind in addition to the shear stress due to the bottom friction. The wind stress is commonly ignored in river problems; however, it plays a prominent role in estuaries.

II. B. Equation for Mass Transport

The basic equation describing the mass transport of conservative and non-conservative constituents can be written for a stream or canal system as

$$\frac{1}{A}\frac{\partial}{\partial t}(AL) = -\frac{1}{A}\frac{\partial}{\partial x}(QL) + \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{\partial L}{\partial x}\right) + \text{source} + \text{sink} \qquad (3)$$

where

A = cross-sectional area

Q = flow rate

L = concentration of a given substance

E = Longitudinal dispersion coefficient

x = distance along the channel

t = time

Equation (3) is the general form of the one-dimensional mass transfer for non-conservative substance. It is assumed to be valid for unsteady, nonuniform flows within the restriction of the one-dimensional approximation. Its derivation is given in standard reference works (e.g., Metcalf and Eddy, Inc., 1972).

Equation (3) has wide application in the analysis of water quality data. The most significant example of its application is in the analysis of the spatial distribution of the concentration of dissolved oxygen (DO) and biochemical oxygen demand (BOD) in rivers and estuaries.

II. C. Multi-Stage Consecutive Reactions

Modeling the transport of DO and BOD by means of numerical solution of Eq. (3) is an example of a two-stage reaction. There are also several phenomena of importance in water quality management that can be represented by a multi-stage reaction model which incorporates feedback effects. For example, the discharge of nitrogenous material into natural waters produces a variety of changes in water quality. Changes occur not only in the various forms of nitrogen, but also in the substances with which the nitrogen may react.

If C_o, C_B, C_2, C_3, C_4 and C_5 represent dissolved oxygen, biochemical oxygen demand, ammonia nitrogen, nitrite plus nitrate nitrogen, algal nitrogen and organic nitrogen respectively, the differential equations for this six-stage system are given as a system of equations (4)

$$\left.\begin{aligned}
&\frac{1}{A}\frac{\partial}{\partial t}(AC_o) + \frac{1}{A}\frac{\partial}{\partial x}(QC_o) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{\partial C_o}{\partial x}\right) + Ka\,(C_s - C_o) \\
&\qquad -K_1\,C_B - K_{25}C_2 \\
&\frac{1}{A}\frac{\partial}{\partial t}(AC_B) + \frac{1}{A}\frac{\partial}{\partial x}(QC_B) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{\partial C_B}{\partial x}\right) - (K_1 + K_3)C_B \\
&\frac{1}{A}\frac{\partial}{\partial t}(AC_2) + \frac{1}{A}\frac{\partial}{\partial x}(QC_2) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{\partial C_2}{\partial x}\right) - K_{22}C_2 + K_{52}C_5 \\
&\frac{1}{A}\frac{\partial}{\partial t}(AC_3) + \frac{1}{A}\frac{\partial}{\partial x}(QC_3) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{\partial C_3}{\partial x}\right) - K_{33}C_3 + K_{23}C_2 \\
&\frac{1}{A}\frac{\partial}{\partial t}(AC_4) + \frac{1}{A}\frac{\partial}{\partial x}(QC_4) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{\partial C_4}{\partial x}\right) - K_{44}C_4 + K_{24}C_2 + K_{34}C_3 \\
&\frac{1}{A}\frac{\partial}{\partial t}(AC_5) + \frac{1}{A}\frac{\partial}{\partial x}(QC_5) = \frac{1}{A}\frac{\partial}{\partial x}\left(AE\frac{C_5}{\partial x}\right) - K_{55}C_5 + K_{45}C_4
\end{aligned}\right\} \quad (4)$$

In these equations, K_a, K_1, K_{25}, K_3, K_{22}, K_{52}, K_{33}, K_{23}, K_{44}, K_{24}, K_{34}, K_{55}, and K_{45} are the reaction coefficients. Other variables are the same as defined previously.

III. SOLUTION TECHNIQUES

III. A. Equations of Unsteady Flow

The numerical model for flow dynamics in the neuse River Estuary is based on the four point implicit method first presented by Amein (1968). Details of the method with application and comparative evaluation are given in the reports by Amein and Fang (1970) and by Amein and Chu (1975). As a companion to the present study, its application to Masonboro Inlet, N. C., is given in the Sea Grant Report (Amein, 1973) and has been summarized in a paper (Amein, 1975).

For the sake of convenience, an outline of the method will be given as follows. To develop the flow model, consider a non-uniform rectangular grid on the x (distance), t (time) plane as shown in Fig. 1. Distances along the channel are represented by abscissas and times are represented by ordinates. It is assumed that all the variables are known at all points x_i and at time t^j. It is desired to determine the values of the variables for time t^{j+1} at all points x_i under given boundary conditions. The differential equations are simulated for a finite time Δt and for a finite distance Δx. The partial derivatives are replaced by finite differences at a point M located on the time ordinate t^{j+1}, midway between the abscissas x_i and x_{i+1}.

The equation of continuity is simulated by

$$\frac{Q_{i+1}^{j+1} - Q_i^{j+1}}{\Delta x} + \frac{\bar{A}_{i+1/2}^{j+1} - \bar{A}_{i+1/2}^{j+1}}{\Delta t} - q_{i+1/2}^{j+1} = 0 \qquad (5)$$

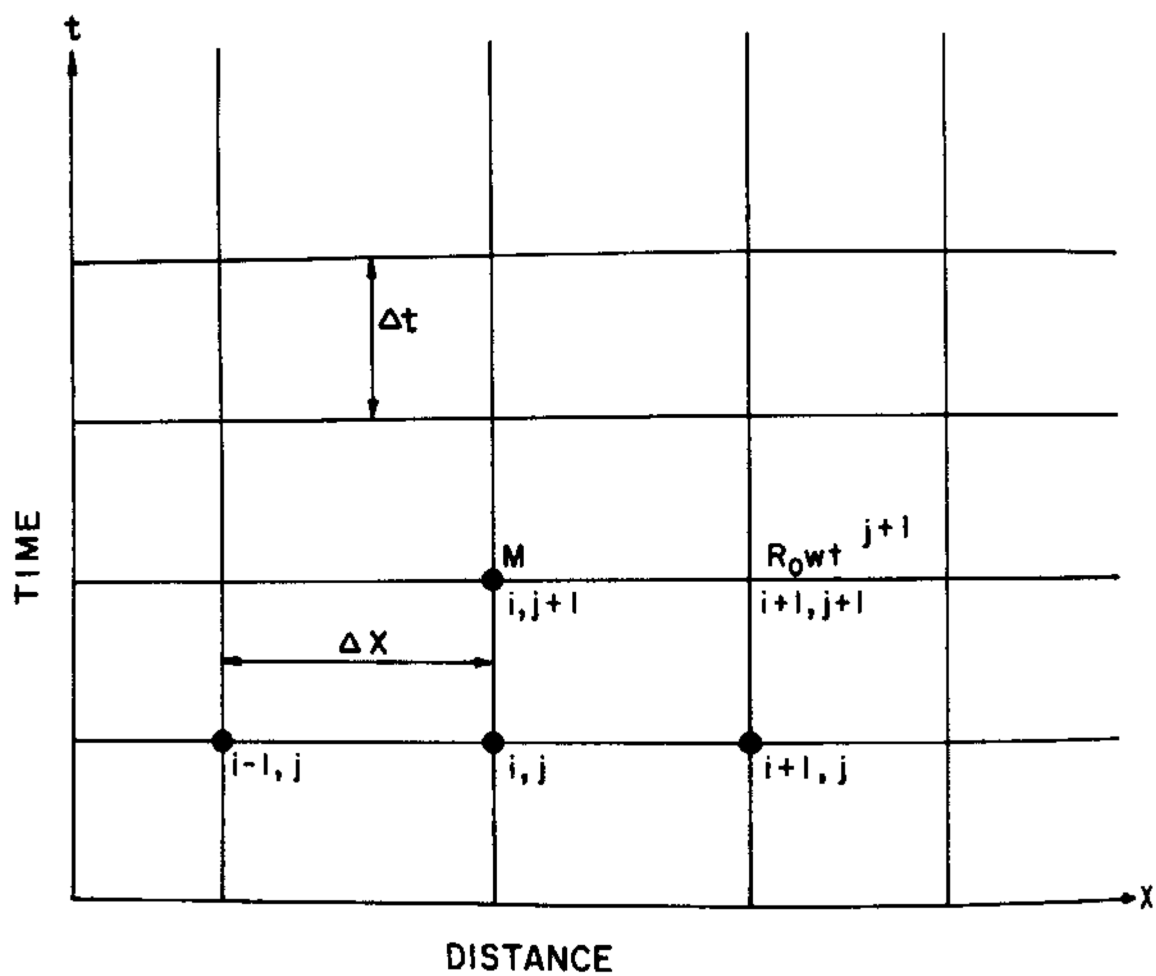

Fig. 1. Non-uniform rectangular grid, with distance (x) and time (t) planes, for unsteady flow.

where

$$\bar{A}_{i+1/2} = \frac{1}{\Delta x} \int_{x_i}^{x_{i+1}} A(x)\Delta x \qquad (6)$$

A reasonable approximation to $\bar{A}_{i+1/2}$ is

$$\bar{A}_{i+1/2} \simeq \frac{1}{2} \{A_i + A_{i+1}\} \qquad (7)$$

The equation for the conservation of momentum is simulated by

$$\frac{1}{\bar{A}^{j}_{i+1/2}} \frac{\bar{Q}^{j+1}_{i+1/2} - \bar{Q}^{j}_{i+1/2}}{\Delta t} + \frac{1}{\Delta x} \left\{ \frac{(Q^{j+1}_{i+1})^2}{A^{j+1}_{i+1}} - \frac{(Q^{j+1}_{i})^2}{A^{j+1}_{i}} \right\} \cdot \frac{1}{\bar{A}^{j+1}_{i+1/2}}$$

$$+ g \frac{(y^{j+1}_{i+1} + z^{j+1}_{i+1}) - (y^{j+1}_{i} + z_i)}{\Delta x} + g \bar{S}_{f}{}^{j+}_{i+1/2} = 0 \qquad (8)$$

In the above equations

$$\bar{Q}^{j+1}_{i+1/2} = \frac{1}{\Delta x} \int_{x_i}^{x_{i+1}} Q(x,t)\, dx \qquad (9)$$

$$\bar{S}_{f}{}^{j+1}_{i+1/2} = \frac{1}{\Delta x} \int_{x_i}^{x_{i+1}} S_f(x,t)\, dx \qquad (10)$$

Reasonable approximations to $\bar{Q}$ and $\bar{S}_f$ are

$$\bar{S}_{f}{}^{j+1}_{i+1/2} \simeq \frac{1}{2} \{S_{f_i}^{j+1} + S_{f_{i+1}}^{j+1}\} \qquad (11)$$

$$\bar{Q}^{j+1}_{i+1/2} \simeq \frac{1}{2} \{Q_i{}^{j+1} + Q^{j+1}_{i+1}\} \qquad (12)$$

In Equations (5) and (8) all the variables with supercripts (j+1) are unknown. The unknowns consist of the values of Q (volume flow rate), y (depth), v (velocity), A (area), P (wetted perimeter), S_f (friction slope), and B (top width).

However, all the unknowns are not independent. If Q and y are chosen as the indepent variables, then other variables can be expressed as functions of Q and y. Equations (5) and (8) contain four independent unknowns, the unknowns being the values of the discharge and stage at grid points (i, j+1) and (i+1, j+1). The distance increment $\Delta x = x_{i+1} - x_i$ and the time increment $\Delta t = t^{j+1} - t^j$ need not be constant and can be varied in accordance with the field data.

Equations (5) and (8) constitute a system of two nonlinear algebraic equations in four unknowns. By themselves they are not sufficient to evaluate the unknowns at points (i, j+1) and (i+1, j+1). However, the unknowns are common to any two adjacent channel reaches. If the entire channel is subdivided into reaches, a number of equations will be obtained that together with the additional equations provided by the boundary conditions will make the system determinate.

If the channel reach is divided into subreaches by N stations, there will be N-1 subreaches and the two equations (5) and (8) can be written at each subreach providing 2(N-1) equations relating the unknown variables. The unknowns are basically the discharge and stage at each station. Therefore, there are 2N unknowns and 2(N-1) equations. The additional two equations furnished by the boundary conditions. The upstream boundary condition can be given as either: (1) discharge as function of time; or (2) stage as function of time.

The downstream boundary condition can be given as (1) discharge as function time, or (2) stage as function of time or (3) stage-discharge relationship. The last alternative could take the form of a rating curve or a weir formula if a weir controls the flow.

The application of the four-point implicit method to solve the equations of unsteady flow is seen to require the solution of a system of nonlinear algebraic equations. The system can be solved very efficiently using the generalized

Newton iteration. There are two basic reasons why the implicit system is efficient. First, large time steps can be used in the computations. Secondly, the coefficient matrices encountered in the solutions are diagonal and sparse so that fast methods of solution can be employed. A recent study by Price (1974) has demonstrated that the four point implicit method is the most efficient technique for the solution of the equations of unsteady flow. It has the advantages of stability and accuracy. Details of the procedure are given in the paper by Amein and Fang, (1970) and summarized in the paper by Amein (1975).

III. B. Equations of Mass Transport

An explicit method is used to develop a numerical model for the equations of mass transport. The method is well known in the literature of numerical analysis and has been applied to the solution of the mass-balance equation by (Jeglic, 1966; and Bunce and Hetling, 1966). A survey of water quality models for application to estuaries is given by Tracor Inc. (1971). To illustrate the procedure in this study, consider the non-uniform rectangular grid on the {x(distance), t (time)} plane as shown on Fig. 2. Again, distances along the waterway are represented by abscissas and times are represented by ordinates, the subscript i identifying the location and the superscript j identifying the time. It is assumed that all the variables are known at all points x_i and at times t^j. It is desired to develop a numerical model for equation (3) to evaluate the water quality parameter L at all points x_i at time step t^{j+1} under given boundary conditions. The partial derivatives are replaced by finite differences at a point P located on the time ordinate t^j, at $x = x_i$.

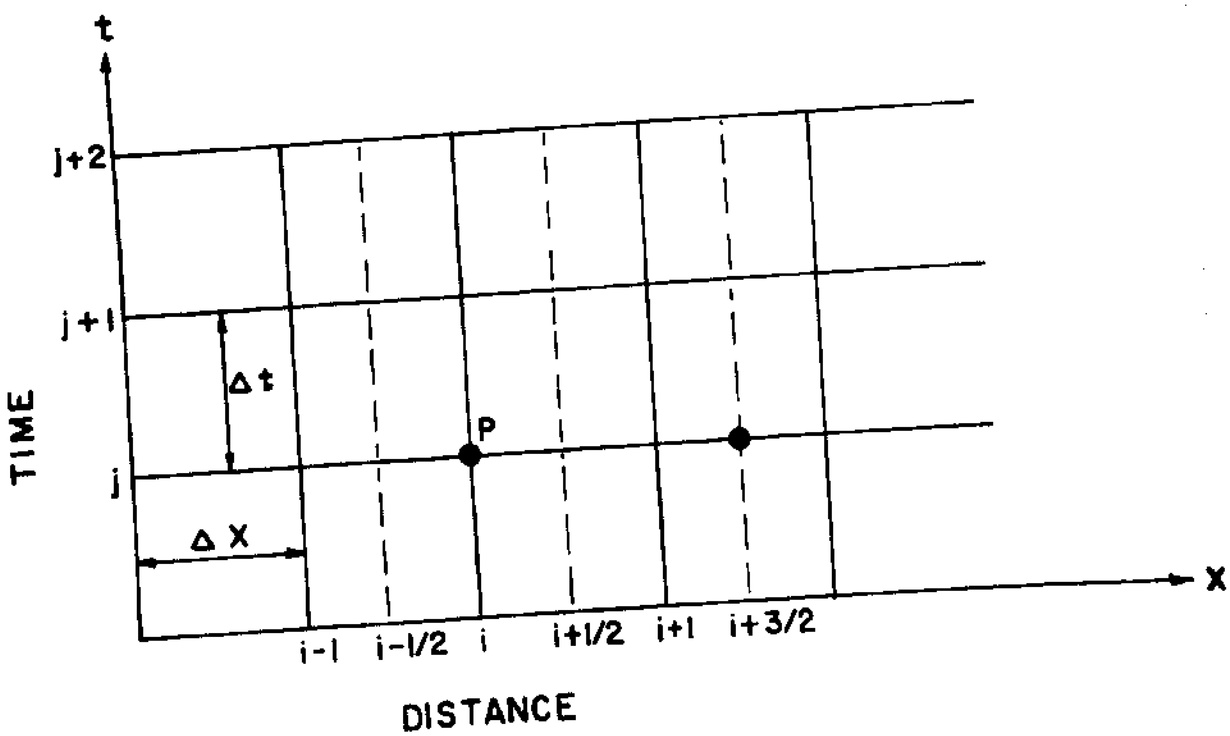

Fig. 2. Non-uniform rectangular grid, with distance (x) and time (t) planes, for mass transport.

The finite difference representation of the advective term can be given as

$$\frac{\partial}{\partial x}(QL) = \left[(\alpha_i^j\, L_i^j\, Q_i^j + \beta_{i+1}^j\, L_{i+1}^j\, Q_{i+1}^j) - (\alpha_{i+1}^j\, L_{i-1}^j\, Q_{i-1}^j + \beta_i^j\, L_i^j\, Q_i^j) \right] \frac{\Delta t}{\Delta x} \cdot \frac{2}{A_i^j + A_{i+1}^j} \qquad (13)$$

where α and β are weighting factors, and $\beta = (1-\alpha)$.

The finite difference representation of the dispersion term can be given as

$$\frac{\partial^2}{\partial x^2}(EAL) = E_{i+1}^j\, A_{i+1}^j \cdot (L_{i+1}^j - L_i^j) - E_{i-1}^j\, A_{i-1}^j \cdot (L_i^j - L_{i-1}^j) \cdot \frac{2\Delta t}{(\Delta x)^2 (A_{i+1} + A_{i-1})} \qquad (14)$$

The left-hand side of equation (3) which consists of the time varying term can be represented as

$$\frac{1}{A}\frac{\partial}{\partial t}(AL) = \frac{L_i^{j+1} - L_i^j}{\Delta t} \qquad (15)$$

It should be noted that with $\alpha = 1$, $\beta = 0$, the finite difference scheme for advection becomes a backward difference scheme while with $\alpha = 0$, $\beta = 1$, it becomes a forward difference scheme and with $\alpha = 1/2$ it becomes a centered finite difference scheme.

Using $\alpha = 1$, $\beta = 0$, and combining equations (13), (14) and (15), the finite difference representation of equation (3), the mass-balance equation, becomes

$$\frac{L_i^{j+1} - L_i^j}{\Delta t} = \frac{}{(A^j_{i+1} + A^j_{i-1})} \cdot \Delta x \ \{(QL)^j_{i+1} - (QL)^j_{i-1}\}$$

$$+ \frac{2}{(A^j_{i+1} + A^j_{i-1})} \cdot \frac{1}{(\Delta x)^2} \cdot \{E_{i+1}A_{i+1}(L^j_{i+1} - L^j_i)$$

$$- E^j_{i-1} \ A^j_{i-1} \ (L^j_i - L^j_{i-1}) \} + \text{sources} + \text{sinks} \tag{16}$$

The use of the weighting factor α can be interpreted also in the following manner (Thomann, 1972). Equation (16) is a numerical model for the mass-balance equation (3). It is required that positive values for the concentration L should be obtained. One method for accomplishing this objective is to introduce a variable finite difference weight for the advective term in the equation. Thus an expression for the values of L at the boundaries of a segment contained between x_i and x_{i+1} can be written as:

$$L_{i+1} = \alpha_{i+1} \ L_{i+1/2} + (1 - \alpha_{i+1}) \ L_{i+3/2}$$

$$L_i = \alpha_i L_{i-1/2} + (1 - \alpha_i) \ L_{i+1/2}$$

where α represents the fraction of the upstream concentration L physically advected into the downstream section. For solutions that must be positive everywhere (the physical condition required here) it is necessary that

$$\alpha > 1 - \frac{EA}{Q\Delta x} \tag{17}$$

Once the criterion given by (17) is met, the solutions are stable and relatively insensitive to the weighting factor. If a lower bound of $\alpha = 1/2$ is used, as practiced by many investigators, then Δx must be adjusted to satisfy (17).

III. C. Selection of Time Step

In using the explicit scheme, the smaller of the following was used for the time step (Bella and Dobbins, 1968):

$$\Delta t \leq \frac{\Delta x}{V_{max}} \tag{18}$$

and

$$\Delta t \leq \frac{(\Delta x)^2}{gE_{max}} \tag{19}$$

where V_{max} is the maximum velocity.

The time step given by equation (18) is smaller than that given by (19) with the expected values of velocity and dispersion coefficients in the Neuse estuary. Therefore, equation (19) was used for selecting the time step. A reasonable value for Δt is 30 hours which can also be used in the hydrodynamic equation with the implicit method. However, to minimize numerical errors, if any, the computations were run with $\Delta t = 6$ hours and $\Delta t = 12$ hours.

IV. INPUT DATA

Basic data needed for the simulation of water quality are the channel section parameters such as the cross-sectional area, channel bottom elevation, distance between the stations, and upstream and downstream flow data at some reasonable specified intervals of time. In addition to the above data, the quality data such as temperature, dissolved oxygen, biochemical oxygen demand, the nitrogen series, etc. are also needed. In spite of the lack of sufficient flow and quality data, the quality model was developed to be applied in the future to simulate the behavior of a prototype system within reasonable limits of accuracy with a minimal amount of time and effort on the user's part. The utility of the model will depend upon the following factors:

(1) the degree to which the spatial details and flow data are provided for the model;

(2) the degree to which temporal details (time-varying inputs) are provided; and

(3) the realiability of the basic data required to describe the characteristics of the prototype system and all essential inputs.

IV. A. Channel Data

The basic geometric data for the Neuse Estuary are given in Table 1. The estuary was subdivided into forty (40) segments by 41 stations as shown on Fig. 3. Segment 41 is the downstream boundary and is located in Pamlico Sound. Table 1 contains the area-depth relationship at each station, the distance at each station along the estuary axis, the bottom elevation and ϕ (the angle between the estuary axis and the east-west line). The angle ϕ is used to find the angle between the wind direction and the direction of water flow needed for the evaluation of the wind stress.

Table 1. Channel Section Parameters

Station No.	Area Equation (ft^2)	Distance (miles)	Bottom Elev. (ft.)	Angle θ (degrees)
1	7667y - 38005	0	9.0	-51
2	7207y - 33044	1	10.0	-51
3	6748y - 28083	2	10.0	-51
4	6288y - 23122	3	8.0	-51
5	7617y - 36152	4	8.0	-51
6	10597y - 65794	5	9.75	-51
7	13491y - 77552	6	11.5	-51
8	16277y - 66547	7	10.75	-51
9	16914y - 57440	8	10.0	-51
10	17203y - 48641	9	10.0	-36
11	17491y - 39843	10	9.15	-36
12	17979y - 34187	11	8.32	-36
13	18780y - 33659	12	7.49	-36
14	18701y - 36934	13	6.66	-36
15	17927y - 43244	14	5.83	-36
16	17154y - 49553	15	5.0	0.0
17	16381y - 55863	16	5.0	0.0
18	15608y - 62173	17	5.0	0.0
19	14835y - 68482	18	5.0	34
20	14062y - 74792	19	5.0	34
21	14480y - 86294	20	5.0	34
22	16137y - 103200	21	4.75	34
23	17796y - 120107	22	4.50	34
24	19454y - 137013	23	4.25	34
25	20286y - 147027	24	4.0	34
26	19742y - 146118	25	3.70	34
27	19197y - 145209	26	3.40	34
28	18635y - 144300	27	3.0	34
29	18108y - 14339	28	2.5	34
30	17563y - 142482	29	2.0	34
31	17018y - 141573	30	1.5	48
32	17555y - 144199	31	1.0	48
33	18814y - 149191	32	0.8	48
34	20073y - 154183	33	0.65	48
35	21332y - 159175	34	0.525	48
36	22591y - 164167	35	0.40	48
37	23850y - 169159	36	0.375	48
38	25109y - 174151	37	0.25	48
39	26368y - 179143	38	0.125	48
40	27627y - 184135	39	0.0	48
41	29199y - 181723	40	0.0	48

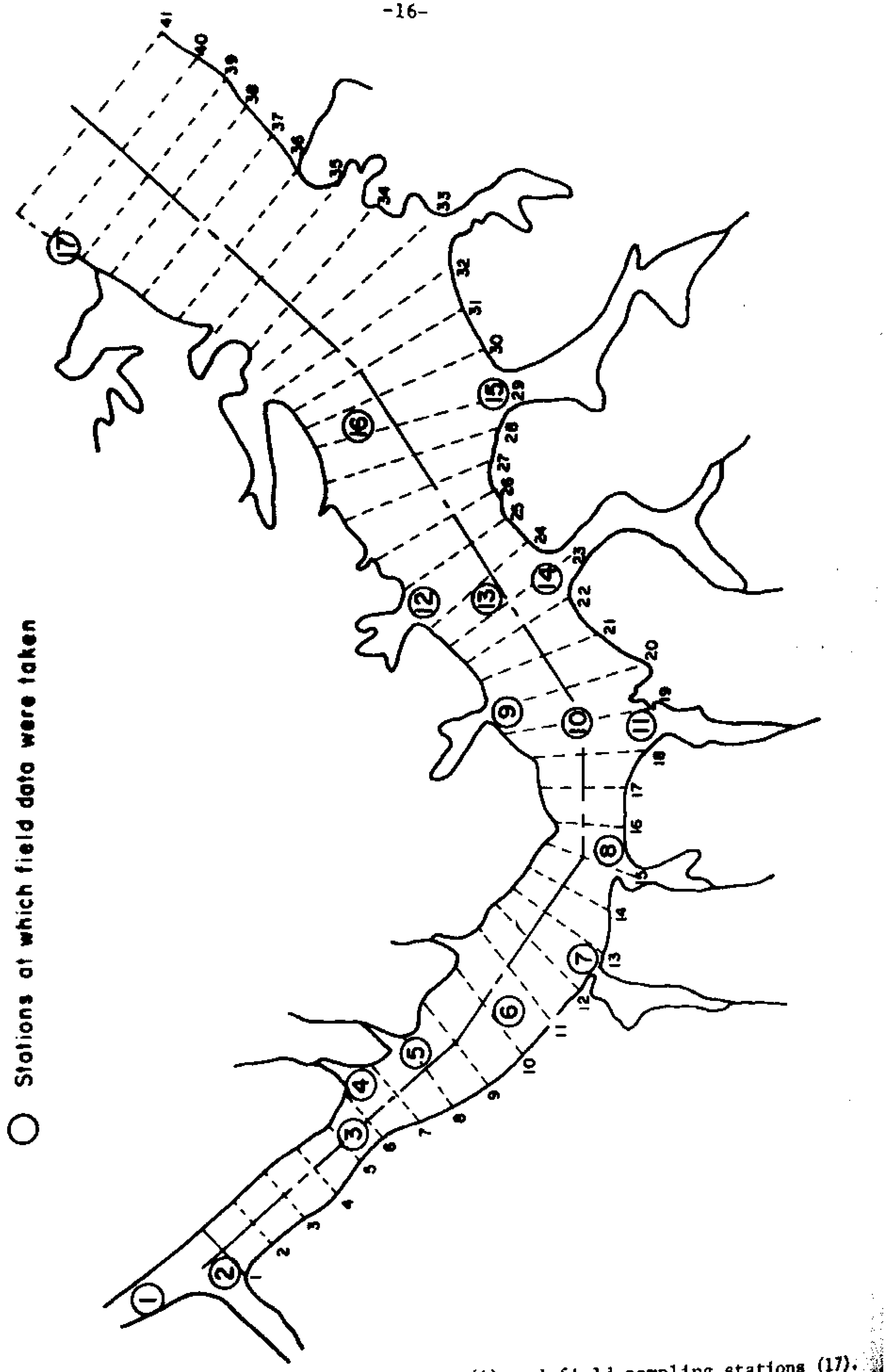

Fig. 3. Neuse River Estuary with segments (4) and field sampling stations (17).

IV. B. Discharge Data

The discharge values for each month at the upstream end (station No. 1) of Neuse River Estuary were obtained by adding the discharge of Neuse River at Kinston to the discharges of several tributaries which join the Neuse River downstream of Kinston. In addition to these discharges, the runoff from the drainage area of about 200 square miles (Fig. 4) was also estimated using the observed relationship between the drainage area and flow. This runoff was added to the above discharges, thus the total mean monthly flow at Station No. 1 was computed. The data for flow of the Neuse River and its tributaries can be obtained from Surface Records for N. C., United States Department of the Interior, Geological Survey.

IV. C. Quality Data

Quality data on dissolved oxygen, NO_2-N, NO_3-N, NH_3-N, etc. at the given station (see Fig. 3) were obtained from the Department of Zoology, North Carolina State University. Initial BOD concentration in the estuary and lateral inflow and its concentration of BOD were obtained by personal communication with personnel of the N. C. State Department of Natural and Economic Resources.

IV. D. Reaeration

One of the major phenomena contributing to the biochemical oxidation in waters containing degradable materials is atmospheric reaeration. Many theories have been proposed and a large number of techniques and equations have been used to estimate the reaeration coefficient; however, there is no universally accepted method for doing so. Langbein and Durum (1967) expressed reaeration coefficient as

$$K_2^{20} = 3.3\,\overline{u}/D^{1.33} \qquad (20)$$

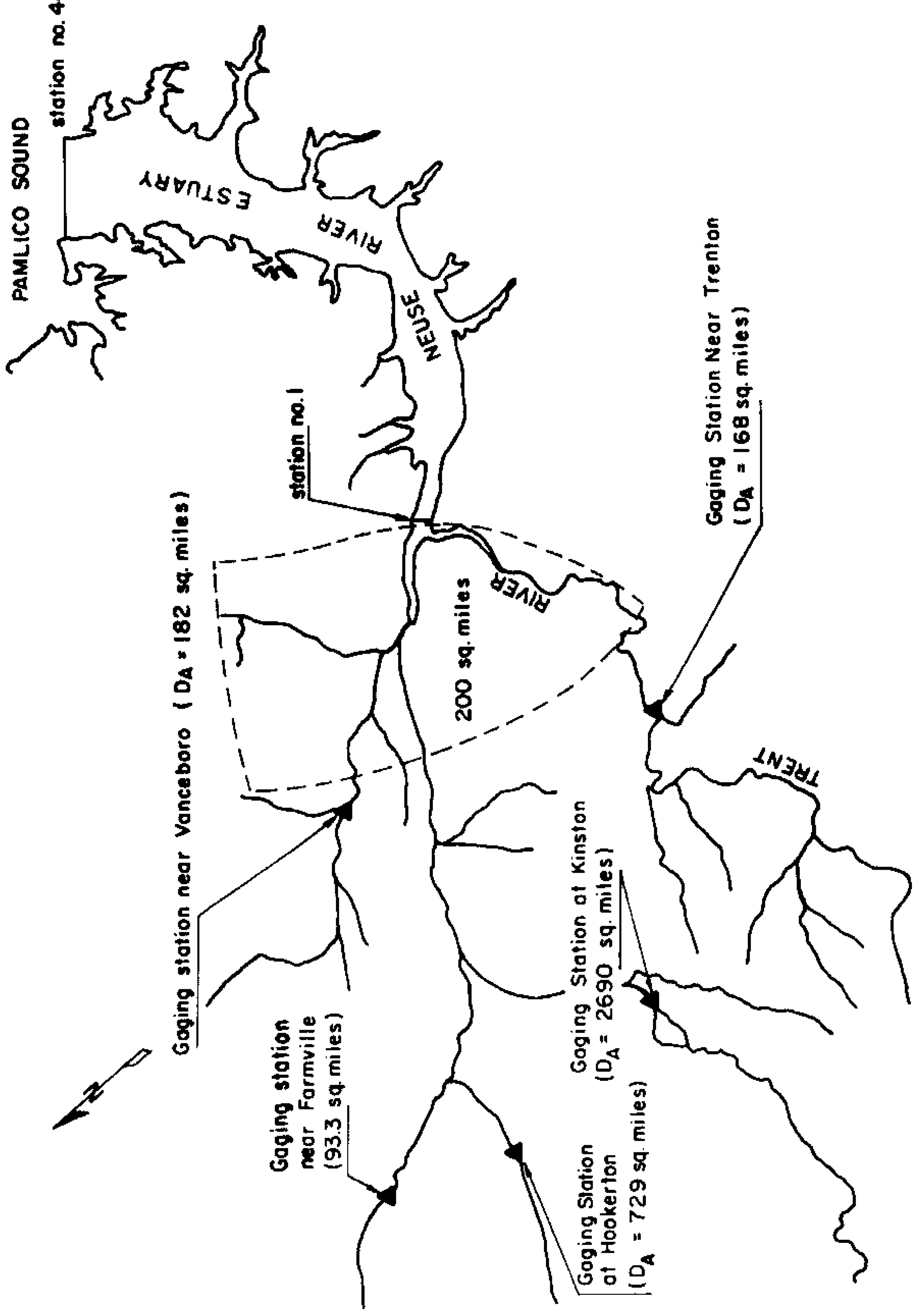

Fig. 4 Neuse River drainage area, with USGS gaging sites.

where

$\bar{u}$ = Mean velocity, ft/sec

D = Mean depth, ft, and

K_2 = Reaeration coefficient, 1/days.

The value of reaeration coefficient has been found (Weber, 1971) to vary with temperature as

$$K_2^T = K_2^{20}(1.047)^{(T-20)} \qquad (21)$$

where T is the temperature of the water in ^oC.

The reaeration coefficient computed for the Neuse Estuary is very small when computed by (20). This formula is not valid for estuaries, but restricted to rivers with velocities higher than 1 ft/sec. In the computation of dissolved oxygen for the Neuse Estuary, the following formula

$$K_2 = \frac{0.2668}{y} \times \frac{1}{(1 - .2006\sqrt{W})} \qquad (22)$$

was used, where K_2 is the reaeration coefficient in (1 day), y is the depth in ft., and W is the wind speed in mph. This formula is given by Kanwisher (1963).

IV. E. Decay Coefficient

Thomas (1948) gives values of decay coefficient K_1 for BOD as

$$K_1 = .06 \text{ to } .36 \text{ per day} \qquad (23)$$

K_1 is also affected by temperature and has been found to vary as

$$K_1^T = K_1^{20}(1.075)^{(T-20)} \qquad (24)$$

where T is the temperature of the water in ^oC.

IV. F. Longitudinal Dispersion Coefficient

For a wide channel the equation for dispersion coefficient based on Elder's expression (Elder, 1959) is given as

$$D_L = 22.6 \, \overline{nu} \, D^{.833} \qquad (25)$$

where

D_L = Longitudinal dispersion coefficient, $ft^2/sec.$

n = Manning's roughness coefficient,

$\overline{u}$ = Mean velocity, ft/sec and

D = Mean depth, ft.

IV. G. Temperature

The spatial distribution of temperature is usually associated with the sources of thermal pollution. At the present there is no such variation of temperature along the estuary. To give some approximate picture that how surface water temperature for the Neuse River Estuary varies annually, the average variation of temperature in degrees centigrade as a function of time can be described by Equation (25)

$$\text{Temp} = 6.545 - 7.9026 \times 10^{-2} + 3.3213 \times 10^{-3} t^2 - 1.6294 \times 10^{-5} t^3 + 2.128 \times 10^{-8} t^4 \qquad (25)$$

where t is time in days measured from month of January. The graph of Equation (25) together with the data from the Institute of Marine Science, N. C. and the Department of Zoology, North Carolina State University is shown in Fig. 5. It should be noted that the variation described by Equation (13) should not be considered absolutely predictive.

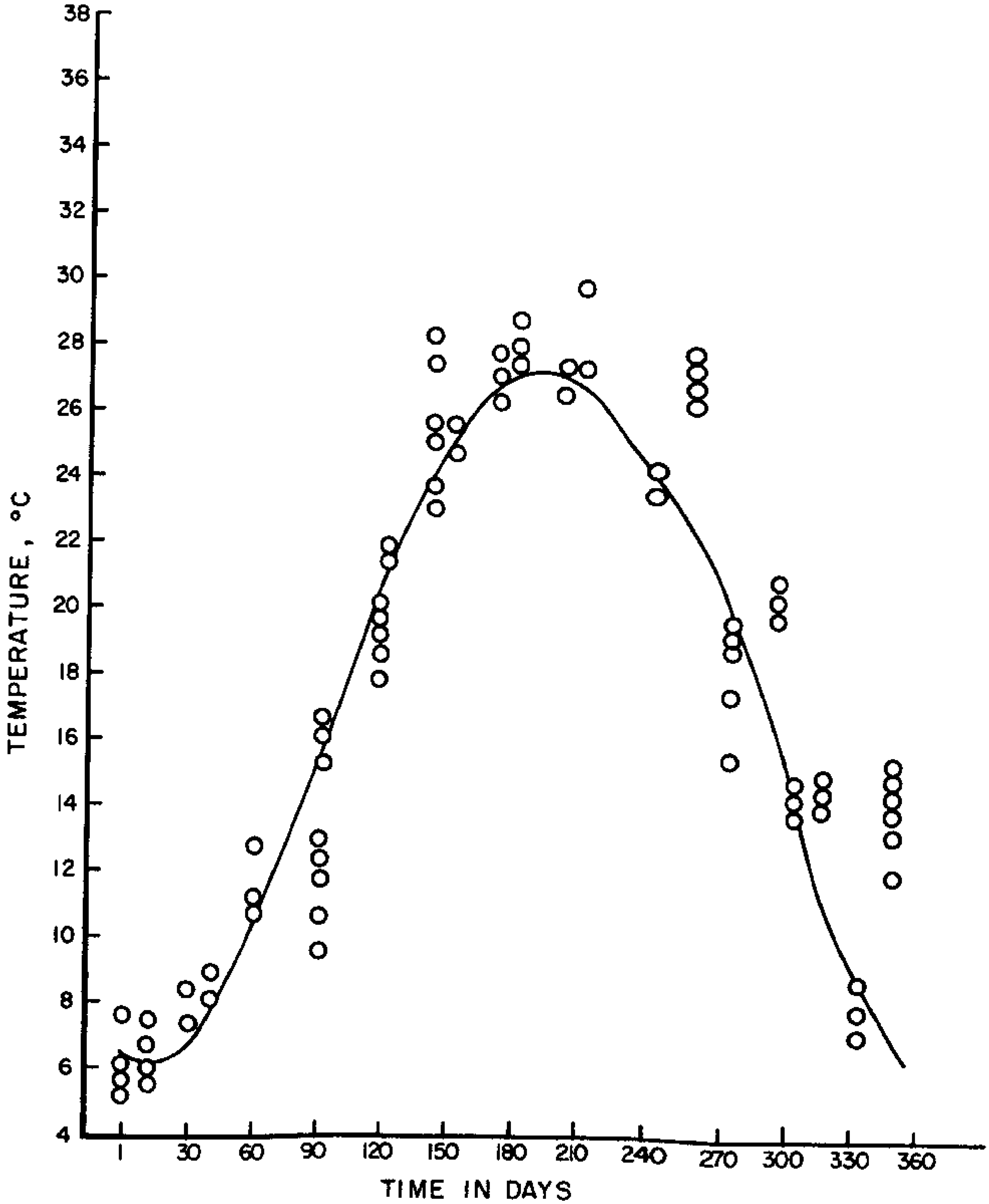

Fig. 5. Water temperature (C) in the Neuse River Estuary. The line gives the predicted value from equation (25) and the circles give actual field data.

All the above factors such as K_a, K_1, K_3, temperature, dispersion coefficient and other decay constants, used in the program are important in water-quality consideration. The values for most of the constants were taken from other related studies because they were not available for the Neuse estuary.

IV. H. Boundary Conditions

The boundary conditions for flow equations were prescribed as discharge at the upstream boundary and depth at the downstream boundary. Since the depth and discharge values were not available at downstream boundaries, the depth value corresponding to initial flow condition at station 41 was provided as a downstream depth and it was assumed to remain constant throughout the simulation. The reason for the above assumption is that the estuary at station 41 is very wide, and therefore upstream flow condition will not change the depth at this station significantly.

For mass transport equation the upstrem boundary values of the variables such as DO, BOD, etc. at station No. 1 were prescribed as a function of time and at the downstream the values of the variables were extrapolated from the interior using constant slope interpolation. For example,

$$L^{j+1}(41) = 2 \cdot L^{j+1}(40) - L^{j+1}(39) \tag{26}$$

where station 41 is the downstream station and $L^{j+1}(41)$ is the concentration at downstream station at time j+1.

The boundary data at upstream boundary as a function of time for both flow and mass transport equations were provided (Table 2) by interpolating the values of the variable at the interval of 29 hours from October 20, 1970, to November 17, 1970 (i.e., 24 time steps).

Table 2. Values of Variables on October 20, 1970, and November 17, 1970

	Q ft^3/sec	DO* (ppm)	C_2* (ppm)	C_3* (ppm)	C_4* (ppm)	C_5* (ppm)
Oct. 20, 1970	476	8.175	0.2818	0.0939	0	0
Nov. 17, 1970	2800	5.562	0.2034	0.6145	0	0

*Source of data: Department of Zoology, North Carolina State University, Raleigh, N. C.

Data for C_4 and C_5 were not available. The variables were defined in IIC.

IV. I. Initial Conditions

For many cases of river or estuary flows initial conditions for Q and y are not explicitly available. Often an initial condition of steady state is assumed for the purpose of analysis. Based on the steady state assumption the initial depths could be supplied by backwater calculation at each station and are shown in Table 3. The initial values of DO, BOD and etc. corresponding to t = 0 (i.e., Oct. 20, 1974) were calculated at each segment from field data taken at specific stations along the Neuse River Estuary.

Initial time t = 0 hour corresponding to October 20, 1970. The computations are terminated at t = 696 hour corresponding to November 17, 1970.

IV. J. Lateral Flows and Waste Loadings

Lateral inflows (QL) and their corresponding concentration (CL) were also obtained by personal communication with personnel of N. C. State Department of Natural and Economic Resources, and were assumed to remain constant during the simulation period. Their values are shown in Table 3.

Table 3. Initial Values of Water Depth, Discharge, Lateral Flow and Lateral Concentration

Station No.	Discharge (ft^3/sec)	Depth (ft)	Lateral Flow (ft^3/sec)	Lateral Concentration of BOD ppm
1	476	14.1	0.0	0.0
2	476	13.0	7.0	50.0
3	476	13.0	0.0	0.0
4	476	15.0	0.0	0.0
5	476	15.0	0.0	0.0
6	476	13.25	0.0	0.0
7	476	11.50	0.16	75.0
8	476	12.25	0.0	0.0
9	476	13.0	0.0	0.0
10	476	13.0	0.0	0.0
11	476	13.85	0.0	0.0
12	476	14.68	0.0	0.0
13	476	15.51	0.0	0.0
14	476	16.34	0.0	0.0
15	476	17.17	0.62	200.0
16	476	18.0	0.0	0.0
17	476	18.0	0.0	0.0
18	476	18.0	2.80	200.0
19	476	18.0	0.0	0.0
20	476	18.0	0.0	0.0
21	476	18.0	0.0	0.0
22	476	18.25	0.0	0.0
23	476	18.50	0.0	0.0
24	476	18.75	0.0	0.0
25	476	19.0	0.0	0.0
26	476	19.30	0.0	0.0
27	476	19.60	0.0	0.0
28	476	20.0	0.0	0.0
29	476	20.5	0.0	0.0
30	476	21.0	0.0	0.0
31	476	21.5	0.0	0.0
32	476	22.0	0.0	0.0
33	476	22.5	0.0	0.0
34	476	22.35	0.0	0.0
35	476	22.475	0.0	0.0
36	476	22.60	0.0	0.0
37	476	22.625	0.0	0.0
38	476	22.75	0.0	0.0
39	476	22.875	0.0	0.0
40	476	23.0	0.0	0.0
41	476	23.0	0.0	0.0

V. OUTPUT

A computer program to simulate the water quality in the Neuse River Estuary system on the basis of the numerical integration of the equation of unsteady flow by the implicit method, coupled with explicit integration of the equation of mass transport, was prepared. The data needed to obtain the solutions consist of the basic channel data, water quality data and their corresponding boundary data. The objective of the computation was to predict the general trend of the distribution of various constituents (DO, BOD, etc.) along the Neuse River Estuary. The results of the computations are presented in Figs. 6, 7 and 8. The water quality was simulated for a period of 29 days (696 hours).

The values of the coefficients used in this study are listed as follows:

Temperature, $T = 16^{\circ}$

Manning's coefficient of friction, $n = .025$

Decay coefficient of "BOD", $K_1 = .16$

Coefficient for "BOD" removal by sedimentation, $K_{33} = 0.0$

Decay coefficient of NH_N-N, $K_{22} = 0.13$

Coefficient of conversion of organic nitrogen to NH_3-N, $K_{52} = 0.04$

Decay coefficient of $(NO_2\text{-}N) + (NO_3\text{-}N)$, $K_{33} = 0.04$

Conversion rate of $(NO_2\text{-}N) + (NO_3\text{-}N)$ to algal nitrogen, $K_{34} = 0.04$

Conversion rate of NH_3-N to algal nitrogen, $K_{24} = 0.01$

Conversation rate of NH_3-N to "DO," K_{25} = 0.54

Conversation rate of algal nitrogen to organic nitrogen, K_{45} = 0.05

Decay Coefficient of algal nitrogen, K_{44} = 0.05

Decay Coefficient of organic nitrogen, K_{55} = 0.08

Saturation value of dissolved oxygen at 20^{o}C, C_s = 9.5 (mg/1)

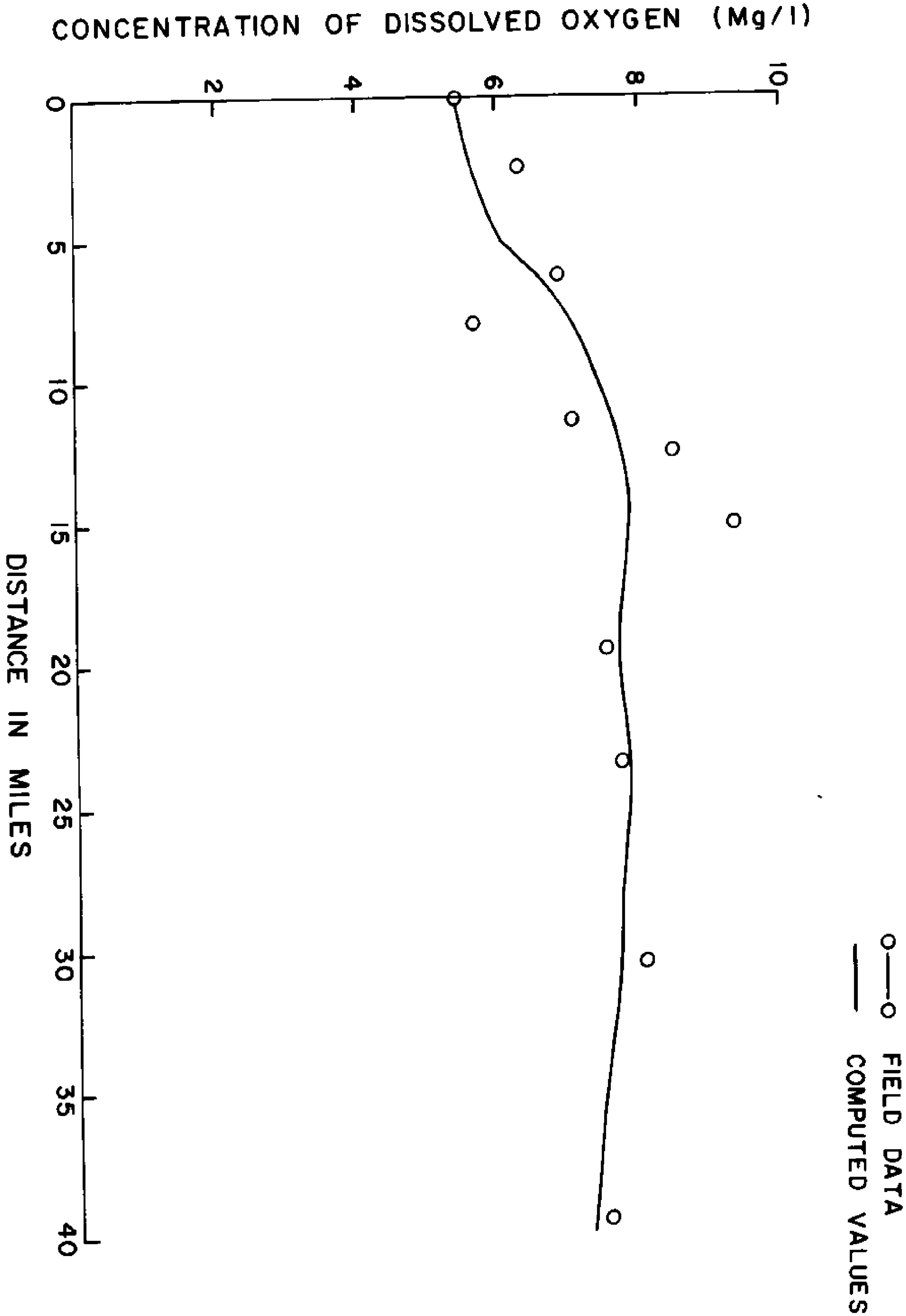

Fig. 6. Dissolved oxygen (mg/l) along the length of the Neuse River Estuary. The line gives the model output and the circles are actual field data.

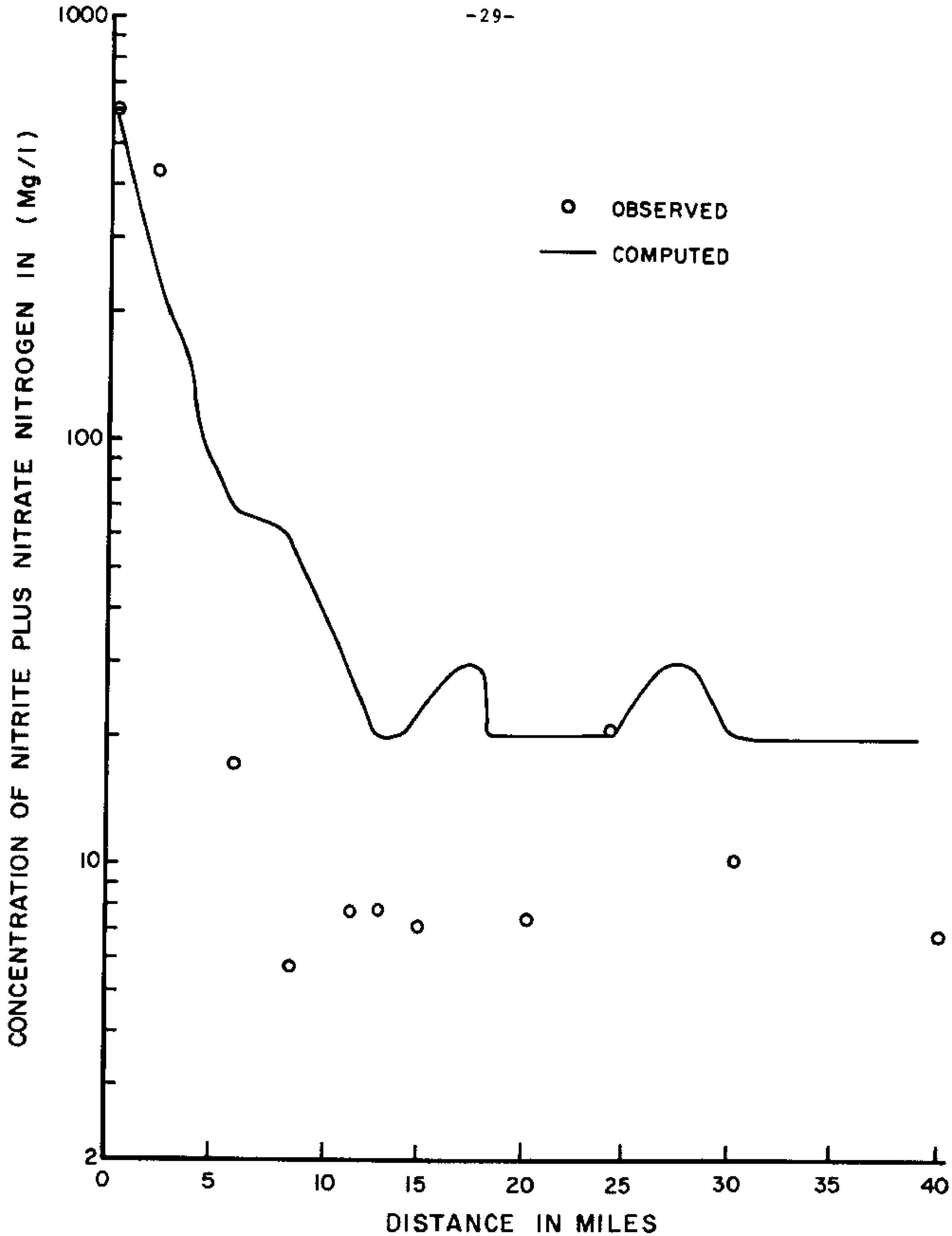

Fig. 7. Nitrate (+ nitrite) nitrogen (mg/l x 1000) along the length of the Neuse River Estuary. The line gives the model output and the circles are actual field data.

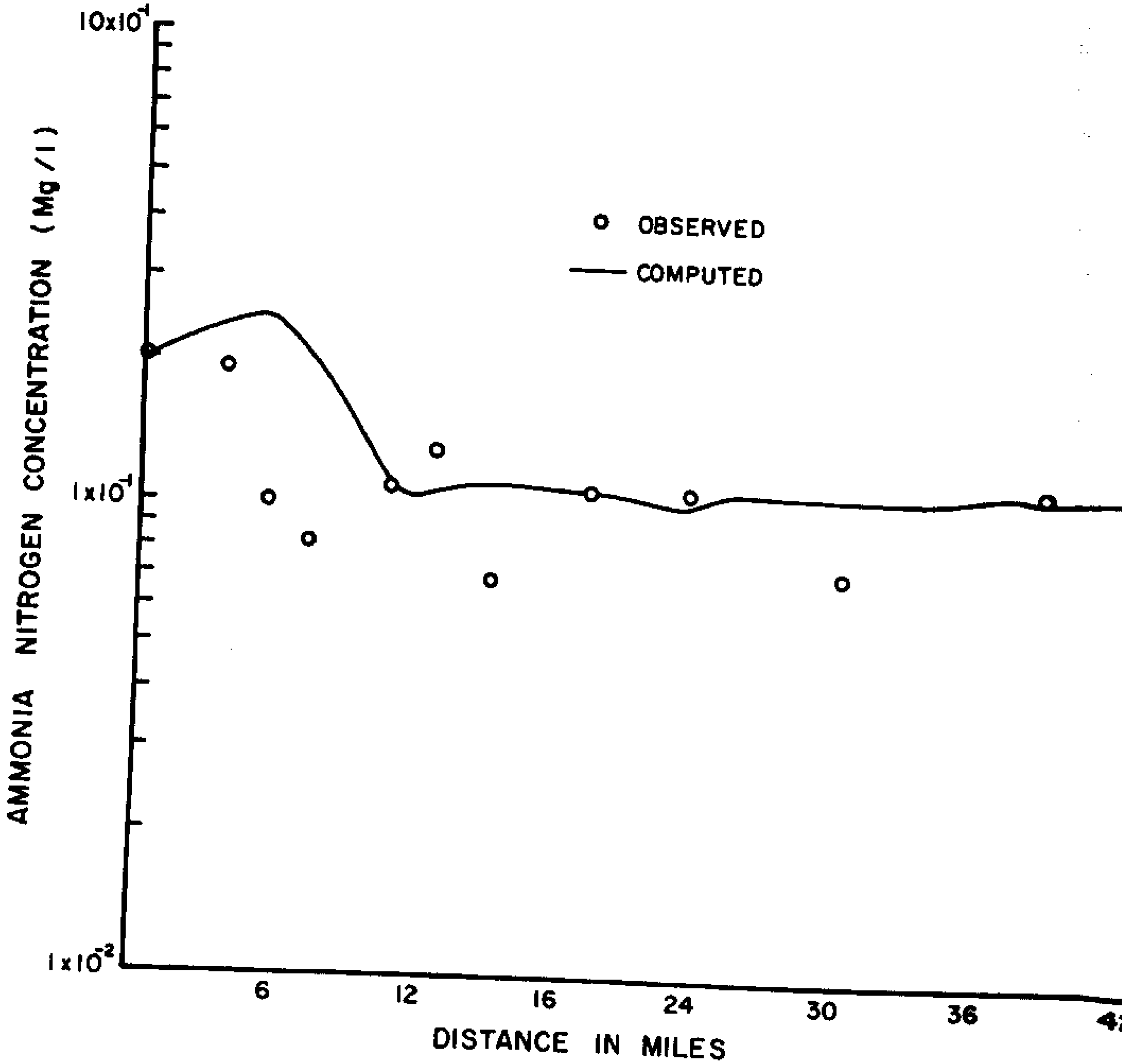

Fig. 8. Ammonia nitrogen (mg/l) along the length of the Neuse River Estuary. The line gives the model output and the circles are actual field data.

VI. CONCLUSIONS AND RECOMMENDATIONS

The computed values of dissolved oxygen, ammonia nitrogen, and nitrite plus nitrate nitrogen were obtained by numerical solution of the equation of mass transport and they are plotted together with the field data in Figs. 6, 7 and 8. In general the field data follow the trend of the computed values. The reliability of the results depends upon the accuracy of the reaction coefficients, dispersion coefficients, waste loadings, withdrawals, and other basic data. The model prepared in this study provides the foundation for simulating water quality in an estuary. For best results, the model must be calibrated with accurate data. It is recommended that the data sampling include the following:

1. Meteorological variables, e.g., precipitation, wind.
2. Continuous stage-discharge relationship at both upstream and downstream boundaries.
3. An estimate of the dispersion coefficient along the estuary.
4. Waste loadings and withdrawals.
5. Reaction coefficients and other special variables related to specific waste discharges.

It is hoped that with the availability of the above data, the program developed in this study can be used to simulate the behavior of the prototype system within reasonable limit of accuracy and with a minimal amount of time and effort on the user's part.

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VIII. COMPUTER PROGRAMS

A program listing is provided to give pertinent information to users. The computer program is written in Fortran IV language and was run on an IBM 370/165 model. The program consists of two parts: (1) FLOW and (2) WQUAL.

FLOW uses an implicit finite difference scheme, for the solution of unsteady flow equation in open channels, while WQUAL uses an explicit finite difference scheme, used for the solution of the mass transport equation. The operation of the program produces a time history and longitudinal variation in depths, velocity, discharge, and concentration of BOD (biochemical oxygen demand), DO (dissolved oxygen), NH_3, NO_2-N, NO_3-N, algal nitrogen and organic nitrogen. The program, if desired, can be used to compute surges due to wind in the Neuse River Estuary. To obtain results, the initial and boundary conditions must be provided by the user. The following are the definitions of the terms used in the program.

The user should be warned that only values for DO, BOD, NH_3-N and NO_2-N + NO_3-N have been computed with the computer program. Neither the equations nor the coefficients for other water quality parameters such as organic nitrogen and algal nitrogen have been tested nor documented. Of course, the variables C_4 and C_5 can represent some other parameter at the user's choice.

DEFINITIONS

Y = depth of water above a given datum. In this program y is measured above the mean sea level.

I = index identifying stationing along the estuary. I = 1 is the upstream and I = 41 is the downstream boundary.

A(Y,I) = equation for area A as function of depth Y at station I.

HR(Y,I) = equation for hydraulic radius HR as a function of depth y at station I.

B(Y,I) = equation for top width at station I as a function of depth y.

WP(Y,I) = equation for wetted parameter as a function of depth Y at station I.

DHR(Y,I) = equation for derivative of hydraulic radius with respect to depth.

DBDY(Y,I) = equation for derivative of top width with respect to depth.

CM(Y,I) = equation for Manning's coefficient of friction at a function of depth at station I.

TFIN = Specified time in (hours) at which computations will be terminated.

N = No. of stations along the axis of estuary, in this case, N is 41.

MN = No. of points on the time axis. This denotes the number of times at which the data are given at the upstream boundary.

G = Gravitational constant in ft/sec^2.

DELX = Length of each segment along the estuary, in miles.

J = is an index identifying time in the computations.

V(I) = Velocity at station I in ft/sec at time J+1.

Q(I) = Discharge at station I in ft^3/sec at time J+1.

VIN(I) = Velocity at station I in ft/sec at time J.

QIN(I) = Discharge at station I in ft^3/sec at time J.

DIST(I) = Distance along the estuary to station I in miles measured from station 1.

QL(I) = Lateral inflow at station I in units of ft^3/sec per lineal ft of the estuary.

STAGE(I) = Elevation of the channel bottom with respect to a horizontal datum at station (I).

NZ = Numbers identifying zones for the Neuse River Estuary.

VWS(I,KT) = Variable wind speed at station I and time KT in mph.

VWD(I,K) = Variable wind direction at station I and time KT in mph.

SWX(I) = Wind stress at station (I) in (lbs/ft^2)

PHI(I) = Angle which Neuse River Estuary makes with East-West in degrees.

WSC = Wind stress coefficient = 2.15 $\rho a/\rho_a$ = density of air, ρ = density of water, Ka = 3.0×10^{-3} and 2.15 is a conversion factor from mph to ft/sec.

CU = Concentration of dissolved oxygen at upstream boundary in (mg/ℓ)

CO = Concentration of dissolved oxygen at initial time along the estuary (mg/ℓ)

RK2 = Reaeration coefficient per day.

E(I) = Longitudinal dispersion coefficient (ft^2/sec) at station (I)

CB = Concentration of BOD at initial time along the estuary in (mg/ℓ)

C2 = Concentration of NH_3 at the initial time along the estuary in (mg/ℓ)

C3 = Concentration of NO_2-N + NO_3-N at initial time along the estuary in (mg/ℓ)

C4 = Concentration of algal nitrogen at initial time along the estuary in (mg/ℓ)

C5 = Concentration of organic nitrogen at initial time along the estuary in (mg/ℓ)

CBU, C2U, C3U, C4U, and C5U are concentration at upstream boundary of CB, C2, C3, C4, and C5 respectively. (mg/ℓ)

CL(I) = Lateral concentration of BOD in QL(I).

T(K) = Time at which computations are made (hrs.)

QUST(K) = Given discharge at upstream boundary at time T(K), in CFS.

DUST(K)	=	Given depth at upstream boundary at time T(K) in ft.
QDST(K)	=	Given discharge at downstream boundary at time T(K) in CFS.
DDST(K)	=	Given depth at downstream boundary at time T(K) in ft.
DC(J)	=	Given coefficient of rating curve at downstream boundary.
AA(J)	=	Matrix of coeffients.
C(K)	=	Vector of residues, in Program FLOW
ID	=	Index for identification of the boundary conditions
QO(I,J)	=	Discharge at station (I) and at time t^j in CFS.
YO(I,J)	=	Depth at station (I) and at time t^j in ft.
AO(I,J)	=	Area at station (I) and at time t^j in ft^2.
C(I)	=	Computed values of CO, CB, C2, C3, C4 or C5 at next time step. At the completion of computations, C's are converted to C_0, C_B, ..., C_5 and another set is computed.
CCS	=	Saturation value of dissolved oxygen in (mg/ℓ)
K1	=	Decay coefficient of BOD (per day)
K3	=	Rate of BOD removal by sedimentation (per day)
K22	=	Decay coefficient of ammonia nitrogen (per day)
K52	=	Conversion rate of organic nitrogen to ammonia nitrogen (per day)
K33	=	Decay coefficient of nitrate plus nitrite nitrogen (per day)
K23	=	Conversion rate of ammonia nitrogen to nitrate nitrogen.
K44	=	Decay coefficient of algal nitrogen (per day)
K24	=	Conversion rate of ammonia nitrogen to algal nitrogen (per day)
K55	=	Decay coefficient of algal nitrogen (per day)
K45	=	Conversion rate of algal nitrogen to organic nitrogen.

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**                                               **
**       DYNAMIC  WATER  QUALITY  MODEL          **
**                                               **
**                                               **
**                                               **
**           THE  NEUSE  ESTUARY                 **
**                                               **
**             NORTH  CAROLINA                   **
**                                               **
**                                               **
**         PART I:  FLOW  DYNAMICS               **
**                                               **
***************************************************
***************************************************


               PROGRAM NAME: FLOW

                METHOD: IMPLICIT

=======================DEFINITIONS================================


N         =NO. OF POINTS GIVEN ON X-AXIS(NO.OF STATIONS)
MN        =NO. OF POINTS GIVEN ON T-AXIS
TFIN      =FINAL TIME IN HOURS
EVERY GRID POINT IS IDENTIFIED BY THE NOTATION(I,J), WHERE
(I) REFERS TO THE DISTANCE (OR STATIONING) AND (J) REFERS TO TIME
Y(I)      =DEPTH FROM THE WATER SURFACE TO A REFERENCE LINE
           AT GRID POINT (I,J+1), IN FT.


V(I)      =VELOCITY AT GRID POINT(I,J+1) IN FT/SEC.
Q(I)      =DISCHARGE AT GRID POINT (I,J+1),IN CFS
YIN(I)    =DEPTH FROM THE WATER SURFACE TO A REFERENCE LINE
          AT GRID POINT (I,J), IN FT.
VIN(I)    =VELOCITY AT GRID POINT(I,J),IN FT/SEC.
QIN(I)    =DISCHARGE AT GRID POINT (I,J),IN CFS.


 YEPS     =TOLERANCE LIMIT FOR Y(I)
 QEPS     =TOLERANCE LIMIT FOR Q(I)
DIST(I)   =DISTANCE AT STATION (I) FROM THE FIRST STATION,IN MILES
QL(I)     =LATERAL INFLOW AT STATION (I),IN CFS PER LENGHT OF A
           SEGMENT


STAGE(I)=ELEVATION OF THE WATER SURFACE WITH REFERENCE TO
           AN ESTABLISHED HORIZONTAL DATUM, IN FT.
Z(I)=     ELEVATION OF THE CHANNEL BOTTOM WITH RESPECT TO A
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DELX      =INCREMENT OF DISTANCE IN MILES
A(Y,I)    =EQUATION FOR AREA AT STATION (I) AS A FUNCTION OF
           DEPTH Y(I)

HR(Y,I) =EQUATION FOR HYDAULIC RADIUS AT STATION(I) AS A
           FUNCTION OF DEPTH Y(I)
B(Y,I)    =EQUATION FOR TOP WIDTH AT STATION (I) AS A FUNCTION
           OF DEPTH Y(I)
WP(Y,I) =EQUATION FOR WETTED PERIMETER AT STATION (I) AS A
           FUNCTION OF DEPTH Y(I)

DHR(Y,I)=DERIVATIVE OF HYDRAULIC RADIUS WITH RESPECT TO DEPTH
DBDY(Y,I)=DERIVATIVE OF TOP WIDTH WITH RESPECT TO DEPTH
CM(Y,I) =MANNING'S FRICTIONAL COEFFS AT STATION I
G         =GRAVITATIONAL CONSTANT
NZ=DIFF. ZONES FOR NEUSE RIVER ESTUARY SUBJECTED TO VARIABLE WIND
I,K OR NS=INDEX FOR  STATION OR SEGMENT
VWS(I,KT)=VARIABLE WIND SPEED AT STATION I AND TIME KT (MPH)
VWD(I,KT)=VARIABLE WIND DIRECTION AT STATION I AND TIME KT (DEG.)

SWX(I)=WIND STRESS AT STSTION I (LB/SQ FT)
PHI(I)=ANGLE WHICH NEUSE RIVER MAKES WITH THE X-AXIX (IE EAST)
PHI IS IN DEG.
WSC=WIND STRESS COEFFICIENT
TPRINT=TIME AT WHICH THE RESULTS ARE PRINTED(HOURS)

T(K)      =TIME AT WHICH COMPUTATION ARE MADE, IN HRS.

QUST(K) =GIVEN DISCHARGE AT UPSTREAM BOUNDARY AT TIME T(K),IN CFS.
DUST(K) =GIVEN DEPTH AT UPSTREAM BOUNDARY AT TMIE T(K),IN FT.
QDST(K) =GIVEN DISCHARGE AT DOWNSTREAM BOUNDARY AT TIME T(K)
DDST(K) =GIVEN DEPTH AT DOWNSTREAM BOUNDARY AT TIME T(K)
DC(J)     =GIVEN COEFFS OF THE RATING CURVE AT DOWNSTREAM BOUNDARY
MSIMQ=A SUBROUTINE FOR OBTAINING SOLUTION OF A SET OF SIMULTANEOUS
LINEAR EQUATIONS AX=C ,IT WAS OBTAINED BY MODIFYING SIMQ WHICH
IS A BUILT-IN PROGRAM IN IBM COMPUTER 360/75
AA(I,J) =ELEMENTS OF COEFFICIENT MATRIX
C(K)      =VECTOR OF RESIDUES

ID        =INDEX FOR IDENFICATION OF THE BOUNDARY CONDITIONS:
           ID=1 DISCHARGES ARE GIVEN BOTH AT UPSTREAM AND
                DOWNSTREAM BOUNDARIES
           ID=2 DISCHARGES ARE GIVEN AT UPSTREAM BOUNDARY AND
                DEPTHS ARE GIVEN AT DOWNSTREAM BOUNDARY
           ID=3 DEPTHS ARE GIVEN AT UPSTREAM BOUNDARY AND
                DISCHARGES ARE GIVEN AT DOWNSTREAM BOUNDARY
           ID=4 DEPTHS ARE GIVEN BOTH AT UPSTREAM AND DOWNSTREAM
                BOUNDARIES
           ID=5 DISCHARGES ARE GIVEN AT UPSTREAM BOUNDARY AND
```

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         A RATING CURVE EQUATION IS GIVEN AT DOWNSTREAM
         BOUNDARY
    ID=6 DEPTHS ARE GIVEN AT UPSTREAM BOUNDARY AND A RATING
         CURVE EQUATION IS GIVEN DOWNSTREAM BOUNDARY

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                        ************
                        MAIN PROGRAM
                        ************

 COMMON/PARAM/ARO(50),AR1(50),AR2(50),CM(50),DC(6)
 COMMON/HPRAM/Q(50),Y(50),V(50),VIN(50),QIN(50),YIN(50),STAGE(50),
*A(50),Z(50),AA(100,100),C(100),QUST(100),QDST(100),DUST(100),
*DDST(100),QL(50)
 COMMON/INTRC/DQ(100),DY(100),SWX(50),DIST(50)
 COMMON/VINPUT/T(100),TFIN,TIME,TPRINT,MN,L,N,NN,NL,ID,DT
 COMMON/WINDC/VWS(10,100),VWD(10,100),VWX(50,100),WD(50,100),
*WX(50,100),PHI(50),NZ

                    ***********************
                      LABELS  AND  TITLES
2 FORMAT(//35X,'=INPUT DATA=')
3 FORMAT(8F10.3)
4 FORMAT(///35X,'UNSTEADY FLOW COMPUTATIONS BY THE IMPLICIT METHOD')
5 FORMAT(3F10.4,4I5)
6 FORMAT(//15X,'FINAL TIME          TFIN=',F10.3,'HOURS',
 1       /15X,'TOLER LIMIT OF DY YEPS=',F10.3,'FT',
 2       /15X,'TOLER LIMIT OF DQ QEPS=',F10.3,'CFS',
 1       /15X,'NO. OF TIME POINTS  MN=',I10,
 1       /15X,'NO. OF STATIONS      N=',I10,
 1       /15X,'NO. OF ZONES        NZ=',I10,
 1       /15X,'INPUT INDEX         ID=',I10/)
7 FORMAT(5X,'(',I2,')',5X,F10.3,7X,F10.3,5X,F10.3,2(5X,F6.2),7X,
 1F10.3)
8 FORMAT(8F10.3)
9 FORMAT(///45X,'VALUES OF VARIABLES')
10 FORMAT(///13X,'STAT',8X,'DISTANCE',10X,'STAGE',10X,'VELOCITY',
 15X,'DISCHARGE',8X,'AREA',11X,'DEPTH',8X,'ELEVA'/)
11 FORMAT(12X,'(.NO.)',8X,'(MILES)',11X,'(FT)',11X,
 1'(FT/SEC)',7X,'(CFS)',10X,'(SQ FT)',9X,'(FT)',9X,'(FT)'/)
12 FORMAT(1H,11X,I2,5(3X,F13.4),2(3X,F10.2))
13 FORMAT(8E10.4)
14 FORMAT(//5X,'STAT',5X,'REF.LINE ELV.',5X,'INIT.DEPTH',5X,'INIT.DIS
 1CH',5X,'DIST.',5X,'ANG.PHI',5X,'LATERAL INFLOW',//
 218X,'FT.',14X,'FT.',12X,'CFS',9X,'MILES',5X,'DEGREES',10X,'CFS',
 1//)
15 FORMAT(//20X,'INPUT UPSTREAM BOUNDARY DISCHARGE IN CFS'/)
16 FORMAT(//20X,'INPUT DOWNSTREAM BOUNDARY DISCHARGE'/)
17 FORMAT(//20X,'INPUT DOWNSTREAM BOUNDARY DEPTH IN FT.'/)
18 FORMAT(20X,'INPUT UPSTREAM BOUNDARY DEPTH'/)
19 FORMAT(//25X,'INPUT TIME INTERVALS IN HOURS'/)
20 FORMAT(//15X,'INPUT DOWNSTREAM BOUNDARY RATING CURVE'/)
21 FORMAT(//13X,'NUMBER OF ITERATIONS=',I2)
```

```
 22 FORMAT(5(5X,E10.4))
 23 FORMAT(//5X,'ITER=',I2,5X,'YIN(',I2,')=',F10.3,'Y(',I2,')=',F10.3)
 25 FORMAT(/10X,'*PROCESS DOES NOT CONVERGE AFTER 10 ITERATIONS'/)
 26 FORMAT(//13X,'TIME IN HOUR=',F10.2)

                          *************************
                          INITIAL AND BOUNDARY VALUES
                          *************************

    WRITE(3,2)
    READ(1,5) TFIN,YEPS,QEPS,MN,N,NZ,ID
    WRITE(3,6) TFIN,YEPS,QEPS,MN,N,NZ,ID
    READ(1,8) (DIST(I),I=1,N)
    READ(1,8) (QL(I),I=1,N)
    READ(1,3) (T(K),K=1,MN)
    WRITE(3,19)
    WRITE(3,3) (T(K),K=1,MN)
    GO TO (100,105,110,115,116,117),ID


       BOUNDARY CONDITION :ID=1

100 READ(1,3)(QUST(K),K=1,MN)
    WRITE(3,15)
    WRITE(3,3)(QUST(K),K=1,MN)
    READ(1,3) (QDST(K),K=1,MN)
    WRITE(3,16)
    WRITE(3,3) (QDST(K),K=1,MN)
    GO TO 120


       BOUNDARY CONDITION :ID=2

105 READ(1,3)(QUST(K),K=1,MN)
    WRITE(3,15)
    WRITE(3,3)(QUST(K),K=1,MN)
    READ(1,3) (DDST(K),K=1,MN)
    WRITE(3,17)
    WRITE(3,3)(DDST(K),K=1,MN)
    GO TO 120


       BOUNDARY CONDITION :ID=3

110 READ(1,3)(DUST(K),K=1,MN)
    WRITE(3,18)
    WRITE(3,3)(DUST(K),K=1,MN)
    READ(1,3) (QDST(K),K=1,MN)
    WRITE(3,16)
    WRITE(3,3) (QDST(K),K=1,MN)
    GO TO 120


       BOUNDARY CONDITION :ID=4

115 READ(1,3)(DUST(K),K=1,MN)
```

```
      WRITE(3,18)
      WRITE(3,3)(DUST(K),K=1,MN)
      READ(1,3) (DDST(K),K=1,MN)
      WRITE(3,17)
      WRITE(3,3)(DDST(K),K=1,MN)
      GO TO 120

         BOUNDARY CONDITION :ID=5

  116 READ(1,3)(QUST(K),K=1,MN)
      WRITE(3,15)
      WRITE(3,3)(QUST(K),K=1,MN)
      READ(1,13) (DC(J),J=1,3)
      WRITE(3,20)
      WRITE(3,22) (DC(J),J=1,3)
      GO TO 120

         BOUNDARY CONDITION :ID=6

  117 READ(1,3)(DUST(K),K=1,MN)
      WRITE(3,18)
      WRITE(3,3)(DUST(K),K=1,MN)
      READ(1,13) (DC(J),J=1,3)
      WRITE(3,20)
      WRITE(3,22) (DC(J),J=1,3)

       READ STATEMENTS FOR CHANNEL BOTTOM ELEV. Z(I), INITIAL DEPTH
       YIN(I),INITIAL DISCHARGE QIN(I) AND ANGLE PHI(I)

  120 READ(1,8) (Z(I),I=1,N)
      READ(1,8) (YIN(I),I=1,N)
      READ(1,8) (QIN(I),I=1,N)
  423 READ(1,203) (PHI(I),I=1,N)
  203 FORMAT(20F4.0)
  119 FORMAT(F10.7)
      READ(1,119)WSC
      DO 200 I=1,NZ
      READ(1,201) (VWS(I,KT),KT=1,MN)
  200 READ(1,201) (VWD(I,KT),KT=1,MN)
  205 FORMAT(//5X,'(',I2,')',20(1X,F4.0))
  201 FORMAT(20F4.0)
  420 WRITE(3,14)
  424 DO 118 I=1,N
  118 WRITE(3,7) I,Z(I),YIN(I),QIN(I),DIST(I),PHI(I),QL(I)
  512 FORMAT(//5X,'(NZ) WIND SPEED IN MPH AT INPUT TIMES(HOURS)')
      WRITE(3,512)
  425 DO 204 I=1,NZ
  204 WRITE(3,205) I,(VWS(I,KT),KT=1,MN)
  513 FORMAT(//5X,'(NZ) WIND DIRECTION IN DEGREES AT INPUT TIME INTERVAL
     1S(HOURS)')
      WRITE(3,513)
      DO 206 I=1,NZ
  206 WRITE(3,205) I,(VWD(I,KT),KT=1,MN)
```

```
      SUBROUTINE FOR THE CROSS-SECTIONAL AREA COEFFICIENTS
421 CALL COEFS

      SUBROUTINE FOR THE MANNING COEFFICIENT
422 CALL FRIC

                                  ************
                                  COMPUTATIONS
                                  ************
124 L=1
    DO 125 I=1,N
    Q(I)=QIN(I)
125 Y(I)=YIN(I)
134 WRITE(3,4)
    WRITE(3,9)
    NL=2.*N
    NN=N-1
    TIME=T(1)
    CALL WIND

                   ESTABLISH AND SOLVE SYSTEM OF EQUATIONS
                             AT GIVEN TIME STEP

136 READ(1,137) TPRINT
137 FORMAT(F10.2)
135 L=L+1
    DELT=T(L)-T(L-1)
    DT=DELT*3600.
    TIME=TIME+DT/3600.

                                  BEGIN ITERATION
    ITER=1
 65 DO 70 I=1,NL
    DO 70 J=1,NL
 70 AA(I,J)=0.

    DO 211 I=1,N
211 SWX(I)=WX(I,L)*WSC
                      FIND MATRIX OF COEFFICIENTS
    CALL BOUND
    CALL INTER
    CALL ARRAY(2,NL,NL,100,100,AA,AA)
    CALL MSIMQ(AA,C,NL,KS)
    CALL ARRAY(1,NL,NL,100,100,AA,AA)

                               COMPUTED VALUES
    KK=NL-1
    DO 210 J=1,KK,2
    I=(J+1)/2
    DY(I)=C(J)
210 DQ(I)=C(J+1)
                   VARIATIONS IN ONE TIME STEP
    DO 220 I=1,N
```

```
      Y(I)=Y(I)-DY(I)
  220 Q(I)=Q(I)-DQ(I)
      DO 225 I=1,N
      Y1=Y(I)
      IF(Y1) 221,221,225
  221 WRITE(3,23) ITER,I,YIN(I),I,Y(I)
  225 CONTINUE
                   TEST IF ADDITIONAL ITERATION IS REQUIRED
      DO 260 I=1,N
      ER1=DY(I)
      ER2=DQ(I)
      IF(ABS(ER1)-YEPS) 250,250,245
  250 IF(ABS(ER2)-QEPS) 260,260,245
  245 ITER=ITER+1
                              TEST FOR CONVERGENCE
      IF(ITER-10) 65,65,255
  255 WRITE(3,25)
      GO TO 265
  260 CONTINUE
  265 DO 270 I=1,N
      YIN(I)=Y(I)
      Y1=Y(I)
      A(I)=AR(Y1,I)
      STAGE(I)=Y(I)+Z(I)
      VIN(I)=Q(I)/A(I)
  270 QIN(I)=Q(I)
      IF(TIME-TPRINT) 135,281,281

                                PRINT RESULTS
  281 WRITE(3,21) ITER
      WRITE(3,26)TIME
      WRITE(3,10)
      WRITE(3,11)
      DO 280 I=1,N
  280 WRITE(3,12) I,DIST(I),STAGE(I),VIN(I),Q(I),A(I),Y(I),Z(I)
      IF(TIME-TFIN)136,310,310
  310 CALL EXIT
      END
```

```
      SUBROUTINE WIND

         WIND STRESS COMPUTATION

      COMMON/VINPUT/T(100),TFIN,TIME,TPRINT,MN,L,N,NN,NL,ID,DT
      COMMON/WINDC/VWS(10,100),VWD(10,100),VWX(50,100),WD(50,100),
     *WX(50,100),PHI(50),NZ
      DO 100 I=1,10
      DO 100 KT=1,MN
      N2=1
      VWX(I,KT)=VWS(N2,KT)
  100 WD(I,KT)=VWD(N2,KT)
      DO 101 I=11,20
      DO 101 KT=1,MN
      N2=NZ-2
      VWX(I,KT)=VWS(N2,KT)
  101 WD(I,KT)=VWD(N2,KT)
      DO 102 I=21,30
      DO 102 KT=1,MN
      N2=NZ-1
      VWX(I,KT)=VWS(N2,KT)
  102 WD(I,KT)=VWD(N2,KT)
      DO 103 I=31,41
      DO 103 KT=1,MN
      N2=NZ
      VWX(I,KT)=VWS(N2,KT)
  103 WD(I,KT)=VWD(N2,KT)
      PI=3.14159
      DO 90 I=1,N
      DO 90 KT=1,MN
   90 WX(I,KT)=VWX(I,KT)*VWX(I,KT)*COS((WD(I,KT)-PHI(I))*PI/180.)
      RETURN
      END
```

```
      SUBROUTINE INTER
                          COMPUTATIONS AT INTERIOR POINTS
                          *******************************

      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      COMMON/HPRAM/Q(50),Y(50),V(50),VIN(50),QIN(50),YIN(50),STAGE(50),
     *A(50),Z(50),AA(100,100),C(100),QUST(100),QDST(100),DUST(100),
     *DDST(100),QL(50)
      COMMON/INTRC/DQ(100),DY(100),SWX(50),DIST(50)
      COMMON/VINPUT/T(100),TFIN,TIME,TPRINT,MN,L,N,NN,NL,ID,DT

      G=32.2

  100 DO 150 I=1,NN
      M=2*I
      J=2*I-1
      DELX=ABS(DIST(I+1)-DIST(I))
      DX=DELX*5280.
      DXDT=DX/DT
      DTDX=DT/DX
      YB1=YIN(I)
      YB2=YIN(I+1)
      Y1=Y(I)
      Y2=Y(I+1)
      QB1=QIN(I)
      QB2=QIN(I+1)
      Q1=Q(I)
      Q2=Q(I+1)
      A1=AR(Y1,I)
      A2=AR(Y2,I+1)
      B1=B(Y1,I)
      B2=B(Y2,I+1)
      DB1=DBDY(Y1,I)
      BM=(B1+B2)/2.
      DB2=DBDY(Y2,I+1)

       WST IS THE TERM DUE TO WIND
       WSTY1,WSTY2,WSTQ1 AND WSTQ2 ARE THE DERIVATIVES OF WST WITH
       RESPECT TO Y1,Y2,Q1 AND Q2 RESPECTIVELY

  102 SWM=(SWX(I)+SWX(I+1))/2.
      WST=SWM*DX*BM/G
      WSTY1=(SWM*DX*DB1)/(2.*G)
      WSTY2=(SWM*DX*DB2)/(2.*G)
  101 WSTQ1=0.0
      WSTQ2=0.0
      H1=HR(Y1,I)
      H2=HR(Y2,I+1)
      Z1=Z(I)
      Z2=Z(I+1)
      F1=CM(I)
      F2=CM(I+1)
      DHR1=DHR(Y1,I)
      DHR2=DHR(Y2,I+1)
      W=.5*(A1+A2)/A1
```

```
      DWY1=-.5*A2*B1/A1**2
      DWY2=.5*B2/A1
      QM=(Q1+Q2)/2.
      AM=(A1+A2)/2.
      RM=(H1+H2)/2.
      CF=(F1+F2)/2.

C     SFM IS THE FRICTION TERM

      SFM=CF*CF*(QM/AM)*ABS(QM/AM)/(2.2082*RM**(4./3.))
      DSFY1=-2.*SFM*DHR1/(3.*RM)-SFM*B1/AM
      DSFY2=-2.*SFM*DHR2/(3.*RM)-SFM*B2/AM
      DSFQ1=CF*CF*QM/(2.2082*AM*AM*RM**(4./3.))
      DSFQ2=DSFQ1
      IF((Q1/A1)) 110,110,120
  110 DSFY1=-DSFY1
      DSFQ1=-DSFQ1
  120 IF((Q2/A2)) 130,130,140
  130 DSFY2=-DSFY2
      DSFQ2=-DSFQ2
  140 QD=Q2-Q1
      DELY=0.5*((Y1-YB1)+(B2/B1)*(Y2-YB2))
      X1=Y1+Z1
      X2=Y2+Z2
      QT=-.5*DXDT*(Q1-QB1+Q2-QB2)/G
      QX=(Q1*Q1)/(G*A1)-(Q2*Q2)/(G*A2)
      DQTY1=0.0
      DQTY2=0.0
      DQTQ1=-.5*DXDT/G
      DQTQ2=-.5*DXDT/G
      DQXY1=-(Q1*Q1*B1)/(G*A1*A1)
      DQXY2=(Q2*Q2*B2)/(G*A2*A2)
      DQXQ1=2.*Q1/(A1*G)
      DQXQ2=-2.*Q2/(A2*G)


C     DR1 IS THE RESIDUE FROM CONTINUITY EQUATION

      DR1=DELY+QD/(B1*DXDT)-QL(I)*DTDX/B1
      DR1Y1=.5-(DB1/(B1*B1))*(.5*B2*(Y2-YB2)+QD*DTDX-QL(I)*DTDX)
      DR1Y2=.5*B2/B1+.5*DB2*(Y2-YB2)/B1
      DR1Q1=-DTDX/B1
      DR1Q2=DTDX/B1

C     DR2 IS THE RESIDUE FROM MOMENTUM EQUATION

      DR2=QT+QX+(X1-X2)*A1*W-SFM*DX*A1*W+WST
      DR2Y1=DQTY1+DQXY1+(X1-X2)*(A1*DWY1+W*B1)-DX*A1*W*DSFY1+A1*W
     1-SFM*DX*(A1*DWY1+W*B1)+WSTY1
      DR2Y2=DQTY2+DQXY2-A1*W+(X1-X2)*(A1*DWY2)-SFM*DX*A1*DWY2-DX*A1*W
     1*DSFY2+WSTY2
      DR2Q1=DQTQ1+DQXQ1-DSFQ1*DX*A1*W+WSTQ1
      DR2Q2=DQTQ2+DQXQ2-DSFQ2*DX*A1*W+WSTQ2

C     FOLLOWING ARE THE ELEMENTS OF THE COEFFICIENT MATRIX
C     (I.E. AA(I,J) )
```

```
      AA(M,J)=DR1Y1
      AA(M,J+1)=DR1Q1
      AA(M,J+2)=DR1Y2
      AA(M,J+3)=DR1Q2
      AA(M+1,J)=DR2Y1
      AA(M+1,J+1)=DR2Q1
      AA(M+1,J+2)=DR2Y2
      AA(M+1,J+3)=DR2Q2
      C(M)=DR1
  150 C(M+1)=DR2
      RETURN
      END
```

```
      SUBROUTINE BOUND
                         ********************************
                         COMPUTATIONS AT UPSTREAM BOUNDARY
                             AND DOWNSTREAM BOUNDARY

      COMMON/HPRAM/Q(50),Y(50),V(50),VIN(50),QIN(50),YIN(50),STAGF(50),
     *A(50),Z(50),AA(100,100),C(100),QUST(100),QDST(100),DUST(100),
     *DDST(100),QL(50)
      COMMON/VINPUT/T(100),TFIN,TIME,TPRINT,MN,L,N,NN,NL,ID,DT


      GO TO (75,80,85,90,95,100),ID

         BOUNDARY CONDITION :ID=1

   75 Q(1)=QUST(L)
      Q(N)=QDST(L)
      DR1=Q(1)-QUST(L)
      DRN=Q(N)-QDST(L)
      DR1DY=0.0
      DR1DQ=1.
      DRNDY=0.0
      DRNDQ=1.
      GO TO 200

         BOUNDARY CONDITION :ID=2

   80 Q(1)=QUST(L)
      Y(N)=DDST(L)
      DR1=Q(1)-QUST(L)
      DRN=Y(N)-DDST(L)
      DR1DY=0.0
      DR1DQ=1.
      DRNDY=1.0
      DRNDQ=0.
      GO TO 200

         BOUNDARY CONDITION :ID=3

   85 Y(1)=DUST(L)
      Q(N)=QDST(L)
      DR1=Y(1)-DUST(L)
      DRN=Q(N)-QDST(L)
      DR1DY=1.0
      DR1DQ=0.
      DRNDY=0.0
      DRNDQ=1.
      GO TO 200

         BOUNDARY CONDITION :ID=4

   90 Y(1)=DUST(L)
      Y(N)=DDST(L)
      DR1=Y(1)-DUST(L)
      DRN=Y(N)-DDST(L)
      DR1DY=1.0
```

```
      DR1DQ=0.
      DRNDY=1.0
      DRNDQ=0.
      GO TO 200
C
C        BOUNDARY CONDITION :ID=5
C
   95 Q(1)=QUST(L)
      QN=Q(N)
      YN=Y(N)
      DR1=Q(1)-QUST(L)
      DRN=QN-RC(YN)
      DR1DY=0.0
      DR1DQ=1.
      DRNDY=-DRCY(YN)
      DRNDQ=1.
      GO TO 200
C
C        BOUNDARY CONDITION :ID=6
C
  100 Y(1)=DUST(L)
      YN=Y(N)
      QN=Q(N)
      DR1=Y(1)-DUST(L)
      DRN=QN-RC(YN)
      DR1DY=1.0
      DR1DQ=0.
      DRNDY=-DRCY(YN)
      DRNDQ=1.
  200 C(1)=DR1
      C(NL)=DRN
C
C     AA(I,J) ELEMENTS OF THE COEFFICIENTS MATRIX WHICH COME FROM
C       BOUNDARY CONDITIONS
C
      AA(1,1)=DR1DY
      AA(1,2)=DR1DQ
      AA(NL,NL-1)=DRNDY
      AA(NL,NL)=DRNDQ
      RETURN
      END
```

```
      SUBROUTINE MSIMQ (A,B,N,KS)
      DIMENSION A(1),B(1)

              FORWARD  SOLUTION
      TOL=0.0
      KS=0
      JJ=-N
      DO 65 J=1,N
      JY=J+1
      JJ=JJ+N+1
      BIGA=0.
      IT=JJ-J
      L1=J+4
      IF(L1-N) 10,10,12
   12 L1=N
   10 DO 30 I=J,L1

           SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN

      IJ=IT+I
      IF(ABS(BIGA)-ABS(A(IJ))) 20,30,30
   20 BIGA=A(IJ)
      IMAX=I
   30 CONTINUE

          TEST FOR PIVOT LESS THAN TOLENANCE(SINGULAR MATRIX)

   32 IF(ABS(BIGA)-TOL) 35,35,40
   35 KS=1
      RETURN

            INTERCHANGE ROWS IF NECESSARY

   40 I1=J+N*(J-2)
      IT=IMAX-J
      L2=J+4
      IF(L2-N) 42,42,44
   44 L2=N
   42 DO 50 K=J,L2
      I1=I1+N
      I2=I1+IT
      SAVE=A(I1)
      A(I1)=A(I2)
      A(I2)=SAVE

          DIVIDE EQUATION BY LEADING COEFFICIENT

   50 A(I1)=A(I1)/BIGA
   52 SAVE=B(IMAX)
      B(IMAX)=B(J)
      B(J)=SAVE/BIGA

            ELIMINATE NEXT VARIABLE

      IF(J-N) 55,70,55
   55 IOS=N*(J-1)
```

```
      L3=JY+4
      IF(L3-N) 57,57,59
   59 L3=N
   57 DO 65 IX=JY,L3
      IXJ=IOS+IX
      IT=J-IX
      DO 60 JX=JY,L3
      IXJX=N*(JX-1)+IX
      JJX=IXJX+IT
   60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))
   65 B(IX)=B(IX)-(B(J)*A(IXJ))

           BACK   SOLUTION

   70 NY=N-1
      IT=N*N
      DO 80 J=1,NY
      IA=IT-J
      IB=N-J
      IC=N
      DO 80 K=1,J
      B(IB)=B(IB)-A(IA)*B(IC)
      IA=IA-N
   80 IC=IC-1
      RETURN
      END




      SUBROUTINE COEFS

      READ THE COEFFICIENTS FOR AREA EQUATION

      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      COMMON/VINPUT/T(100),TFIN,TIME,TPRINT,MN,L,N,NN,NL,ID,DT
    8 FORMAT(8F10.2)
   14 FORMAT(17X,'(',I2,')',2(2X,F10.2))
   15 FORMAT(//15X,'COEFF. FOR THE AREA  EQUATIONS')
      WRITE(3,15)
      WRITE(3,13)
      READ(1,8) (AR0(I),I=1,N)
      READ(1,8) (AR1(I),I=1,N)
   13 FORMAT(/15X,'-STAT-',6X,'-AR0-',7X,'-AR1-'/)
      DO 130 I=1,N
  130 WRITE(3,14) I,AR0(I),AR1(I)
      RETURN
      END
```

```
      SUBROUTINE FRIC

C     MANNING COEFFICIENTS ARE SPECIFIED IN THIS SUBROUTINE

      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      COMMON/VINPUT/T(100),TFIN,TIME,TPRINT,MN,L,N,NN,NL,ID,DT
      DO 10 I=1,N
   10 CM(I)=0.025
      RETURN
      END


      FUNCTION RC(Y)
            THIS IS THE EQUATION FOR RATING CURVE WHERE RC IS THE
            DISCHARGE AND DC(1), DC(2), AND DC(3) ARE THE COEFFICIENTS
                       AT EACH STATION
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      RC=DC(1)*Y+DC(2)*Y**DC(3)
      RETURN
      END


      FUNCTION DRCY(Y)

           DRCY  IS THE DERIVATIVE OF THE DISCHARGE WITH RESPECT
            TO DEPTH GIVEN BY THE EQUATION FOR THE RATING CURVE
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      DRCY=DC(1)+DC(2)*DC(3)*Y**(DC(3)-1.)
      RETURN
      END


      FUNCTION AR(Y,I)

            THIS IS THE EQUATION FOR AREA AS A FUNCTION OF DEPTH
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      AR=AR0(I)+AR1(I)*Y
      RETURN
      END


      FUNCTION B(Y,I)

            THIS IS THE EQUATION OF WIDTH AS A FUNCTION OF DEPTH
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      B=Y+AR1(I)-Y
      RETURN
      END
```

```
      FUNCTION HR(Y,I)
           THIS IS THE EQUATION OF THE HYDRAULIC RADIUS AS A FUNCTION OF
                                     DEPTH
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      HR=(AR0(I)/AR1(I))+Y
   30 RETURN
      END


      FUNCTION DHR(Y,I)

           THIS IS THE EQUATION FOR THE DERIVATIVE OF HYDRAULIC RADIUS
                          WITH RESPECT TO DEPTH
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      DHR=Y+I+1.-Y-I
      RETURN
      END


      FUNCTION DBDY(Y,I)
           THIS IS THE EQUATION FOR THE DERIVATIVE OF WIDTH WITH
                               RESPECT TO DEPTH
      COMMON/PARAM/AR0(50),AR1(50),AR2(50),CM(50),DC(6)
      DBDY=I+Y+0.-I-Y
      RETURN
      END
```

```
**************************************************
**************************************************
**                                              **
**       DYNAMIC  WATER  QUALITY  MODEL         **
**                                              **
**                                              **
**           THE  NEUSE  ESTUARY                **
**                                              **
**              NORTH  CAROLINA                 **
**                                              **
**                                              **
**          PART II:  WATER  QUALITY            **
**                                              **
**************************************************
**************************************************


              PROGRAM NAME: WQUAL

               METHOD: EXPLICIT


   WQUAL IS AN EXPLICIT NUMERICAL MODEL FOR THE
     SOLUTION OF THE MASS-BALANCE EQUATION

THE PROCEDURE STARTS WITH KNOWN VALUES OF THE VARIABLES AT THE
CURRENT TIME STEP AND COMPUTES VALUESS AT THE NEXT TIME STEP

          **  DEFINITIONS  **

   N  = NO. OF STATIONS
   DX   = DISTANCE BETWEEN STATIONS IN FT.
   DELX = DISTANCE BETWEEN STATIONS IN MILES
   M  = NO. OF GIVEN DATA POINTS AT UPSTREAM BOUNDARY
   DELT = TIME INTERVAL BETWEEN DATA AT UPSTREAM BOUNDARY, IN HOURS
   DT   = COMPUTATION TIME STEP IN SECS.
   DTDAY = COMPUTATION TIME STEP IN DAYS
   TIME  = TIME OF COMPUTED VALUES, IN HOURS,
   I = AN INDEX IDENTIFYING STATIONS
   A  = X-SECTION AREA AT CURRENT TIME, IN SQ FT.
   Q  = DISCHARGE AT CURRENT TIME, IN CFS
   Y  =  WATER  DEPTH  ,IN  FT.
   T = TIME AT WHICH UPSTREAM DATA ARE READ, IN HOURS
   QUST = UPSTREAM  DISCHARGE,  IN CFS
   QDST = DOWNSTREAM  DISCHARGE, IN CFS
   L = AN INDEX IDENTIFYING T FOR UPSTREAM DATA
   E = DISPERSION COEFFICIENT, IN SQ. FT./SEC
   COU = UPSTREAM DO AT TIME
   CL  = LATERAL INPUT OF MATERIAL PER UNIT LENGTH OF ESTUARY
   CBLA = DISTRIBUTED BOD , IN MG/L PER DAY
   CB = BOD AT CURRENT TIME, IN MG/L
   CO = DO AT CURRENT TIME, IN MG/L
   CCS = SATURATION VALUE OF DO, IN MG/L
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          CM    = MANNING'S  COEFFICIENT  OF  FRICTION
          TEM =  TEMPERATURE  , IN C
          C2  = NH3-N
          C3  = (NO2 + NO3)-N
          C4  = ALGAL  NITROGEN
          C5  = ORGANIC  NITROGEN
          K 'S  = THESE ARE DECAY AND REACTION RATES DEFINED UNDER DATA
          C  = COMPUTED VALUE OF CONCENTRATION IN MG/L; IT REPRESENTS
                 DIFFERENT PARAMETERS AT EACH OPERATION
          ALPHA=  A  WEIGHTING  FACTOR
          BETA=  A  WEIGHTING  FACTOR
          TPRINT = TIME FOR PRINTOUT, IN HOURS
          DPRINT = TIME INTERVAL BETWEEN PRINTOUTS, IN HOURS
          RK2 = REAERATION  RATE IN (/DAY)
 REAL  K1,K3,K22,K23,K0,K33,K34,K44,K45,K52,K55
 DIMENSION  A(200),Q(200),X(200),ALPHA(200),BETA(200),
2            Y(200),Z(200),V(200),T(200),RK2(200),
3            QUST(200),QDST(200),QL(200),CM(200),
4            CL(200),CBLA(200),E(200),
5            CO(200),CB(200),C2(200),C3(200),C4(200),C5(200),
6            CBU(200),COU(200),C2U(200),C3U(200),C4U(200),C5U(200)
 DIMENSION C(200),W(200)


 READ(1,1)  M,N,DELX,DELT
1 FORMAT (2I5,2F5.2)
 DT=43200.
 DPRINT=12.
 NN=N-1
 MM=M-1
 DX=DELX*5280.
 DTDX=DT/DX
 DTDAY=DT/(24.*3600.)
 TEM=16.
 TFIN=696.
 ALPHA(1)=1.
 BETA(1)=0.
 CM(1)=0.035
 CCS=9.5
 WRITE(3,3) N,M,DELX,DELT
3 FORMAT(/T6,'N,NO. OF STATIONS=',I5,
 1/T6,'M,NO. OF INPUT TIMES=',I5,
 2/T6,'DELX,LENGTH OF SEGMENT=',F5.2,'MILE',
 3/T6,'DELT, TIME INTERVAL FOR INPUT DATA=',F5.2,'HOURS')

                    S E C T I O N    I
                       D  A  T  A

                   RATES  AND  COEFFICIENTS

 READ (1,11)  K1,K3,K22,K23,K24,K25
 READ(1,11) K33,K34,K44,K45,K52,K55
 WRITE(3,4)   K1,K3,K22,K52,K33,K23,K24,K34,K25,K45,K44,K55,CCS
4 FORMAT(//10X,'DECAY COEFF. OF BOD                        K1=',F10.2/
1   10X,'COEFF. ACCOUNT FOR BOD REMOVAL                  K3=',F10.2/
2   10X,'DECAY COEFF. OF C2                              K22=',F10.2/
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  3  10X,'COEF. FOR RATE OF CONVERSION OF C5 TO C2  K52=',F10.2/
  4  10X,'DECAY COEFF. FOR C3                       K33=',F10.2/
  5  10X,'COEF. FOR RATE OF CONVERSION OF C2 TO C3  K23=',F10.2/
  6  10X,'COEF. FOR RATE OF CONVERSION OF C2 TO C4  K24=',F10.2/
  7  10X,'COEF. FOR RATE OF CONVERSION OF C3 TO C4  K34=',F10.2/
  8  10X,'COEF. FOR RATE OF CONVERSION OF C2 TO C0  K25=',F10.2/
  9  10X,'COEF. FOR RATE OF CONVERSION OF C4 TO C5  K45=',F10.2/
  *  10X,'DECAY COEFF. OF C4                        K44=',F10.2/
  *  10X,'DECAY COEFF. OF C5                        K55=',F10.2/
  *10X,'SATURATION  OF DO AT A GIVEN TEMP           CCS=',F10.2)

 5 FORMAT(8F10.5)
   WRITE(3,7)
 7 FORMAT(/5X,'NOTE:   CO=DISSOLVED OXYGEN',/13X,'CB= BOD',
  1/13X,'C2 = NH3N',/13X,'C3 = (NO2+NO3)-N',/13X,'C4 = ALGAL NITROGEN
  2',/13X,'C5 = ORGANIC NITROGEN')
   WRITE (3,8)
 8 FORMAT(/57X,'INPUT  DATA',//54X,'BOUNDARY  VALUES'///)
11 FORMAT (6F10.3)
   WRITE (3,12)
12 FORMAT(T6,'TIME',T13,'DISCHARGE',T26,'DISCHARGE',T39,'WIND',
  1T50,'CO',  T60,'CB', T70,'C2',T80,'C3', T90,'C4',T100,'C5'
  2/T12,'(UPSTREAM)',  T25,'(DOWNSTREAM)'
  3///T5,'(HOUR)',T14,'(CFS)',T28,'(CFS)',T38,'(MPH)',T48,'(MG/L)',
  4T58,'(MG/L)',T68,'(MG/L)',T78,'(MG/L)',T88,'(MG/L)',T98,'(MG/L)'
  5//)

                CROSS  SECTIONAL  AREAS
   READ (1,13)(A(I),I=1,N)

                              DEPTHS
   READ (1,13) (Y(I),I=1,N)

                           INPUT  TIMES

   READ (1,13) (T(K),K=1,M)

                        UPSTREAM  DISCHARGE

   READ (1,13) (QUST(K),K=1,M)

                      DOWNSTREAM  DISCHARGE
   READ (1,13) (QDST(K),K=1,M)
                           WIND  SPEED
   READ(1,5)(W(K),K=1,M)
13 FORMAT (8F10.2)
     UPSTREAM  TIME  VARIABLE  WATER  QUALITY  INPUT  DATA
   READ (1,5) (COU(K),K=1,M)
   READ (1,5) (CBU(K),K=1,M)
   READ (1,5) (C2U(K),K=1,M)
   READ(1,5) (C3U(K),K=1,M)
   READ (1,5) (C4U(K),K=1,M)
   READ (1,5) (C5U(K),K=1,M)

   DO 14 K=1,M
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      THIS IS A TEST FOR REAERATION DUE TO A 5 MPH WIND.  WHEN WIND DATA
      ARE GIVEN AS INPUT, THEN THE FOLLOWING CARD MUST BE REMOVED
      W(K)=5.

   14 WRITE (3,15)  (T(K),QUST(K),QDST(K),W(K),COU(K),CBU(K),C2U(K),
     1C3U(K),C4U(K),C5U(K))
   15 FORMAT(3X,F7.1,2X,F10.2,3X,F10.2,7(F10.2))
              INITIAL  WATER  QUALITY  PARAMETERS
      READ(1,5)(C0(I),I=1,N)
      READ (1,5)(CB(I),I=1,N)
      READ (1,5)(C2(I),I=1,N)
      READ (1,5) (C3(I),I=1,N)
      READ(1,5)(C4(I),I=1,N)
      READ (1,5)(C5(I),I=1,N)


      X(1)=0.
      DO  20 I=1,NN
   20 X(I+1)=X(I)+DELX
      DO 40  I=1,N
      BETA(I)=BETA(1)
      C(I)=0.
      CL(I)=0.
      EI=I
      EN=N
      Q(I)=QUST(1)  +(QDST(1)-QUST(1))*(EI-1)/(EN-1)
      CM(I)=CM(1)
      RK2(I)=0.268614/Y(I)
      E(I)=22.6*CM(I)*(Q(I)/A(I))/(Y(I)**1.3333)
   40 ALPHA(I)=ALPHA(1)
      L=2

       TEMPERATURE  CORRECTION  FOR  RATES  AND  COEFFICIENTS

      CCS=14.652-0.410222*TEM+0.007991*(TEM)**2-0.00007777*(TEM)**3
      CORR=1.075**(TEM-20)
      K22=CORR*K22
      K52=CORR*K52
      K33=CORR*K33
      K23=CORR*K23
      K44=CORR*K44
      K24=CORR*K24
      K34=CORR*K34
      K25=CORR*K25
      K55=CORR*K55
      K45=CORR*K45
      K1=CORR*K1
   49 FORMAT(///7X,'TIME=',F10.2,'    HOURS'//)
   50 FORMAT(20X,'TIME=',I5,' ND  DAY      ',F5.1,' TH  HOUR')
      TPRINT=T(1)
      TIME=T(1)
      WRITE(3,61)
   61 FORMAT(///48X,'WATER  QUALITY  PARAMETERS'///)

                           INITIAL  VALUES

      WRITE(3,62)
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N.NO. OF STATIONS= 41
M.NO. OF INPUT TIMES= 17
DELX.LENGTH OF SEGMENT= 1.00MILE
DELT. TIME INTERVAL FOR INPUT DATA= 1.00HOURS

DECAY COEFF. OF BOD	K1=	0.16
COEFF. ACCOUNT FOR BOD REMOVAL	K3=	0.0
DECAY COEFF. OF C2	K22=	0.13
COEF. FOR RATE OF CONVERSION OF C5 TO C2	K52=	0.04
DECAY COEFF. FOR C3	K33=	0.04
COEF. FOR RATE OF CONVERSION OF C2 TO C3	K23=	0.12
COEF. FOR RATE OF CONVERSION OF C2 TO C4	K24=	0.01
COEF. FOR RATE OF CONVERSION OF C3 TO C4	K34=	0.04
COEF. FOR RATE OF CONVERSION OF C2 TO C0	K25=	0.54
COEF. FOR RATE OF CONVERSION OF C4 TO C5	K45=	0.05
DECAY COEFF. OF C4	K44=	0.05
DECAY COEFF. OF C5	K55=	0.08
SATURATION OF DO AT A GIVEN TEMP	CCS=	9.50

NOTE: C0=DISSOLVED OXYGEN
C8= BOD
C2 = NH3N
C3 = (NO2+NO3)-N
C4 = ALGAL NITROGEN
C5 = ORGANIC NITROGEN

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62 FORMAT(T8,'INDEX',T15,'STATION',T26,'AREA',T35,'DEPTH',T43,
  1'DISCHARGE',T54,'DISPERSION',T66,'REAERATION',T79,'DO',T88,'BOD'
  2,T98,'C2',T107,'C3',T118,'C4',T129,'C5',/T57,'RATE',T69,'RATE',
  3//T15,'(MILES)',T24,'(SQ. FT)',T36,'(FT)',T45,'(CFS)',T53,
  4'(SQ. FT/DAY)',T67,'(/DAY)',T77,'(MG/L)',T86,'(MG/L)',
  5T96,'(MG/L)',T105,'(MG/L)',T116,'(MG/L)',T127,'(MG/L)'//)
65 FORMAT(5X,I5,12F 10.2)
   WRITE(3,65)  ((I,X(I),A(I),Y(I),Q(I),E(I),RK2(I),CO(I),CB(I),
  1C2(I),C3(I),C4(I),C5(I)) ,I=1,N)

                    S E C T I O N    II

                 C O M P U T A T I O N S

   TIME=TIME+DT/3600.
70 IF (TIME-T(L)) 80,80,75
75 L=L+1
   GO TO 70
80 QU=QUST(L-1)+((QUST(L)-QUST(L-1))/(T(L)-T(L-1)))*(TIME-T(L-1))
   QD=QDST(L-1)+((QDST(L)-QDST(L-1))/(T(L)-T(L-1)))*(TIME-T(L-1))
   WIND=W(L-1)+((W(L)-W(L-1))/(T(L)-T(L-1)))*(TIME-T(L-1))
   DO  90  I=1,N
   EI=I
   EN=N
   Q(I)=QU+(QD-QU)*(EI-1)/(EN-1)
   CBLA(I)=Q(I)*CL(I)/(A(I)*DX)

       DISPERSION  COEFFICIENTS  BY  FORMULA
   E(I)=22.6*CM(I)*(Q(I)/A(I))/(Y(I)**1.3333)

        REAERATION  COEFFICIENTS  BY  FORMULA
   RK2(I)=0.268614/Y(I)
   RK2(I)=RK2(I)/(1.-0.2006*SQRT(WIND))
90 RK2(I)=CORR*RK2(I)

            C O M P U T A T I O N  O F   B O D

                      UPSTREAM  BOUNDARY
   C(1)=CBU(L-1)  +((CBU(L)-CBU(L-1))/(T(L)-T(L-1)))*(T(L)-TIME)

                    INTERIOR  STATIONS

   DO 100 I=2,NN

                             ADVECTION
   ADV=BETA(I+1)*CB(I+1)*Q(I+1)+ALPHA(I)*CB(I)*Q(I)
  1-(ALPHA(I-1)*CB(I-1)*Q(I-1)+BETA(I)*CB(I)*Q(I))
   ADV=ADV*DTDX*2./(A(I+1)+A(I-1))

                           DISPERSION
   DISP=E(I+1)*A(I+1)*(CB(I+1)-CB(I))
  1-E(I-1)*A(I-1)*(CB(I)-CB(I-1))
   DISP=(DISP/DX)*DTDX*2./(A(I+1)+A(I-1))
   DECAY=K1*CB(I)*DTDAY
   SOURCE=CBLA(I)*DTDAY
                 ADSORPTION  AND  SEDIMENTATION
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      ADS=K3*CB(I)*DTDAY
  100 C(I)=CB(I) - ADV + DISP - DECAY + SOURCE - ADS
      C(N)=2.*C(N-1)-C(N-2)
      DO 101 I=1,N
  101 CB(I)=C(I)

                COMPUTATION OF DISSPLVED OXYGEN

                         UPSTREAM  BOUNDARY
      C(1)=COU(L-1)+((COU(L)-COU(L-1))/(T(L)-T(L-1)))*(T(L)-TIME)
                        INTERIOR  STATIONS
      DO 200 I=2,NN
                                ADVECTION
      ADV=BETA(I+1)*CO(I+1)*Q(I+1)+ALPHA(I)*CO(I)*Q(I)
     1-(ALPHA(I-1)*CO(I-1)*Q(I-1) + BETA(I)*CO(I)*Q(I))
      ADV=ADV*DTDX*2./(A(I+1)+A(I-1))
                             DISPERSION
      DISP=E(I+1)*A(I+1)*(CO(I+1)-CO(I))-
     1E(I-1)*A(I-1)*(CO(I)-CO(I-1))
      DISP=(DISP/DX)*DTDX*2./(A(I+1)+A(I-1))
      DECAY=K1*CB(I)*DTDAY
      IF (CO(I) - CCS) 149,149,145
  145 REAER=0.
      GO TO 200
  149 REAER=RK2(I)*(CCS-CO(I))*DTDAY
  200 C(I)=CO(I) - ADV + DISP - DECAY + REAER
                         DOWNSTREAM  BOUNDARY
      C(N)=2.*C(N-1)-C(N-2)

        INITIALIZATION  FOR  THE  NEXT  TIME  STEP

      DO 201 I=1,N
  201 CO(I)=C(I)


                     COMPUTATION  OF  AMMONIA

                         UPSTREAM  BOUNDARY
      C(1)=C2U(L-1)  +((C2U(L)-C2U(L-1))/(T(L)-T(L-1)))*(T(L)-TIME)
      K25=0.05
      DO 300 I=2,NN
      ADV=BETA(I+1)*C2(I+1)*Q(I+1)+ALPHA(I)*C2(I)*Q(I)
     1-(ALPHA(I-1)*C2(I-1)*Q(I-1)+BETA(I)*C2(I)*Q(I))
      ADV=ADV*DTDX*2./(A(I+1)+A(I-1))
      DISP=E(I+1)*A(I+1)*(C2(I+1)-C2(I))
     1-E(I-1)*A(I-1)*(C2(I)-C2(I-1))
      DISP=(DISP/DX)*DTDX*2./(A(I+1)+A(I-1))
      DECAY=K25*C2(I)*DTDAY
      CONV=K23*C2(I)*DTDAY
  300 C(I)=C2(I)  - ADV + DISP - DECAY - CONV
      C(N)=2.*C(N-1)-C(N-2)
      DO 301 I=1,N
  301 C2(I)=C(I)


        COMPUTATION  OF  NITRITE PLUS  NITRATE  NITROGEN
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      C(I)=C3U(L-1)  +  ((C3U(L)-C3U(L-1))/(T(L) - T(L-1)))*(T(L)-TIME)
      K33=0.40
      DO 400 I=2,NN
      ADV=BETA(I+1)*C3(I+1)*Q(I+1)+ALPHA(I)*C3(I)*Q(I)
     1-(ALPHA(I-1)*C3(I-1)*Q(I-1)+BETA(I)*C3(I)*Q(I))
      ADV=ADV*DTDX*2./(A(I+1)+A(I-1))
      DISP=E(I+1)*A(I+1)*(C3(I+1)-C3(I))-
     1E(I-1)*A(I-1)*(C3(I)-C3(I-1))
      DISP=(DISP/DX)*DTDX*2./(A(I+1)+A(I-1))
      DECAY=K33*C3(I)*DTDAY
C              CONV= CONVERSION OF C2  TO  C3
      CONV=K23*C2(I)*DTDAY
  400 C(I)=C3(I)  -  ADV  +  DISP  - DECAY + CONV
      C(N)=2.*C(N-1)-C(N-2)
      DO 401 I=1,N
  401 C3(I)=C(I)
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S E C T I O N   III

O U T P U T

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 2000 IF (TIME - TPRINT ) 4000,3020,3020
 3020 WRITE(3,49)TIME
      DIV=TIME/24.
      IDAY=DIV
      HR=(DIV-IDAY)*24.0
      WRITE(3,50) IDAY,HR
C        PRINT THE RESULTS

      WRITE(3,62)
      WRITE(3,65)  ((I,X(I),A(I),Y(I),Q(I),E(I),RK2(I),CO(I),CB(I),
     1C2(I),C3(I),C4(I),C5(I))  ,I=1,N)

      TPRINT=TPRINT+DPRINT

      IF(TIME - TFIN) 4000,5000,5000
 4000 TIME=TIME + DT/3600.
      GO TO 70
 5000 STOP
      END
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