6-1-1977

Water Quality Models of Back and Poquoson Rivers, Virginia

Paul V. Hyer
Virginia Institute of Marine Science

Albert Y. Kuo
Virginia Institute of Marine Science

Bruce J. Neilson
Virginia Institute of Marine Science

Follow this and additional works at: https://scholarworks.wm.edu/reports

Part of the Marine Biology Commons

Recommended Citation
WATER QUALITY MODELS OF BACK AND POQUOSON RIVERS, VIRGINIA

by

Paul V. Hyer,
Albert Y. Kuo
and
Bruce J. Neilson

Special Report No. 144
in Applied Marine Science and Ocean Engineering

Virginia Institute of Marine Science
Gloucester Point, Virginia 23062

William J. Hargis, Jr.
Director

June, 1977
WATER QUALITY MODELS OF
BACK AND POQUOSON RIVERS, VIRGINIA

by

Paul V. Hyer,
Albert Y. Kuo
and
Bruce J. Neilson

A Report to the Hampton Roads Water Quality Agency

Special Report No. 144
in Applied Marine Science and
Ocean Engineering

The preparation of this report was financed through
a grant from the U. S. Environmental Protection Agency
under Section 208 of the Federal Water Pollution
Control Act Amendments of 1972.

Virginia Institute of Marine Science
Gloucester Point, Virginia 23062

William J. Hargis, Jr.,
Director

June, 1977
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapter 1. Introduction</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chapter 2. A Description of the Water Quality Model</td>
<td>5</td>
</tr>
<tr>
<td>A. Basic Equations</td>
<td>5</td>
</tr>
<tr>
<td>B. Finite Difference Approximation</td>
<td>12</td>
</tr>
<tr>
<td>C. Method of Solution</td>
<td>19</td>
</tr>
<tr>
<td>D. Evaluation of Parameters and Rate Constants</td>
<td>22</td>
</tr>
<tr>
<td>Chapter 3. Model Calibration</td>
<td>31</td>
</tr>
<tr>
<td>A. Calibration Procedure</td>
<td>34</td>
</tr>
<tr>
<td>B. Model Sensitivity</td>
<td>36</td>
</tr>
<tr>
<td>C. Discussion</td>
<td>39</td>
</tr>
<tr>
<td>Appendix A. Input Constants</td>
<td>42</td>
</tr>
<tr>
<td>Appendix B. Observed and Predicted Values of Model Components for the Back River</td>
<td>53</td>
</tr>
<tr>
<td>Appendix C. Observed and Predicted Values of Model Components for the Poquoson River</td>
<td>65</td>
</tr>
</tbody>
</table>
Introduction

Section 208 of the Federal Water Pollution Control Act Amendments of 1972 provides for the development and implementation of areawide waste treatment management plans. In addition to industrial and municipal waste water treatment facilities, the plans are to account for nonpoint sources of pollution, such as urban runoff, runoff from agriculture and silviculture, pollution due to construction activities and so on. The basic tool used in developing a management plan is a mathematical model of water quality for the estuary which receives the waste streams and land runoff. Once an appropriate model has been calibrated and verified for the water body under consideration, it can be used to simulate the response of the receiving waters to various combinations of point and nonpoint loadings. In this manner, it is possible to assess the impact of future loadings, proposed changes in treatment levels and other management alternatives.

The Hampton Roads 208 study area, shown in Figure 1, consists of the Peninsula and Southeastern Virginia Planning Districts. The Poquoson River and Back River are located on the Virginia Peninsula, generally flow from west to east and empty into Chesapeake Bay between the York and James Rivers. The Poquoson River basin lies primarily in York County and the City of Poquoson, while the Back River drainage basin includes much of the cities of Poquoson and Hampton and a small portion of the city of Newport News, as can be seen in
Figure 1. Tidewater Virginia showing the Hampton Roads 208 Study Area.
Figure 2. During the summer of 1975, field surveys were conducted in these rivers to determine present water quality conditions and to collect the data necessary to calibrate a mathematical model of water quality in these water bodies. The field program and an analysis of water quality conditions have been presented in an earlier report to the Hampton Roads Water Quality Agency (Neilson, 1976).

The purpose of this report is to describe the model which was applied to the Back and Poquoson Rivers and to document the calibration results. A detailed description of the model, its many components, internal interactions and the various assumptions employed is given in Chapter 2. This discussion is of a rather technical nature, since it is intended to provide a definitive presentation of the model and its inner workings. A more general presentation of the model and how it works will be given in future reports on the results of the modelling studies. Chapter 3 includes a description of the calibration procedures and the sensitivity of the model to various factors. The actual results of the calibration process are given in appendices as graphs showing field observations and model predictions for each river and the entire suite of model components.
Figure 2. The Hampton Roads area, including the Back and Poquoson Rivers.
Chapter 2.

A Description of the Water Quality Model

The water quality model used for this study is a one-dimensional, intra-tidal model which simulates the longitudinal distribution of cross-sectional average concentrations of water quality parameters, including the temporal variation of these concentration fields in response to tidal oscillation. The water quality parameters simulated in the model include dissolved oxygen, carbonaceous oxygen demand, organic nitrogen, ammonia nitrogen, nitrite-nitrate nitrogen, organic phosphorus, inorganic phosphorus, chlorophyll 'a' as phytoplankton, coliform bacteria, and salinity. Temperature, turbidity, and light intensity are important parameters for the biochemical interactions taking place, but are not modeled directly. They are input to the model and their influence on the biochemical reaction rates is taken into account.

A. Basic Equations

The model is based on the one-dimensional equation describing the mass-balance of a dissolved or suspended substance in a water body.

$$\frac{\partial}{\partial t} (AC) + \frac{\partial}{\partial x} (QC) = \frac{\partial}{\partial x} (EA \frac{\partial C}{\partial x}) + A \cdot Se + A \cdot Si$$  \hspace{1cm} (1)

where

t is time,
x is the distance along the axis of the estuary,
A is the cross-sectional area
Q is discharge,

C is the concentration of dissolved or suspended substance,

E is the dispersion coefficient

Se is the time rate of external addition (or withdrawal) of mass across the boundaries, i.e., free surface, bottom, and lateral boundary,

Si is the time rate of increase or decrease of mass of a particular substance by biochemical reaction processes.

The advective term, the second term on the left hand side of the equation, represents advection of mass by water movement; the dispersive, the first term on the right hand side, represents dispersion of mass by turbulence and shearing flow. These two terms represent the physical transport processes in the flow field and, are identical for all dissolved and suspended substances in the water. The last two terms of the equation represent the external additions and internal biochemical reactions and differ for different substances.

The model treats the nitrogen, phosphorus, oxygen demanding material and dissolved oxygen with an interacting system of eight components. The schematic diagram (Figure 3) shows the interaction of these components. Each rectangular box represents one component being simulated by the model, with its name in the computer program shown in parentheses. The arrow between components represent the biochemical transformation of one substance to the other. The arrows with one end not attached to any component represent the external sources (or sinks) or the internal sources (or sinks) due to the biochemical reactions.
Figure 3. Schematic Diagram of Interaction of Ecosystem Model
The mathematical representation of the terms $S_e$ and $S_i$ for each of the eight components are explained in the following:

(1) **Phytoplankton concentration, $C$, measured as $\mu g/\ell$ of chlorophyll 'a'**

\[ S_e = -k_{cs} \cdot C \]

where $k_{cs}$ is the settling rate of phytoplankton.

\[ S_i = (g-d-kg)C \]

where $g$ and $d$ are the growth and endogenous respiration rates of phytoplankton respectively, $kg$ is the grazing of phytoplankton by zooplankton.

(2) **Organic Nitrogen, $N_l$ in mg/\ell**

\[ S_e = W_{n1} - k_{n1l} \cdot N_l \]

where $W_{n1}$ is the wasteload from point and non-point sources and $k_{n1l}$ is the settling rate.

\[ S_i = -k_{n12} \cdot N_l + a_n \cdot (d + 0.4 kg) \]

where $k_{n12}$ is the hydrolysis rate of organic nitrogen to ammonia nitrogen and $a_n$ is the ratio of nitrogen to chlorophyll 'a' in mg-N/$\mu g$-C.

(3) **Ammonia Nitrogen, $N_2$ in mg/\ell**

\[ S_e = W_{n2} \]

where $W_{n2}$ is the wasteload from point and non-point sources.

\[ S_i = k_{n12} \cdot N_l - k_{n23} \cdot N_2 - a_n \cdot g \cdot C \cdot Pr \]
where $k_{n23}$ is the $\text{NH}_3$ to $\text{NO}_3$ nitrification rate, $P_r$ is ammonia preference by phytoplankton given by

$$P_r = \frac{N2}{N2 + K_{mn}}$$

$K_{mn}$ is the Michaelis constant.

(4) Nitrite - Nitrate Nitrogen, N3 in mg/l

$$S_e = W_{n3} - k_{n33} \cdot N3$$

where $W_{n3}$ is wasteload from point and non-point sources, $k_{n33}$ is the nitrate escape rate.

$$S_i = k_{n23} \cdot N2 - (1 - P_r) \cdot a_n \cdot g \cdot C$$

where the first term represents the nitrification of ammonia nitrogen and the second term represents the uptake by phytoplankton.

(5) Organic Phosphorus, P1 in mg/l

$$S_e = W_{pl} - k_{pl1} \cdot P1$$

where $W_{pl}$ is wasteload from point and non-point sources, $k_{pl}$ is the settling rate.

$$S_i = -k_{pl2} \cdot P1 + a_p (d + 0.4 \text{ kg})$$

where $k_{pl2}$ is the organic P to inorganic P conversion rate, $a_p$ is the phosphorus to chlorophyll ratio, in mg - P/µg-C.
(6) Inorganic Phosphorus, P2 in mg/l

\[ Se = W_{p2} - k_{p22} \cdot P2 \]

where \( W_{p2} \) is wasteload from point and non-point sources, \( k_{p22} \) is settling rate.

\[ Si = k_{p12} \cdot P1 - a_p \cdot g \cdot C \]

where the first term represents the conversion of organic phosphorus to inorganic phosphorus, the second term represents the uptake by phytoplankton.

(7) Carbonaceous Biochemical Oxygen Demand, CBOD in mg/l

\[ Se = W_b - k_s \cdot CBOD \]

where \( W_b \) is the wasteload from point and non-point sources, \( k_s \) is the settling rate.

\[ Si = -k_l \cdot CBOD + 2.67 \cdot a_c \cdot 0.4 \cdot kg \cdot C \]

where \( k_l \) is the oxidation rate of CBOD, \( a_c \) is the carbon-chlorophyll ratio.

(8) Dissolved Oxygen, DO in mg/l

\[ Se = k_2 \cdot (DO_s - DO) - BEN \]

where \( k_2 \) is reaeration rate, \( DO_s \) is the saturated oxygen concentration, \( BEN \) is the benthic oxygen demand.

\[ Si = -k_l \cdot CBOD - 4.57 \cdot k_{n23} \cdot N2 \\
+ a_d \cdot g \cdot C - a_r \cdot d \cdot C \]
where the first two terms represent the oxygen demands by oxidation of CBOD and by nitrification of ammonia nitrogen, the last two terms represents the source and sink due to photosynthesis and respiration of phytoplankton, \( a_d \) (or \( a_r \)) is the amount of oxygen produced per unit chlorophyll synthesized in the photosynthesis process.

The model treats the salinity and coliform bacteria as independent systems. The simulation of salinity distribution not only serves to calibrate the dispersion coefficient for the model, but also furnishes the required parameter to calculate saturated oxygen content of saline water.

(9) Salinity, \( S \) in parts per thousand

\[
Se = 0 \\
Si = 0
\]

(10) Coliform Bacteria, \( BAC \) in MPN/100 ml

\[
Se = W_{bac} \\
Si = -k_b \cdot BAC
\]

where \( W_{bac} \) is the loading from point and non-point sources.

where \( k_b \) is the die-off rate.
B. Finite Difference Approximation

To facilitate the numerical computation, equation (1) needs to be written in terms of finite difference form. This may be done by dividing the river into a number of volume elements, called reaches, with a series of lateral transects perpendicular to its axis and by integrating equation (1) with respect to x over each of the reaches. Considering the mth reach of the river bounded by the mth and (m+1)th transects as shown in the sketch below:

\[
\frac{\partial}{\partial t} (C_m V_m) = Q_m C_m^* - Q_{m+1} C_{m+1}^* + (EA \frac{\partial C}{\partial x})_{m+1} \\
- (EA \frac{\partial C}{\partial x})_m + S_{em} \cdot V_m + S_{im} \cdot V_m
\]
where

- \( C_m \) is the volume average concentration of the mth reach,
- \( V_m \) is the volume of water in the mth reach,
- \( Q_m \) is the discharge through the mth transect,
- \( C_m^* \) is the concentration of the water, flowing through the mth transect,
- \( \text{EA}(\frac{\partial C}{\partial x})_m \) is the dispersive flux through the mth transect.

The time rate of change of water volume may be expressed as

\[
\frac{\partial V_m}{\partial t} = Q_m - Q_{m+1} + Q_l
\]  

(3)

where \( Q_l \) is lateral inflow, including natural runoff, \( Q_t \), and sewage flow, \( Q_{\text{sew}} \).

Substituting equation (3) into equation (2) and dividing the resulting equation by \( V_m \), it is obtained that

\[
\frac{\partial C_m}{\partial t} = \frac{Q_m}{V_m} (C_m^* - C_m) - \frac{Q_{m+1}}{V_m} (C_{m+1}^* - C_m)
\]

\[+ \frac{1}{V_m} (\text{EA}(\frac{\partial C}{\partial x})_m + 1 - \frac{1}{V_m} (\text{EA}(\frac{\partial C}{\partial x})_m\]

\[+ \text{Se}_m + \text{Si}_m - \frac{1}{V_m} \cdot Q_l \cdot C_m
\]

(4)

With proper initial and boundary conditions, equation (4) may be integrated with respect to time to obtain the temporal variations of concentration within each reach of the water body. To solve the equation with a digital computer, it
is integrated numerically over successive finite time intervals. At each integration step over a time increment, the various parameters, such as flow rates, dispersion coefficients, etc., should assume representative values during this particular time interval. An implicit scheme is used to formulate the finite difference equation, i.e., the concentration at the end of the time step as well as that at the beginning of the time step is used to express the right hand side of equation (4).

Equation (4) is approximated by the following finite difference form,

\[
\frac{C_m' - C_m}{\Delta t} = \frac{1}{2} \left\{ \frac{C_m'}{V_m} (C_m^* - C_m') + \frac{Q_m}{V_m} (C_m^* - C_m) \right\}
- \frac{1}{2} \left\{ \frac{Q_{m+1}}{V_m} (C_{m+1}^* - C_m') + \frac{Q_{m+1}}{V_m} (C_{m+1}^* - C_m) \right\}
+ \frac{E_{m+1}A_{m+1}}{V_m} \frac{C_m' - C_m}{\Delta x_m + \Delta x_{m+1}} + \frac{E_{m+1}A_{m+1}}{V_m} \frac{C_{m+1} - C_m}{\Delta x_m + \Delta x_{m+1}}
- \frac{E_A'A_m'}{V_m} \frac{C_m' - C_{m-1}}{\Delta x_m + \Delta x_{m-1}} + \frac{E_A'm}{V_m} \frac{C_m - C_{m-1}}{\Delta x_m + \Delta x_{m-1}}
+ \frac{S_m + S_{m'}}{V_m} Q \bar{C}_m
\]  

(5)

where \(\Delta t\) is the time increment. The primed and unprimed variables designate the parameters evaluated at the end and beginning of time interval respectively, and the over bar represents the average value over the time interval.

The concentration, \(C_m^*\), of the water flowing through the \(m\)th transect is calculated as a weighted average of the
concentrations in the adjacent reaches, $C_{m-1}$ and $C_m$. Thus

$$C_m^* = \alpha C_{m-1} + (1 - \alpha) C_m$$  \hspace{1cm} (6)

$$C_m'^* = \alpha' C_{m-1}' + (1 - \alpha') C_m'$$  \hspace{1cm} (7)

where the weighting factors $\alpha$ and $\alpha'$ depend on the direction of flow through the transect,

\[0.5 \leq \alpha \leq 1 \quad \text{if} \quad Q_m > 0\]
\[0 \leq \alpha \leq 0.5 \quad \text{if} \quad Q_m < 0\]

and

\[0.5 \leq \alpha' \leq 1 \quad \text{if} \quad Q_m' > 0\]
\[0 \leq \alpha' \leq 0.5 \quad \text{if} \quad Q_m' < 0\]

Similarly,

$$C_{m+1}^* = \alpha_2 C_{m+1} + (1 - \alpha_2) C_m$$  \hspace{1cm} (8)

$$C_{m+1}'^* = \alpha'_2 C_{m+1}' + (1 - \alpha'_2) C_m'$$  \hspace{1cm} (9)

and

\[0.5 \leq \alpha_2 \leq 1 \quad \text{if} \quad Q_{m+1} < 0\]
\[0 \leq \alpha_2 \leq 0.5 \quad \text{if} \quad Q_{m+1} > 0\]
\[0.5 \leq \alpha'_2 \leq 1 \quad \text{if} \quad Q_{m+1}' < 0\]
\[0 \leq \alpha'_2 \leq 0.5 \quad \text{if} \quad Q_{m+1}' > 0\]
Substituting equations (6), (7), (8) and (9) into equation (5), it is obtained that

\[
C_m' - C_m = \frac{\Delta t}{2} \left\{ \frac{Q_m'}{V_m} \alpha (C_{m-1}' - C_m') + \frac{Q_m}{V_m} \alpha (C_{m-1} - C_m) \right\}
- \frac{\Delta t}{2} \left\{ \frac{Q_{m+1}'}{V_m} \alpha_2 (C_{m+1}' - C_m') + \frac{Q_{m+1}}{V_m} \alpha_2 (C_{m+1} - C_m) \right\}
+ \frac{E_{m+1} A_{m+1}'}{V_m} \frac{\Delta t}{\Delta x_m + \Delta x_{m+1}} (C_{m+1}' - C_m')
+ \frac{E_{m+1} A_{m+1}}{V_m} \frac{\Delta t}{\Delta x_m + \Delta x_{m+1}} (C_{m+1} - C_m)
+ \frac{E_m A_m'}{V_m} \frac{\Delta t}{\Delta x_m + \Delta x_{m-1}} (C_m' - C_m')
+ \frac{E_m A_m}{V_m} \frac{\Delta t}{\Delta x_m + \Delta x_{m-1}} (C_m - C_{m-1})
+ \Delta t (S_{m+1} + S_m) - \frac{\Delta t}{V_m} Q_m C_m
\]  

(10)

Defining

\[
ADV_m = \frac{\Delta t}{2} \cdot \frac{AC_m}{V_m}
\]

\[
ADV2_m = \frac{\Delta t}{2} \cdot \frac{AC_{m+1}}{V_m}
\]

\[
DIF_m = \frac{\Delta t}{\Delta x_m + \Delta x_{m-1}} \cdot \frac{E_m A_m}{V_m}
\]

\[
DIF2_m = \frac{\Delta t}{\Delta x_m + \Delta x_{m+1}} \cdot \frac{E_{m+1} A_{m+1}}{V_m}
\]
\[ Q_m = AC_m \cdot U_m \]
\[ Q_{m+1} = AC_{m+1} \cdot U_{m+1} \]
\[ U_m = \text{advective velocity} \]
\[ AC_m = \text{conveyancy cross-sectional area} \]

and similarly for the primed variables, equation (10) becomes

\[ C'_m (1 - \alpha'_2 U'_m + \alpha'_1 U'_m \cdot ADV'_m + \DeltaF'_m + \DeltaF'_2) \]
\[ = C'_{m+1} (-\alpha'_2 U'_m \cdot ADV'_2 + \DeltaF'_2) + C'_{m-1} (\alpha'_1 U'_m \cdot ADV'_m) \]
\[ + \DeltaF'_m) + C_m (1 + \alpha'_2 U'_m + \DeltaF'_m) + C_m (\alpha'_1 \DeltaF'_m + \DeltaF'_2) \]
\[ + \DeltaF'_m) + C_{m+1} (\alpha'_2 U'_m + \DeltaF'_m) \]
\[ + C_m (\alpha'_1 \DeltaF'_m + \DeltaF'_m) \]  

Equation (11) is further simplified to

\[ (1 + \text{COE}_m) C'_m = \text{COE2}_m \cdot C'_{m+1} + \text{COE1}_m \cdot C'_{m-1} \]
\[ + \text{CON}_m \cdot C_m + \text{CON2}_m \cdot C_{m+1} + \text{CON1}_m \cdot C_{m-1} \]
\[ + \Delta t (S_{e_m} + S_{i_m}) - \frac{\Delta t}{V_m} Q_\lambda C_m \]

where

\[ \text{COE}_m = \alpha'_1 U'_m - \alpha'_2 U'_m + \DeltaF'_m + \DeltaF'_2 \]
\[ \text{COE1}_m = \alpha'_1 U'_m + \DeltaF'_m \]
\[ \text{COE2}_m = -\alpha'_2 U'_m + \DeltaF'_2 \]
The lateral inflow, \( Q_L \), may be written as

\[
Q_L = Q_t + Q_{sew}
\]

where \( Q_t \) is the natural runoff (e.g. flow from tributaries) and \( Q_{sew} \) is the sewage flow. In a tidal estuary, \( Q_t \) may be positive or negative, depending on the phase of tide, with an average value over tidal cycle \( Q_f \), the net freshwater inflow. Without the detailed information about the time variation of \( Q_t \) over tidal cycle, the net effect of lateral inflow is approximated by a constant value, \( Q_f + Q_{sew} \). Therefore, the last term of equation (12) becomes

\[
\frac{\Delta t}{V_m} (Q_f + Q_{sew}) C_m
\]

The terms \( \overline{Se}_m \) and \( \overline{Si}_m \) will differ for different parameters. It is shown in the previous section that all the mathematical expressions for \( Se \) and \( Si \) are algebraic functions, and no finite difference approximation is necessary. However, there are choices in expressing \( \overline{Se} \) and \( \overline{Si} \) in terms of concentrations at the beginning or end of time increment. In order to avoid introducing extra unknown into the finite difference equation, \( \overline{Se} \) and \( \overline{Si} \) are expressed in terms of known concentrations of water quality parameters other than the one under consideration.
In case $S_e$ and/or $S_i$ depends on the concentration of the water quality parameter under consideration, the average of the concentrations at the beginning and end of time step is used.

In general, equation (12) may be written as

$$C'_m = a_mC'_{m+1} + b_mC'_{m-1} + c_m$$

(13)

where

$$a_m = \frac{COE2_m}{(1 + COE_m + \frac{\Delta t}{2} k)}$$

$$b_m = \frac{COE1_m}{(1 + COE_m + \frac{\Delta t}{2} k)}$$

$$c_m = \left\{ C_m \left( CON_m - \frac{\Delta t}{2} k - \frac{Q_f + Q_{sew}}{v_m} \cdot \Delta t \right) 
+ C_{m+1} \cdot CON2_m + C_{m-1} \cdot CON1_m 
+ \Delta t \left( S_{e*,m} + S_{i*,m} \right) \right\} / (1 + COE_m + \frac{\Delta t}{2} k)$$

$$S_{e*,m} + S_{i*,m} = S_{e_m} + S_{i_m} - k (C_m + C'_m)/2$$

(14)

In the above expression, $S_e + S_i$ is separated into two parts, one depends on the average concentration of the water quality parameter under consideration and the other is the remainder.

C. Method of Solution

Because of advective and dispersive transport across the transects bounding each end of a particular reach of the estuary, the concentration of a substance in one reach will depend on the concentrations in two adjacent reaches. This interdependence of concentrations at neighboring reaches is
manifested in equation (13). Therefore, the equation cannot be solved for the concentration at the \( m \)th reach by itself. Equations must be written for every reach of the estuary and solved for the concentrations in every reach simultaneously.

Suppose that the total length of the estuary to be modeled is divided into \( N \) reaches. \((N-2)\) equations will be obtained by writing equation (13), for \( m = ML+1 \) to \( m = MU-1 \), where the \( ML\)th and \( MU\)th reaches are the most upstream and downstream ones, respectively. Since there are \((N-2)\) equations for \( N \) unknowns, two boundary conditions must be specified. The principal operation of numerical computations in the model is then to compute the concentrations in each reach at time \( t_0 + \Delta t \) with a given initial concentration field at time \( t_0 \) and appropriate boundary conditions. The computed concentration field at \( t_0 + \Delta t \) will then be used as the initial condition to compute the concentration field at time \( t_0 + 2\Delta t \), and so forth. Each computation cycle will advance the time by the increment of \( \Delta t \). Within each computation cycle, the \((N-2)\) simultaneous equations are solved by an elimination method.

Given the upstream boundary condition \( C'_{ML} \), \( C'_{ML+1} \) may be expressed in terms of \( C'_{ML+2} \) through equation (13) with \( m = ML+1 \), i.e.

\[
C'_{ML+1} = a_{ML+1}C'_{ML+2} + b_{ML+1}C'_{ML} + c_{ML+1}
\] (15)

where the only unknown on the right hand side of the equation is \( C'_{ML+2} \). Equation (15) may, in turn, be substituted back into equation (13) with \( m = ML+2 \), and thus one arrives at an
expression for $C'_{ML+2}$ in terms of $C'_{ML+3}$. In general, there exists the following relation

$$C'_m = P_m C'_{m+1} + O_m$$  \hspace{1cm} (16)

where the recursion coefficients $P_m$ and $O_m$ may be calculated from the upstream boundary condition $C'_{ML}$.

With subscript $m-1$, equation (16) becomes

$$C'_{m-1} = P_{m-1} C'_{m} + O_{m-1}$$

Substituting this expression for $C'_{m-1}$ in equation (13), it becomes

$$C'_m = a_m C'_{m+1} + b_m (P_{m-1} C'_m + O_{m-1}) + c_m$$

or

$$C'_m = \frac{a_m}{1 - b_m \cdot P_{m-1}} C'_{m+1} + \frac{b_m O_{m-1} + c_m}{1 - b_m \cdot P_{m-1}}$$ \hspace{1cm} (17)

The comparison between equations (16) and (17) gives

$$P_m = \frac{a_m}{1 - b_m \cdot P_{m-1}}$$

$$O_m = \frac{b_m \cdot O_{m-1} + c_m}{1 - b_m \cdot P_{m-1}}$$ \hspace{1cm} (18)

Since $C'_{ML}$ is a known quantity, the comparison between equation (15) and (16) with $m = ML+1$ gives

$$P_{ML+1} = a_{ML+1}$$

$$O_{ML+1} = b_{ML+1} \cdot C'_{ML} + c_{ML+1}$$
and thus

\[ P_{ML} = 0, \quad O_{ML} = C'_{ML} \]

In summary, the recursion coefficients and equation are

\[ P_m = \frac{a_m}{1 - b_m \cdot P_{m-1}} \]

\[ O_m = \frac{c_m + b_m \cdot O_{m-1}}{1 - b_m \cdot P_{m-1}} \]

and

\[ C'_m = P_m C'_{m+1} + O_m \]

with \( m = ML+1, ML+2, \ldots, MU-1 \).

Then, the order of numerical computations is (1) calculate the recursion coefficients by applying equations (18) repeatedly with \( m = ML+1, ML+2, \ldots, MU-1 \), and (2) with \( C'_{MU} \) given as the downstream boundary condition, the concentrations of the interior reaches are calculated by applying equation (16) repeatedly with \( m = MU-1, MU-2, \ldots, ML+1 \).

D. Evaluation of Parameters and Rate Constants

(1) Velocity \( U \): In an estuary, the current velocity may be divided into two parts,

\[ U_m(t) = U_F m + U_t m(t) \]
where $UF$ is the non-tidal component generated by freshwater discharge and $Ut$ is the oscillating tidal component. In the model, the tidal current is approximated by a sinusoidal function of time with period $T$ and phase $\phi$

$$Ut_m(t) = UT_m \sin \left\{ \frac{2\pi}{T} t + \phi_m \right\}$$  \hspace{1cm} (20)

where $UT$ is the amplitude. $UT_m$ and $\phi_m$ are obtained from field data. The non-tidal component $UF$ is calculated by the equation

$$UF_m = \frac{Q_m}{AC_m}$$ \hspace{1cm} (21)

where $Q_m$ is the freshwater discharge from a drainage area upstream of the $m$th transect. Since the stream in question is ungauged, freshwater inflow is estimated from drainage area and flow data from other watersheds.

(2) Dispersion coefficient $E$: The dominant mechanism of longitudinal dispersion is the interaction between turbulent diffusion and shearing current. Taylor's (1954) formulation of one-dimensional dispersion has been successfully modified and extended to homogeneous estuaries (Holley, et al., 1970; Harleman, 1971). The dispersion coefficient in the freshwater portion of a tidal estuary may be expressed as

$$E = \nu n |U|^\frac{5}{6}$$  \hspace{1cm} (22)

where $n$ is Manning's friction coefficient, $|U|$ is the absolute value of velocity, $R$ is hydraulic radius, and $\nu$ is a constant on the order of 100. It is known that the presence of density
stratification due to salinity intrusion enhances the vertical shear while suppressing the turbulence, and therefore, increases the dispersion coefficient. Equation (22) is modified to

$$E = v' n |U| R^{5/6} (1 + v'S)$$

(23)

where $v'$ is a constant and $S$ is the salinity. $v'$ is determined by the model calibration, i.e. adjusting $v'$ until the model results agree satisfactorily with the salinity distribution measured in the field.

(3) Reaeration coefficient $k_2$: O'Connor and Dobbins (1956) presented a theoretical derivation of the reaeration coefficient, in which fundamental turbulence parameters were taken into account. They derived the following formula

$$k_2 = \frac{(D_c U)^{1/2}}{H^{3/2}}$$

(24)

where $D_c$ is the molecular diffusivity of oxygen in water, $U$ and $H$ are the cross-sectional mean velocity and depth respectively, and $(k_2)_{20}$ is the reaeration coefficient at 20°C. This formula has been shown to give a satisfactory estimate of $k_2$ for a reach of river with cross-sectional mean depth and velocity more or less uniform throughout the reach. In case the cross-section varies appreciably within a single reach, there is no reason to expect a satisfactory estimate from the formula by using the values of $U$ and $H$ at the two bounding transects of the reach. Therefore, equation
(24) is modified as stated in the following paragraph. Assuming that the O'Connor and Dobbins formula is valid locally then

\[ f = k_2 h = \frac{(D_c u)^{1/2}}{h^{1/2}} \]  \hspace{1cm} (25)

where \( f \) is the exchange coefficient, i.e., the exchange rate of oxygen through unit water surface area, \( u \) is the local depth-mean velocity and \( h \) is local depth. \( M \), the exchange rate of oxygen through the water surface over an entire reach is

\[ M = \int f (D_{OS} - DO) \, dAh \]  \hspace{1cm} (26)

where \( Ah \) is the total surface area over a reach. By definition of \( k_2 \),

\[ M = (k_2) \frac{V}{20} (D_{OS} - DO) \]  \hspace{1cm} (27)

thus,

\[ (k_2) = \frac{D_c^{1/2}}{V} \int \frac{u^{1/2}}{Ah \, h^{1/2}} \, dAh = D_c^{1/2} \frac{u^{1/2}}{\langle h^{1/2} \rangle} \frac{Ah}{V} \]

\[ = D_c^{1/2} \frac{\langle u^{1/2} \rangle}{\langle h^{1/2} \rangle} \frac{1}{\langle h \rangle} \]  \hspace{1cm} (28)

where \( \langle \cdot \rangle \) indicates the average over the surface area \( Ah \), and \( \langle h \rangle \) is the mean depth of the reach. Since the velocity data are available only at the end transects of a reach, no true \( \frac{\langle u^{1/2} \rangle}{\langle h^{1/2} \rangle} \) may be estimated. In this model, the average value
\[ \frac{u^{1/2}}{H^{1/2}} \] at the two end-transects is used.

To adjust \( k_2 \) for temperatures other than 20°C, Elmore and West's (1961) formula is used

\[ k_2 = (k_2)_{20} \cdot 1.024(T-20) \]  \hspace{1cm} (29)

where \( T \) is the water temperature in centigrade degrees.

(4) CBOD oxidation rate, \( k_1 \): The oxidation rate of CBOD (carbonaceous biochemical oxygen demand) normally ranges from 0.1 to 0.5 per day. The rate also depends on water temperature; the following formula is used for this temperature dependence,

\[ k_1 = (k_1)_{20} \cdot 1.047(T-20) \]  \hspace{1cm} (30)

(5) CBOD settling rate, \( k_s \): \( k_s \) is usually negligible.

(6) Saturated oxygen content, \( D_{0S} \): The saturation concentration of dissolved oxygen depends on temperature and salinity. From tables of saturation concentration (Carritt and Green, 1967) a polynomial equation was determined by a least-squares method.

\[ D_{0S} = 14.6244 - 0.367134T + 0.0044972T^2 \]
\[ - 0.0966S + 0.00205TS + 0.0002739S^2 \]

where \( S \) is salinity in parts per thousand and \( D_{0S} \) is in mg/liter.

(7) Benthic oxygen demand, BEN: The bottom sediment of an estuary may vary from deep deposits of sewage or industrial
waste origin to relatively shallow deposits of natural material of plant origin and finally to clean rock and sand. The oxygen consumption rate of the bottom deposits must be determined with field measurements. Field data were used wherever they are available. A value of 1.0 gm/m²/day at 20°C is typical average for most estuaries. The temperature effect was simulated by Thomann, 1972.

\[
\text{BEN} = (\text{BEN})_{20} \cdot 1.065^{(T-20)}
\]

where \((\text{BEN})_{20}\) is the benthic demand at 20°C.

(8) Coliform bacteria dieoff rate, \(k_b\)

\[
k_b = (k_b)_{20} \cdot 1.040^{(T-20)}
\]

where \((k_b)_{20}\) is the dieoff rate at 20°C and \(T\) is temperature in degrees centigrade. The normal range of \((k_b)_{20}\) is 0.5-4.0/day.

(9) Settling rate of organic nitrogen, \(k_{n11}\)

\[k_{n11} \text{ is of order of } 0.1/\text{day}\]

(10) Organic N to NH₃ hydrolysis rate, \(k_{n12}\)

\[k_{n12} = aT\]

where \(a\) is of order of 0.007/day/degree

(11) NH₃ to NO₃ nitrification rate, \(k_{n23}\)

\[k_{n23} = aT\]

where \(a\) is of order of 0.01/day/degree
(12) NO$_3$ escaping rate, $k_{n33}$

$k_{n33}$ is usually negligible

(13) Organic phosphorus settling rate, $k_{p11}$

$k_{p11}$ is order of 0.1/day

(14) Organic P to inorganic P conversion rate, $k_{p12}$

$k_{p12} = aT$

where $a$ is of order of 0.007/day/degree

(15) Inorganic phosphorus settling rate, $k_{p22}$

$k_{p22}$ is of order of 0.1/day

(16) Nitrogen-chlorophyll ratio, $a_n$

$a_n$ is of order of 0.01 mg N/µg C

(17) Phosphorus-chlorophyll ratio, $a_p$

$a_p$ is of order of 0.001 mg P/µg C

(18) Carbon-chlorophyll ratio, $a_c$

$a_c$ is of order of 0.05 mg carbon/µg C

(19) Oxygen produced per unit of chlorophyll growth, $a_d$

$a_d = 2.67 \cdot a_c \cdot PQ$

where PQ is photosynthesis quotient, PQ = 1 ~ 1.4.

(20) Oxygen consumed per unit of chlorophyll respired, $a_r$

$a_r = 2.67 \cdot a_c/RQ$

where RQ is respiration ratio.

(21) Phytoplankton settling rate, $k_{cs}$

$k_{cs} = S_{sl}/h$

where $S_{sl}$ is settling velocity, whose normal range is 15 to 150 cm/day (0.5 to 5 ft/day).
(22) Zooplankton grazing, $K_g$: In reality, $K_g$ should depend solely on the concentration of herbivorous zooplankton biomass. However, the settling rate has been assumed to be zero. This effect has been included in the grazing rate.

(23) Endogenous respiration rate, $R_s$

$$R_s = aT$$

where $a$ is of order of 0.005/day/degree.

(24) Growth rate, $G_c$: The growth rate expression is that developed by Di-Toro, O'Connor and Thomann (1971) and as used in this model is given by

$$G_c = k_{gr} T \cdot I (I_a, I_s, k_e, C, h) \cdot N (N2, N3, P2)$$

where $k_{gr}$ is the optimum growth rate of the order of 0.1/day/degree. The functional form, $I$, for the light effect incorporates vertical extinction of solar radiation and self-shading effect. The form is

$$I = \frac{2.718}{k_e h} (e^{-\alpha_1} - e^{-\alpha_o})$$

$$k_e = k_e' + 0.0088 \cdot C + 0.054 \cdot C^{0.66}$$

$$\alpha_1 = \frac{I_a}{I_s} e^{-k_e h}$$

$$\alpha_o = \frac{I_a}{I_s}$$

$k_e'$ is the light extinction coefficient at zero chlorophyll concentration, $k_e$ is the overall light extinction
coefficient, $I_a$ is the incoming solar radiation and $I_s$ is the optimum light intensity, about 300 langleys per day. The nutrient effect makes use of product Michaelis-Menten kinetics and is given by

$$N = \frac{N_2 + N_3}{K_{mn} + N_2 + N_3} \cdot \frac{P^2}{K_{mp} + P^2}$$

where $K_{mn}$ is the half saturation concentration for total inorganic nitrogen and $K_{mp}$ is the half saturation concentration for phosphorus. $K_{mn}$ and $K_{mp}$ have been reported to be about 0.3 - 0.4 and 0.03 - 0.05 mg/l respectively, although $K_{mn}$ has been reported as low as 0.008 mg/l and $K_{mp}$ has been reported as low as 0.015 mg/l.
Chapter 3.

Model Calibration

The first step in a modelling study is to develop the mathematical expressions which incorporate the essential physical, chemical and biological processes which control water quality. While this may be useful for scientific studies, it is not useful for the purpose of developing waste load allocation schemes unless and until the model is calibrated. That is, the model must be adjusted so that it reproduces the behavior observed in the actual estuary. Obviously, a set of field data is required to accomplish this end. Measurements of both independent and interdependent variables must be made sequentially over a period of time and more or less simultaneously at selected locations throughout the area of concern.

Independent variables are those factors which are not modelled, but which are included in the model as known constants or functions. Some of these factors, such as water temperature and solar radiation, can be measured directly. Those factors which cannot be measured directly must be estimated using the scientific literature or they may be derived from field observations (the decay rate for carbonaceous BOD, for example). A list of the independent variables used as inputs to the model as given in Appendix A.

Interdependent variables are the factors which are modelled and are related. For example, the decay of oxygen demanding materials reduces the amount of dissolved oxygen,
and the decay of organic phosphorus results in increased levels of inorganic phosphorus. These components of the model have been described in Chapter 2. The matrix shown in Table 1 indicates the interdependence among variables, in the sense of the existence of a direct mathematical relationship. The fecal coliform and salinity submodels may be calibrated independently, but the remaining eight components must be calibrated simultaneously.

Field observations of estuarine water quality were made during intensive surveys conducted in July of 1975. A description of the field project and a summary of results have been presented in a water quality report. Neither the Back nor the Poquoson River have known point sources of oxygen demanding materials or nutrients. Loadings therefore were solely the result of runoff from the land. Field observations of runoff quality and quantity for a variety of land uses within the 208 study area were made during the period March to October, 1976. These data were used by Malcolm Pirnie Engineers, Inc. to calibrate the math model of land runoff, STORM. Once this model had been calibrated, it was used to generate nonpoint source loadings for each of the drainage basins for the 30 day period prior to the estuarine sampling program. These STORM model outputs were used as inputs to the water quality models of the two estuaries in order to reproduce the water quality conditions which existed on July 23, 1975, the date of the intensive surveys.

The Back and Poquoson models employed no freshwater inflows or loadings above those specified by the STORM output.
Table 1

Ecosystem Component Interdependence Matrix

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Salinity</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic Nitrogen</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ammonia</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nitrate plus Nitrite</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic Phosphorus</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inorganic Phosphorus</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chlorophyll</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CBOD</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dissolved Oxygen</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coliform Bacteria</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: 'X' indicates dependency.
The flows and loadings were input to the model on a daily basis, with the updating taking place at midnight, model time. Baseline runoff between rainfall events was assumed to be zero.

A. Calibration Procedure

Calibration of the model is achieved in stages. The first step is to simulate conservative substances, such as salt or a tracer dye, since the distributions of these substances are solely the result of physical processes. That is, the variations in salinity observed in the estuary are the result of Bay-derived salty water being transported and mixed with land-derived freshwater. Since there is essentially no decay of salt nor any source other than the ocean, only the physical processes are at work. It is assumed that all substances will be transported and dispersed in a like fashion, but that non-conservative substances will experience bio-chemical transformations during the process. Therefore, the second phase of calibration is to simulate the concentration field of a non-conservative substance. For the water quality model used in this study, the fecal coliform submodel normally would be calibrated next since it is simple having essentially no interactions with other components.

Calibration of the nutrient cycle is difficult since numerous elements and constants are involved. Several constants used in the model were not measured in the field, but instead values were determined by successive trials using literature values as guides. The system used in this trial and error approach was to concentrate on the chlorophyll levels.
In other words, changes in constants were chosen to bring the chlorophyll concentration closer to the observed value. This process was efficient in the sense that most model components were close to calibration by the time that the chlorophyll element was properly adjusted. There remained only some final "tuning" of several rate constants which had minor influence on chlorophyll. A few of the factors which were adjusted in the chlorophyll calibration were the growth and death rates for phytoplankton, and the internal transfer rates among nitrogen and phosphorus species. In many ways the system is very stable. For example, if the rate of transfer from organic to inorganic phosphorus is increased, the portion of phosphorus in organic form will initially decline and the fraction in inorganic form will be increased. However, the greater availability of inorganic phosphorus can stimulate phytoplankton growth, which eventually will result in a larger transfer of dead cells to the organic phosphorus component.

The dissolved oxygen component is the last to be adjusted since the phytoplankton have an effect on DO levels. Changes in the decay rate of oxygen demanding material, including dead plankton, tends to affect the BOD levels more than the oxygen concentrations since reaeration plays a dominant role in the oxygen cycle.

The water quality models of the Back and Poquoson Rivers were calibrated with the field data collected in July, 1975. Some of the constants and transfer rates were derived from actual measurements while other were determined
during the calibration process. Values for these inputs are given in Appendix A: Table A-1 enumerates those inputs derived from field observation while Table A-2 lists those constants which were estimated. Literature values are given for comparison purposes and the references are given in Table A-3. Nonpoint source loadings which were used are those predicted by the mathematical model of runoff, STORM, and were supplied to VIMS by Malcolm Pirnie Engineers, Inc. For the initial trials, the nonpoint loadings were averaged over the 30 day period prior to the intensive survey. This proved to be inadequate, so the final calibration was achieved using time dependent loadings. Graphs of the observed and predicted daily average values are given in Appendices B and C, for the Back and Poquoson Rivers respectively. The segmentation of the river and its tributaries for modelling purposes has been shown as well.

B. Model Sensitivity

Many input constants are included in the model. The model components are very sensitive to some of the constants but less so to others. It is important to establish the sensitivity of model components to changes in input constants for two reasons: first, to prove the potential usefulness of the model once developed, since an insensitive model will not be able to discriminate between widely different input conditions; second, a systematized sensitivity scheme facilitates the calibration process.
In some cases, analysis can be used to predict the sensitivity, but more often sensitivity is determined by experience gathered in the process of calibration. In few cases did a 20% change in a parameter produce a 20% change in any component. There are two reasons for this: first, the relationships tend to be self-buffering, so that a great change in one component is resisted by a negative-feedback effect; second, the system is not closed from outside sources. If any component begins to be depleted, the transport terms bring in reserve quantities across the boundaries.

Based on the experience gained from many computer runs, quantitative estimates of sensitivity to certain inputs can be given. The following table indicates maximum sensitivity to changes in the value of particular parameters. These results are not universal; they depend on the range of parameters used. For example, chlorophyll growth can be inhibited by either a shortage of inorganic phosphorus or a shortage of inorganic nitrogen. Analysis of the field data indicates that nitrogen is the limiting nutrient for both the Back and Poquoson Rivers. Therefore, the responses shown in Table 2 are for nitrogen-limited phytoplankton growth; for the phosphorus-limited case, the responses of individual components would be quite different. The large sensitivity of nitrate plus nitrite stems from the smallness of the base. Observed values were only about two to four times the minimum observable.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Change in Input</th>
<th>N1</th>
<th>N2</th>
<th>N3</th>
<th>P1</th>
<th>P2</th>
<th>C</th>
<th>CBOD</th>
<th>DO</th>
</tr>
</thead>
<tbody>
<tr>
<td>KN12</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>-1.7</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>15.6</td>
<td>0.8</td>
</tr>
<tr>
<td>KN23</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-0.2</td>
</tr>
<tr>
<td>KP12</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-4.3</td>
<td>4.4</td>
<td>0.2</td>
<td>0.07</td>
<td>0.05</td>
</tr>
<tr>
<td>Carbon-C Ratio</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-0.05</td>
<td>12.7</td>
</tr>
<tr>
<td>N-C Ratio</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>2.6</td>
<td>0</td>
<td>-80.</td>
<td>0</td>
<td>4.3</td>
<td>-14.2</td>
</tr>
<tr>
<td>P-C Ratio</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>-0.2</td>
<td>0</td>
<td>9.1</td>
<td>3.4</td>
<td>-8.0</td>
<td>-0.4</td>
</tr>
<tr>
<td>KMN</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>-0.4</td>
<td>4.8</td>
<td>25.0</td>
<td>0</td>
<td>0</td>
<td>-2.1</td>
</tr>
<tr>
<td>KMP</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>-0.2</td>
<td>6.0</td>
<td>18.5</td>
<td>-4.3</td>
<td>4.6</td>
<td>-1.3</td>
</tr>
<tr>
<td>Sat.Growth Rate</td>
<td>+10%</td>
<td>0</td>
<td>0</td>
<td>0.7</td>
<td>-4.8</td>
<td>-33.3</td>
<td>0</td>
<td>-3.8</td>
<td>3.9</td>
</tr>
<tr>
<td>Grazing Rate</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>-0.4</td>
<td>6.0</td>
<td>45.5</td>
<td>0</td>
<td>6.0</td>
<td>-12.9</td>
</tr>
<tr>
<td>Photosyn. Quotient</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Resp. Quotient</td>
<td>+20%</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-5.3</td>
</tr>
</tbody>
</table>

N1 = Organic N  
N2 = Ammonia  
N3 = Nitrate plus Nitrite  
KN12 = Organic N-Ammonia Hydrolysis Rate  
KN23 = Ammonia Nitrofication Rate  
KP12 = Org. to Inorg. P Rate  
P1 = Organic Phosphorus  
P2 = Inorganic Phosphorus  
C = Chlorophyll  
CBOD = Carbonaceous BOD  
DO = Dissolved Oxygen  
KMN, KMP = Nitrogen and Phosphorus Michaelis Constants
C. Discussion

Comparison of field measurements and model predictions indicates that the models are able to reproduce the behavior of the estuaries and that they are calibrated. The only component which showed any appreciable variation between observed and predicted levels was biochemical oxygen demand (BOD), a notoriously imprecise analysis. Predicted levels are within the confidence limits for the observed values.

Observed chlorophyll "a" concentrations often were in the range 8 to 12 micrograms per liter, a mild algal bloom condition. Analysis of the model results indicates that the availability of nutrients was limiting algal growth. This conclusion was supported by several observations. First, the ratio of nitrogen to chlorophyll was low. That is, the amount of nitrogen taken up by the phytoplankton to produce a unit of chlorophyll was much lower than has been observed in many instances. There is a minimum amount of nitrogen required for phytoplankton growth, but often amounts far in excess of this minimum value are consumed, the so called "luxury uptake". The low nitrogen to chlorophyll ratio implies that there was insufficient nitrogen available to support luxury uptake, and that what was available was being used for essential life functions, namely growth. The phosphorus to chlorophyll ratio similarly was low. Additionally, the supply of nitrogen and phosphorus were observed to be limiting the growth of phytoplankton (inhibition factors of about 0.6) as a result of the Michaelis-Menten kinetics of
growth. This occurred despite the fact that the Michaelis constants were at the lower end of the ranges of values found in the literature. All of this indicates that the increased loadings of nitrogen and phosphorus are likely to result in higher standing crops of algae, perhaps to levels that would be considered blooms by most observers.

Dissolved oxygen levels are quite satisfactory under the conditions used for calibration. The runoff loadings are minimal, there are no point sources and oxygen demand from the decay of phytoplankton also has only a small impact on DO levels. Diurnal variations in DO levels due to photosynthesis in the day and respiration during periods of darkness are not insignificant. Maximum variations observed were around 4 mg/l in the Poquoson River and about 3 mg/l in the Back River. This effect is reproduced in the model, although the amplitude of the variations is somewhat reduced. As long as the minimum DO concentrations remain about 4 mg/l, there is not violation of water quality standards nor is there likely to be any strong impact. But when oxygen levels reach 2 mg/l or less, large amounts of nutrients can be released from the sediments exacerbating bloom conditions. Waste load allocation studies should focus on the sources of the nutrients and the levels which can be assimilated without having this situation develop.

The fecal coliform sub-model has only one parameter, the die-off rate. Following rain events coliform counts in the estuary rise dramatically. Model runs indicate that post-rain-event peaks are of the order of several hundred fecal coliforms per 100 mls and that counts are very high in the upstream reaches.
For example, the July 5, 1975 rain event produced coliform counts of over 2000 MPN/100 ml at the upper ends of the estuaries. The magnitude of the peak concentrations is sensitive to die-off rate, but field data to calibrate the model for rain events are lacking. The transport of fecal coliforms in land runoff is apparently the reason that shellfish closure zones exist in both estuaries. Wasteload allocation studies should demonstrate the severity, the extent and the duration of these increased coliform levels resulting from non-point loadings.

Between rain events coliform counts subside to low, background levels which generally were less than 10 MPN/100 ml. However, it must be noted that there was a great deal of scatter in the fecal coliform data and that individual observations at several stations were considerably higher than the daily mean. Nonetheless, much of the estuary is suitable for both primary contact recreation and shellfish culture. The coliform counts predicted by the model for periods between rain events are insensitive to variations in die-off rate.

In summary, use of field observations of estuarine water quality and predictions of stormwater runoff loadings has allowed mathematical models of the Back and Pougoson Rivers to be calibrated. These models accurately reproduce the physical, biological and chemical processes occurring in these water bodies and are able to simulate many aspects of water quality. Although no major water quality problems exist at present, model studies will allow for delineation of the assimilation capacity of these rivers and examination of problem situation which might arise. Since these models have been calibrated, they are suitable for these studies.
APPENDIX A

Input Constants
<table>
<thead>
<tr>
<th>Input</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>River Channel Geometry</td>
<td>VIMS Bathymetry Survey</td>
</tr>
<tr>
<td>Drainage Basin Area</td>
<td>Va. Div. of Water Resources Bulletin</td>
</tr>
<tr>
<td>Tidal Current Amplitude</td>
<td>Current meter measurements simultaneous w/intensive survey</td>
</tr>
<tr>
<td>Fresh Water Inflow</td>
<td>Estimated from rainfall record</td>
</tr>
<tr>
<td>Incident Solar Radiation</td>
<td>Concurrent Pyroheliometer Data taken by VIMS</td>
</tr>
<tr>
<td>Bottom Oxygen Demand</td>
<td>VIMS Surveys July 29 &amp; 31, 1975</td>
</tr>
<tr>
<td>CBOD Decay Rate</td>
<td>VIMS Intensive Survey July, 1975</td>
</tr>
<tr>
<td>Input Constant (Symbol)</td>
<td>Units</td>
</tr>
<tr>
<td>-------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>Saturation Light Intensity (RIS)</td>
<td>langleys day</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Phytoplankton Growth Rate (GSAT)</td>
<td>day^{-1}</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Input Constant (Symbol)</td>
<td>Units</td>
</tr>
<tr>
<td>-------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>Saturation</td>
<td></td>
</tr>
<tr>
<td>Phytoplankton</td>
<td></td>
</tr>
<tr>
<td>Growth Rate (GSAT)</td>
<td></td>
</tr>
<tr>
<td>(cont'd)</td>
<td></td>
</tr>
<tr>
<td>Phosphorus</td>
<td>mg P</td>
</tr>
<tr>
<td>Michaelis Constant (KMP)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Planktonic green algae & diatoms
Artificial fertilization experiment in Fresh Water Lake
Summary of results from several sources
From Scavia & Parks, 1976
Tidal fresh water ecosystem model study
Shortage of extra-cellular P not limiting to growth
Tidal fresh water ecosystem model study
<table>
<thead>
<tr>
<th>Input Constant (Symbol)</th>
<th>Units</th>
<th>Value(s) Used in Models</th>
<th>Literature Values</th>
<th>Reference</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen Michaelis Constant (KMN)</td>
<td>mgN/l</td>
<td>.010-.018</td>
<td>.014-.018</td>
<td>MacIsaac &amp; Dugdale, 1969</td>
<td>Oligotrophic Systems</td>
</tr>
<tr>
<td>Plankton Settling Rate (KCS)</td>
<td>day⁻¹</td>
<td>0.0</td>
<td>0.1</td>
<td>Penumalli, et.al., 1976</td>
<td>Tidal fresh water ecosystem model study</td>
</tr>
<tr>
<td>Endogenous Respiration Rate (RRESP)</td>
<td>day⁻¹</td>
<td>.015</td>
<td>8-10% of optimum photosynthetic rate</td>
<td>Nielsen, 1975</td>
<td>Fresh water phytoplankton</td>
</tr>
<tr>
<td>Carbon-Chlorophyll Ratio (AC)</td>
<td>mg/µg</td>
<td>.05</td>
<td>.015-.02, .019-.097, .027-.049, .05</td>
<td>McAllister, et.al., 1961, Parsons, et.al., 1961, Parsons &amp; Takahashi, 1972, p. 47, Thomann, et.al., 1974</td>
<td>Sea water, Eleven different species examined, Textbook summary from other sources, Tidal fresh water ecosystem model study</td>
</tr>
<tr>
<td>Input Constant (Symbol)</td>
<td>Units</td>
<td>Value(s)</td>
<td>Literature Values</td>
<td>Reference</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------------------</td>
<td>-------</td>
<td>----------</td>
<td>-------------------</td>
<td>-----------</td>
<td>----------</td>
</tr>
<tr>
<td>Nitrogen-Chlorophyll Ratio (AN)</td>
<td>mg/µg</td>
<td>.005</td>
<td>.08-.17 gmN/gm Carbon</td>
<td>Collos &amp; Levin, 1976</td>
<td>Ratio tends to increase as growth rate slows</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.0016-.0045</td>
<td>McAllister, et.al., 1961</td>
<td>Log phase growth</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.008-.016</td>
<td>Parsons &amp; Takahashi, 1972, p. 47</td>
<td>Textbook summary from other sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.004-.014</td>
<td>Parsons, et.al., 1961</td>
<td>Eleven different species examined</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.01</td>
<td>Thomann, et.al., 1974</td>
<td>Tidal fresh water ecosystem model study</td>
</tr>
<tr>
<td>Phosphorus-Chlorophyll Ratio (AP)</td>
<td>mg/µg</td>
<td>.0005</td>
<td>.0008</td>
<td>McAllister, et.al., 1961</td>
<td>Log Phase Growth</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.0014-.0055</td>
<td>Parsons, et.al., 1961</td>
<td>Eleven different species examined</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.0009-.0023</td>
<td>Parsons &amp; Takahashi, 1972, p. 47</td>
<td>Textbook summary from other sources</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>.001</td>
<td>Thomann, et.al., 1974</td>
<td>Tidal fresh water ecosystem model study</td>
</tr>
<tr>
<td>Input Constant (Symbol)</td>
<td>Units</td>
<td>Value(s) Used in Models</td>
<td>Literature Values</td>
<td>Reference</td>
<td>Comments</td>
</tr>
<tr>
<td>------------------------</td>
<td>-------</td>
<td>-------------------------</td>
<td>------------------</td>
<td>-----------</td>
<td>----------</td>
</tr>
<tr>
<td>Organic N- Ammonia Hydrolysis rate Constant (KN12)</td>
<td>day$^{-1}$ OC$^{-1}$</td>
<td>.0025-.003</td>
<td>.015/day</td>
<td>Penumalli, Flake &amp; Fruh, 1976</td>
<td>Nitrogen Cycle model</td>
</tr>
<tr>
<td>Ammonia Nitrification Rate (KN23)</td>
<td>day$^{-1}$ OC$^{-1}$</td>
<td>.02-.03</td>
<td>.025/day</td>
<td>Penumalli, Flake &amp; Fruh, 1976</td>
<td>Nitrogen Cycle model</td>
</tr>
<tr>
<td>Organic Phosphorus to Inorganic Phosphorus rate Const. (KP12)</td>
<td>day$^{-1}$ OC$^{-1}$</td>
<td>.005</td>
<td>.007</td>
<td>Thomann, et al., 1974</td>
<td>Tidal fresh water ecosystem model study</td>
</tr>
<tr>
<td>Grazing Constant (KGRAZ)</td>
<td>day$^{-1}$</td>
<td>.27-.42</td>
<td>.85gm/day</td>
<td>Frederove &amp; Sorokin, 1977</td>
<td>These two models have compartments for zooplankton. Grazing rate of phytoplankton per unit zooplankton per unit time.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Scavia &amp; Park, 1976</td>
<td></td>
</tr>
<tr>
<td>Input Constant</td>
<td>Units</td>
<td>Value(s)</td>
<td>Literature Values</td>
<td>Reference</td>
<td>Comments</td>
</tr>
<tr>
<td>----------------</td>
<td>-------</td>
<td>----------</td>
<td>-------------------</td>
<td>-----------</td>
<td>----------</td>
</tr>
<tr>
<td>Photosynthetic Quotient (PQ)</td>
<td></td>
<td>1.3-1.4</td>
<td>1.25</td>
<td>Schlieper, 1972, p. 303</td>
<td>Average value for marine phytoplankton</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.3</td>
<td>McAllister, et.al., 1961</td>
<td></td>
</tr>
</tbody>
</table>
Table A-3.
References - Ecosystem Model Parameters


APPENDIX B

Observed and Predicted Values of Model Components for the Back River
Figure B-1. The Back River, showing model segments.

Model transects indicated with river mi. (km)

- Model Reach Number
Figure B-2. Longitudinal salinity profiles.
Figure B-3. Longitudinal variation of inorganic phosphorus.
Figure B-4. Longitudinal variation of organic phosphorus.
Back River
Organic Nitrogen
Time-dependent Loading

Figure B-5. Longitudinal variation of organic nitrogen.
Back River
Ammonia Nitrogen
Time-dependent Loading

- Observed Daily Average
- Model Daily Average

Figure B-6. Longitudinal variation of ammonia-nitrogen.
Figure B-7. Longitudinal variation of (nitrate + nitrite)-nitrogen.
Figure B-8. Longitudinal variation of chlorophyll "a".
Figure B-9. Longitudinal variation of carbonaceous BOD.
Figure B-10. Longitudinal variation of dissolved oxygen.
Figure B-11. Longitudinal profiles of fecal coliform concentrations.
APPENDIX C

Observed and Predicted Values of Model Components for the Poquoson River
Poquoson River Model transects indicated with river mi. (km).

Model Reach Number

Figure C-1. Poquoson River, showing model segments.
Figure C-2. Longitudinal profiles of salinity.
Figure C-3. Longitudinal profiles of inorganic phosphorus.
Poquoson River
Organic Phosphorus
Time-dependent Loadings

- Observed Daily Average
- Model Daily Average

Chisman Cr.
Bennett Cr.

Figure C-4. Longitudinal variation of organic phosphorus.
Poquoson River
Nitrate plus Nitrite
Time-dependent Loadings

- Observed Daily Average
- Model Daily Average

Figure C-5. Longitudinal variation of (nitrate + nitrite)-nitrogen.
Poquoson River
Ammonia Nitrogen
Time-dependent Loadings

- Observed Daily Average
- Model Daily Average

Figure C-6. Longitudinal profiles of ammonia-nitrogen.
Figure C-7. Longitudinal variation of organic nitrogen.
Poquoson River
Chlorophyll
Time-dependent Loadings

Figure C-8. Longitudinal profiles of chlorophyll "a".
Figure C-9. Longitudinal variation of carbonaceous BOD.
Figure C-10. Longitudinal profile of dissolved oxygen.
Figure C-11. Longitudinal profiles of fecal coliform densities.