Summary report on the calibration of the water quality models of the Chesapeake Bay system

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SUMMARY REPORT
ON
THE CALIBRATION OF THE WATER QUALITY MODELS
OF
THE CHESAPEAKE BAY SYSTEM

A REPORT TO THE U. S. ENVIRONMENTAL PROTECTION AGENCY
CHESAPEAKE BAY PROGRAM
from
the Department of Physical Oceanography
and Environmental Engineering

Virginia Institute of Marine Science
and
School of Marine Science
College of William and Mary
Gloucester Point, Va. 23062

MARCH 1984

NAUTICAL MILES
SUMMARY REPORT

ON THE CALIBRATION OF THE WATER QUALITY MODELS

OF THE CHESAPEKE BAY SYSTEM

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Project Manager

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CHAPTER I. INTRODUCTION

One of the three areas of emphasis for the U. S. Environmental Protection Agency's Chesapeake Bay Program has been nutrient enrichment, often referred to as eutrophication. Because this program was intended to provide guidance to those persons and agencies that manage the bay, there was the need to not only address important scientific questions, but also to develop tools that would be of value in assessing alternative management strategies. One of those tools is the water quality model of Chesapeake Bay.

The intended use of the water quality model was to predict the levels of important water quality parameters, in particular the dissolved oxygen levels and the algal populations, for alternative sets of nutrient loadings. The goals of the present modelling study were to apply appropriate models to the Chesapeake Bay system, to adjust the models so that they accurately simulated conditions in the prototype, and to use those models to predict conditions under a number of nutrient loading scenarios. This report provides a summary of the work done to satisfy the first two of those three objectives.

It is important to note at this time that the water quality modelling was done under a cooperative agreement between the Environmental Protection Agency and the Virginia Institute of Marine Science of the College of William and Mary. The overall direction of the study was determined primarily by the Bay Program staff with periodic reviews by scientific advisors and the management advisory committee. The Bay Program and individuals and organizations under contract to the Bay Program provided much of the information necessary for operation of the
model, reviewed modelling efforts regularly, and were involved in virtually every aspect of the study. Thus the results of the study are due to the contributions of those individuals and organizations, as well as the scientists who worked with the models at VIMS.

Figure 1. Schematic diagram showing types of processes occurring in a typical water quality model segment.
CHAPTER II. MODELLING APPROACH

The models of the Chesapeake Bay system include both hydrodynamics and water quality submodels. The hydrodynamics models simulate the physical transport processes that control the advection and dispersion of substances in the water. The water quality models include the cycling of nutrients due to bacterial and chemical action, the uptake of nutrients by phytoplankton, and the ensuing growth and death of the algal population. Production and consumption of oxygen by the phytoplankton are incorporated into the dissolved oxygen cycle, along with the bacterial decomposition of organic matter, sediment oxygen demand, and natural reaeration processes (see Figure 1). The rates at which these processes occur are determined in large part by external variables such as environmental conditions.

The Susquehanna, Potomac, and James rivers are the primary sources of freshwater for the Bay supplying roughly one half, one third, and one sixth of the total freshwater inflow respectively. In each of these river basins are activities which contribute nutrients and other pollutants to the river flows. The Potomac River estuary is influenced greatly by the Washington, D. C. metropolitan area, specifically by urban runoff and the treated wastewaters that are discharged to the river. Although Richmond has a smaller population, and therefore a smaller volume of wastewater that is discharged to the James, the James also receives pollutant loads from industries located along the river. Both estuaries have exhibited signs of stress in the past, and for that reason considerable effort has been devoted to simulating water quality conditions in these two estuaries. Of particular importance is the
transformation and transport of pollutants from the tidal freshwater portion of the river, through the brackish reaches, and into Chesapeake Bay. The spatial coverage of the models is shown in Figure 2.

Hydrodynamics

The hydrodynamics models reproduce the transport mechanisms at work in the estuaries through solution of the equations representing conservation of mass and momentum. For the James and the Potomac, the equations are averaged over the river cross-section and in the Chesapeake Bay the equations are averaged over the vertical dimension. Details of the model formulation can be found in Unkelvasapaul (1984) and in Chen (1978a,b). The models are driven primarily by the tidal conditions imposed at the downstream boundary and by freshwater inputs at upriver locations. For the three estuaries of concern, either falls or dams restrict the upriver movement of the tides. Therefore the upstream boundary condition allows no upriver flow.

A model of the bay had been formulated to allow for meteorological forcing of the water surface elevations and flows, and in fact, that model has been used in a study of storm surge in Chesapeake Bay (Chen, 1978a). However, for this project that capability of the model was not employed, because the focus of the study was water quality and there was no readily available mechanism for explicitly incorporating these effects into an already ambitious program. Rather the effects of storms, the passage of meteorological fronts, etc. were incorporated into the model only via mixing or dispersion parameters, plus the direct effects resulting from variations in the freshwater inflow. Accordingly the values of the model coefficients determined through calibration will
Figure 2. Model Coverage.
incorporate the effects of those meteorological events and conditions occurring during the calibration period.

The models used do not explicitly simulate the gravitationally induced circulation in partially stratified estuaries. However, it has been common practice in math model studies to use simplified spatial representations of estuaries which do not allow for complete characterization of the flow patterns. Numerous scientists and engineers have employed one-dimensional models of estuaries in previous studies. Those transport mechanisms which are not explicitly simulated are included nonetheless, because the equations contain dispersion terms which incorporate the remaining processes. It should be noted that specification of these terms becomes increasingly more important and difficult with greater simplification of the temporal and spatial representation of the prototype. For the case at hand, the models employ time steps that are short relative to the tidal and diurnal cycles, and therefore the parameters used in these models incorporate fewer processes than do similar terms in steady state models.

Although vertically averaged models do not provide information on the vertical salinity structure, it is likely that analysis of field data would allow a 'first cut' estimate to be made given the other environmental factors. For example, analysis of the data might show a strong correlation between the vertical and the longitudinal salinity gradients. If that correlation or some other correlation were strong, then the vertical structure could be estimated using both the model predictions and historical field observations.

There is room for honest disagreement concerning the choice of hydrodynamic models for use in this study. It is the opinion of the
scientists involved that the validity of the one-dimensional approach used in the James and the Potomac is well founded. That approach has been found acceptable in numerous instances in the past. The selection of the model for Chesapeake Bay is more controversial. Perhaps a vertical plane 2-D model, such as has been developed by Wang (1983), Blumberg (1977), or others, could have been utilized. In the end, the EPA-Chesapeake Bay Program asked Dr. H. S. Chen and his colleagues to use the 2-D horizontal plane model in a cooperative study. It is the belief of those involved in this project that use of this model is scientifically valid and appropriate for the study of certain types of problems. There is no doubt that the model does not explicitly simulate vertical variations in density and flow, but the model does ‘parameterize’ a number of transport processes that are not modeled explicitly. The results of the calibration efforts must be examined to determine whether that parameterization has or has not been successful.

Water Quality

One of the intended uses of the model is to examine changes in the algal densities for differing nutrient loadings. The water quality models use the chlorophyll concentration to represent the algal biomass. Because there is no differentiation among the algal species, the model does not simulate species changes over the annual cycle or species changes in response to altered nutrient availability. However, we believe that anyone who examines the available data will conclude that the data base simply is not sufficiently detailed to permit any other approach. Indeed, chlorophyll data are sparse, often lacking for many areas and for lengthy periods of time.
The water quality models employed in this study use growth kinetics that are similar to those used in numerous water quality modelling projects of the Chesapeake Bay system and other water bodies. The inter-reactions among the water constituents are shown schematically in Figure 3. The growth of the phytoplankton is reduced from optimum or maximum levels due to light and/or nutrient limitations. The term for limited light conditions includes self-shading and acclimatization to prior light conditions. The term expressing limited availability of nitrogen and phosphorus uses a Michaelis-Menten formulation with ammonia the preferred nitrogen species. The overall growth inhibition effect is a multiplicative combination of the several terms, as opposed to selection of the term most severely limiting growth.

In addition to the uptake of dissolved inorganic forms of nitrogen and phosphorus by phytoplankton, the model includes bacterial transformations and loss to the bottom sediments. Nutrient species are generated via point and nonpoint source additions, bacterial transformations, remineralization in the bottom sediments, and atmospheric fallout.

Dissolved oxygen levels are influenced by not only the phytoplankton kinetics, but also bacterial and physical processes. Photosynthesis and natural reaeration are the primary sources of oxygen. Sinks for dissolved oxygen are phytoplanktonic respiration, bacterial transformations (both the decomposition of BOD and nitrification), and sediment oxygen demand.

Temporal resolution among water quality models varies greatly. Previous studies have emphasized a steady state approach for the upper portion of Chesapeake Bay or have utilized tidal average models. For
Figure 3. Schematic diagram showing the inter-reactions of the constituents. Adapted from Chen (1979).
the present study the models were run in a 'real time' mode. That is,
the time steps employed in the computations are on the order of a few
minutes to an hour and therefore they are much shorter than the tidal or
daily cycle. Thus one can observe the effects of both the tides and the
day-night periods on the water constituents.

Initially it was planned to simulate a few relatively short
periods, say two-week intervals. Consideration of the life cycles and
critical stages of important aquatic organisms was to provide the means
for selecting those intervals. Eventually the Bay Program decided that
a single, longer term simulation period was preferable. One considera-
tion which influenced this decision was the knowledge that spring runoff
from the Susquehanna basin typically delivers a large nitrogen load to
the upper end of the bay and that this pulse of nitrogen-rich water
slowly moves down-bay, exiting to the Atlantic sometime in late summer
or the fall. The time period finally chosen for model simulation is the
March 1 through October 31 period.

In order to examine the interactions in some detail, the cycles
incorporated in the model will be discussed in the following sections.
The full equations used in the model can be found in Chen (1978b).

Phosphorus Cycle

The phosphorus cycle included in the model is relatively simple,
with the primary compartments being phosphorus bound in living algal
cells (C3), organic phosphorus, both particulate and dissolved forms and
including dead phytoplankton (C7), and dissolved inorganic phosphorus
(C8) generally measured in the field as Soluble Reactive Phosphorus.
These compartments and the transfer mechanisms are shown schematically
in Figure 4. The model calculates the internal transformations shown in the figure.

Remineralization = T • OPIOP • C7
Respiration = T • ENRES • PCHLRA • C3
Grazing = T • ZOOGR • ZCK • PCHLRA • C3
Uptake = gr • PCHLRA • C3
Loss = SETTL(7) • C7 or SETTL(8) • C8

The factors included in these transformations are:

T = Temperature in degrees Centigrade
OPIOP = phosphorus mineralization rate (day\(^{-1}\)deg C\(^{-1}\))
C7 = organic phosphorus concentration (mg/l)
ENRES = respiration coefficient (day\(^{-1}\)deg C\(^{-1}\))
PCHLRA = phosphorus to chlorophyll ratio (mg/µg)
C3 = chlorophyll concentration (µg/l)
ZOOGR = zooplankton grazing rate (day\(^{-1}\)deg C\(^{-1}\))
ZCK = efficiency of grazing as a phosphorus transfer mechanism
g = growth rate of phytoplankton including light and nutrient inhibiting factors (day\(^{-1}\))
SETTL(7) = loss of organic phosphorus, including settling (day\(^{-1}\))
SETTL(8) = loss of inorganic phosphorus, including settling (day\(^{-1}\))

The values used in the models in the present study and also in other studies of the Potomac River are given in Table 1.

Nitrogen Cycle

The nitrogen cycle includes more compartments and more transformations than the phosphorus cycle, but otherwise is similar. Nitrite-nitrogen and nitrate-nitrogen are combined in model calculations and ammonia-nitrogen is the inorganic form preferred by phytoplankton.
Phosphorus Interactions

Figure 4. Phosphorus cycle schematic.

Nitrogen Interactions

Figure 5. Nitrogen cycle schematic.
### Table 1.

Parameters Related to Phosphorus Cycle

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Memonic</th>
<th>Ches. Bay</th>
<th>James River</th>
<th>This Study</th>
<th>COG</th>
<th>Clark</th>
<th>Zison et.al.</th>
<th>DiToro Thomann</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phosphorus Mineralization Rate (1/day/deg.C)</td>
<td>OPIOP</td>
<td>0.003</td>
<td>0.001</td>
<td>0.005</td>
<td>0.22/da*</td>
<td>-</td>
<td>-</td>
<td>0.007</td>
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<td>Endogenous Respiration Rate (1/day/deg.C)</td>
<td>ENRES</td>
<td>0.002</td>
<td>0.004</td>
<td>0.004</td>
<td>0.125/da*</td>
<td>0.0076</td>
<td>0.002-.011</td>
<td>0.005</td>
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<td>P to chlorophyll ratio (mg/ug)</td>
<td>PCHLRA</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.025**</td>
<td>-</td>
<td>0.024-0.24**</td>
<td>0.001</td>
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<td>Michaelis P constant (mg/l)</td>
<td>HSCPHO</td>
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<td>0.006</td>
<td>0.001</td>
<td>0.001</td>
<td>-</td>
<td>0.016-0.5</td>
<td>0.005</td>
</tr>
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<td>Zooplankton grazing rate (1/day/deg.C)</td>
<td>ZOOGR</td>
<td>0.002</td>
<td>0.004</td>
<td>0.002</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Phytoplankton Optimum Growth Rate (1/day/deg.C)</td>
<td>OPTGR</td>
<td>0.09</td>
<td>0.121</td>
<td>0.11</td>
<td>2.0/da*</td>
<td>0.081</td>
<td>0.2-3.1/da</td>
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<td>Loss rates (1/day):</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Org. P</td>
<td>SETTL(7)</td>
<td>0</td>
<td>0.01-0.03</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.10</td>
</tr>
<tr>
<td>Inorg P</td>
<td>SETTL(8)</td>
<td>0.01-0.10</td>
<td>0.03</td>
<td>0-0.15</td>
<td>0.0218</td>
<td>-</td>
<td>-</td>
<td></td>
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</tbody>
</table>

* Temperature power law formulation used.
** Phosphorus to Carbon Ratio.
Internal transformations, shown in the schematic diagram (Figure 5), are calculated as follows:

\[
\text{Hydrolysis} = T \times \text{HYDRO} \times C4
\]
\[
\text{Respiration} = T \times \text{ENRES} \times \text{RNOCHL} \times C3
\]
\[
\text{Grazing} = T \times \text{ZOOGR} \times ZCK \times \text{RNOCHL} \times C3
\]
\[
\text{Nitrification} = T \times \text{CNITR} \times C5
\]
\[
\text{Uptake} = gr \times \text{RNOCHL} \times PR \times C3 \text{ (for ammonia)}
\]
\[
= gr \times \text{RNOCHL} \times (1-PR) \times C3 \text{ (for nitrite + nitrate)}
\]
\[
\text{Loss} = \text{SETTL}(4) \times C4, \text{ and SETTL}(6) \times C6
\]

where

\[
\text{HYDRO} = \text{hydrolysis rate (day}^{-1} \text{deg C}^{-1})
\]
\[
C4 = \text{organic nitrogen concentration (mg/1)}
\]
\[
\text{ENRES} = \text{endogenous respiration rate (day}^{-1} \text{deg C}^{-1})
\]
\[
\text{RNOCHL} = \text{nitrogen to chlorophyll ratio (mg/ug)}
\]
\[
C3 = \text{chlorophyll concentration (~g/1)}
\]
\[
\text{ZOOGR} = \text{zooplankton grazing rate (day}^{-1} \text{deg C}^{-1})
\]
\[
ZCK = \text{efficiency of grazing as a nitrogen transfer mechanism}
\]
\[
\text{CNITR} = \text{nitrification rate (day}^{-1} \text{deg C}^{-1})
\]
\[
C5 = \text{ammonia-nitrogen concentration (mg/1)}
\]
\[
gr = \text{phytoplankton growth rate, including light and nutrient inhibiting factors (day}^{-1})
\]
\[
\text{PR} = \text{ammonia preference factor: calculated as}
\]
\[
= C5 / (C5 + \text{HSCTIN})
\]
\[
\text{HSCTIN} = \text{Michaelis constant for nitrogen availibility (mg/1)}
\]
\[
\text{SETTL}(4) = \text{organic nitrogen loss rate (day}^{-1})
\]
\[
\text{SETTL}(6) = \text{nitrite plus nitrate-nitrogen loss rate, that is denitrification rate (day}^{-1})
\]

Values used in this and other studies are given in Table 2.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mnemonic</th>
<th>Ches. Bay</th>
<th>James River</th>
<th>This Study</th>
<th>COG</th>
<th>Clark + Jaworski</th>
<th>Zison et al</th>
<th>DiToro + Thomann</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-Hydrolysis Rate (1/day/deg.C)</td>
<td>HYDRO</td>
<td>0.005</td>
<td>0.0025</td>
<td>0.003</td>
<td>.075/da*</td>
<td>-</td>
<td>-</td>
<td>0.007</td>
</tr>
<tr>
<td>Nitrification Rate (1/day/deg.C)</td>
<td>CNITR</td>
<td>0.01</td>
<td>0.01</td>
<td>0.006</td>
<td>0.09/da*</td>
<td>0.084/da*</td>
<td>.1-.5/da</td>
<td>0.10</td>
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<tr>
<td>Michaelis N Constant (mg/l)</td>
<td>HSCTIN</td>
<td>0.014</td>
<td>0.018</td>
<td>0.025</td>
<td>0.025</td>
<td>-</td>
<td>0.0014</td>
<td>0.025</td>
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<tr>
<td>Nitrogen to Chlorophyll Ratio</td>
<td>RNOCHL</td>
<td>0.015</td>
<td>0.01</td>
<td>0.01</td>
<td><strong>0.25</strong></td>
<td>0.011</td>
<td><strong>0.05-0.17</strong></td>
<td>0.01</td>
</tr>
<tr>
<td>Phytoplankton Optimum Growth Rate (1/day/deg.C)</td>
<td>OPTGR</td>
<td>0.09</td>
<td>0.121</td>
<td>0.11</td>
<td>2.0/da*</td>
<td>0.081</td>
<td>0.2-3.1/da</td>
<td>0.10</td>
</tr>
<tr>
<td>Endogenous Respiration Rate (1/day/deg.C)</td>
<td>ENRES</td>
<td>0.002</td>
<td>0.004</td>
<td>0.004</td>
<td>0.125/da*</td>
<td>0.0076</td>
<td>0.002-0.011</td>
<td>0.005</td>
</tr>
<tr>
<td>Zooplankton Grazing Rate</td>
<td>ZOOGR</td>
<td>0.002</td>
<td>0.004</td>
<td>0.002</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Loss Rates (1/day):</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic N</td>
<td>SETTIL(4)</td>
<td>0.0-0.04</td>
<td>0.02</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.10</td>
</tr>
<tr>
<td>Ammonia N</td>
<td>SETTIL(5)</td>
<td>0.0-0.08</td>
<td>0.0-0.04</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Nitrate + Nitrite-N</td>
<td>SETTIL(6)</td>
<td>0.08-0.16</td>
<td>0.0-0.16</td>
<td>0.06</td>
<td>.075</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

*Temperature power law correction formulation used.

**Nitrogen to carbon Ratio
Phytoplankton Growth Cycle

The standing crop of algae is increased by phytoplankton growth and depleted by death, grazing by zooplankton, and losses from the system, such as settling.

Nitrogen to chlorophyll and phosphorus to chlorophyll ratios are specified in the model to calculate the amount of nutrients taken up by a unit of chlorophyll (phytoplankton). The growth of the algae is affected by a number of factors including the availability of nutrients and light, the amount of solar radiation, the length of the day, the water temperature and prior light conditions. The formula expressing the instantaneous growth rate is:

\[ G = \frac{k_{gr}}{T} \cdot L \cdot N \]

where

- \( k_{gr} \) = optimum growth rate (day\(^{-1}\) deg.\(C\)^{-1})
- \( L \) = light limitation formula (given below)
- \( N \) = nutrient limitation formula (given below)

The light inhibition term is a function of the following variables:

- \( I_a \) = daily total solar radiation (langley per day)
- \( I_s \) = saturation light intensity (langley per day)
- \( k' e \) = extinction coefficient (m\(^{-1}\))
- \( k_ e \) = effective extinction coefficient
- \( C_3 \) = chlorophyll concentration (micrograms per liter)
- \( h \) = mean water depth (m)
- \( t \) = time of day (hour)

The full formula for light inhibition is:

\[ L = \frac{e^{I_0}}{k_ e h} \left( \exp\left(\frac{-I(t)\exp(-k_ e h)}{I_s}\right) - \exp\left(-I(t)/I_s\right) \right), \]
can be approximated by

\[ L = \frac{e^{-k_e h}}{k_e h} \left(1 - \exp\left(\frac{I(t)}{I_s}\right)\right), \]

in cases where the product \( k_e h \) exceeds 2. The model uses this approximate form.

The effective extinction coefficient includes a self-shading term.

\[ k_e = k_e' + 0.0088 \cdot C3 + 0.054 \cdot C3^{0.66} \]

For daylight hours, the instantaneous light intensity is given by

\[ I(t) = \frac{\pi I_a}{2} \sin \left(\frac{\pi (t - \text{SUNR})}{\text{DAYL}}\right) \]

where

- \( t \) = time of day
- \( \text{SUNR} \) = time of sunrise
- \( \text{DAYL} \) = day length

For times of day before sunrise or after sunset, the incoming radiation is, of course, zero. The day length is varied according to time of year by the formula

\[ \text{DAYL} = 12.0 + 2.7 \sin \left(\frac{2\pi}{365} (t' - 20)\right), \]

where \( t' \) is the time from the beginning of the model run, expressed in days. The constant 2.7 was determined from a nomogram in the Handbook of Meteorology (Berry, et al., 1940). The time of sunrise is computed from the day length.
Growth rate also may be limited either by shortage of phosphorus or shortage of nitrogen. That is, the nutrient limitation factor, \( N \), is the product of the nitrogen limitation factor, \( NN \), and the phosphorus limitation factor, \( NP \).

\[ N = NN \cdot NP \]

where

\[ NN = \frac{(C5 + C6)}{(C5 + C6 + KMN)} \] and
\[ NP = \frac{C8}{(C8 + KMP)} \]

in which

\[ C5 = \text{ammonia-nitrogen concentration} \]
\[ C6 = \text{nitrate plus nitrite-nitrogen concentration} \]
\[ KMN = \text{Michaelis constant for nitrogen nutrient limitation} \]
\[ C8 = \text{inorganic phosphorus concentration} \]
\[ KMP = \text{Michaelis constant for phosphorus nutrient limitation} \]

All of the above quantities are expressed in mg/l.

The respiration and grazing rates are linear functions of temperature. The endogenous respiration rate, \( ER \), is:

\[ ER = ENRES \cdot T \]

where \( ENRES \) is a respiration coefficient expressed in day^{-1} deg. C^{-1}. Likewise the grazing rate, \( ZOO \), is:

\[ ZOO = ZOOGR \cdot T \]

where \( ZOOGR \) is a grazing coefficient also expressed in days^{-1} deg. C^{-1}.

A portion of the material that has been grazed is recycled to the organic nitrogen and the organic phosphorus pools, and to the CBOD pool. The so-called efficiency of the grazing is specified as \( ZCK \).

Phytoplankton are also lost from the system by settling. This process is modeled by a decay term, \( KS \), given in days^{-1}. In other words the loss to the system is equal to the product of the loss rate, \( K38 \), and ambient concentration, \( C3 \).

The coefficients related to phytoplankton are summarized in Table 3.
Table 3. Phytoplankton-Related Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mnemonic</th>
<th>Ches. Bay</th>
<th>James River</th>
<th>Potomac River</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phytoplankton Optimum Growth Rate (1/day/deg.C)</td>
<td>OPGTGR</td>
<td>0.09</td>
<td>0.121</td>
<td>0.11</td>
</tr>
<tr>
<td>Extinction Coefficient (m⁻¹)</td>
<td>EXTINC</td>
<td>1.2</td>
<td>1.0</td>
<td>2.7</td>
</tr>
<tr>
<td>Endogenous Respiration Rate (1/day/deg.C)</td>
<td>ENRES</td>
<td>0.002</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>Zooplankton Grazing Rate (1/day/deg.C)</td>
<td>ZOOGR</td>
<td>0.002</td>
<td>0.004</td>
<td>0.002</td>
</tr>
<tr>
<td>Photosynthetic Coefficient</td>
<td>PHOTOQ</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>Respirator-Quotient</td>
<td>RESPIQ</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Carbon to Chlorophyll Ratio (mg/g)</td>
<td>CAOCHR</td>
<td>0.05</td>
<td>0.05</td>
<td>0.042</td>
</tr>
<tr>
<td>Carbon-chlorophyll ratio assumed to be 0.047 (see CTSL TR35)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1970 observations quoted in COE Report</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature power law formulation used.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Dissolved Oxygen Cycle

The dissolved oxygen pool is coupled to many of the other compartments and cycles as illustrated schematically in Figure 6. The primary source of oxygen is the atmosphere through natural reaeration. However, oxygen is also added during photosynthesis but it is consumed by phytoplanktonic respiration. Oxygen is lost in the decomposition of organic matter, including the oxidation of carbonaceous biochemical oxygen demand (CBOD) and nitrification in the water column and processes occurring in the bottom sediments, included in the model as sediment oxygen demand.

The model calculates the dissolved oxygen deficit (C10), from saturation values and the deficit, and then the ambient DO can be determined. The formulae used are:

\[
\text{Reaeration} = \text{REAER} \times C10
\]
\[
\text{Algal respiration} = T \times \text{ENRES} \times \text{CAOCHR} \times 2.67 \times C3/\text{RESPIQ}
\]
\[
\text{Nitrification} = T \times \text{CNITR} \times \text{RNOCHL} \times 4.57 \times C5
\]
\[
\text{Oxidation of CBOD} = \text{OXIDR} \times C9
\]
\[
\text{Photosynthesis} = \text{gr} \times \text{CAOCH} \times 2.67 \times \text{PHOTOQ} \times C3
\]
\[
\text{Settling} = \text{SETTL(10)} \times C10
\]
\[
\text{Sediment Oxygen Demand} = \text{BENT} \times \text{SODTB}^{T-20}
\]

where \( \text{SODTB} \) is the coefficient for temperature correction.

\( \text{CAOCHR} \) = carbon to chlorophyll ratio (mg/ug)

\( \text{RESPIQ} \) = respiration quotient expressing moles of carbon oxidized per mole of oxygen produced

\( \text{PHOTOQ} \) = photosynthetic quotient expressing moles of oxygen produced per mole of carbon fixed.

\( \text{REAER} \) = reaeration rate (day\(^{-1}\)): the O'Connor-Dobbins formula is used,

\( \text{SETTL (10)} \) = loss term for dissolved oxygen deficit, expressing processes such as wind reaeration (day\(^{-1}\)).
The CBOD pool is decreased through oxidation and losses such as settling, but increased due to zooplankton grazing, as well as by point and nonpoint source additions. The internal mechanisms are given by:

Oxidation = C9 * OXIDR
Loss = SETTL(9) * C9
Grazing = T * ZOOGR * ZCK * CAOCHR * 2.67 * C3, where

Values used for DO-related coefficients are summarized in Table 4.

Figure 6. Schematic of dissolved oxygen cycle.
Table 4. Dissolved Oxygen Related Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mnemonic</th>
<th>Ches Bay</th>
<th>James River</th>
<th>This Study</th>
<th>COG</th>
<th>Clark + Jaworski</th>
<th>Zison et al.</th>
<th>DiToro + Thomann</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaeration Coefficient (mSec**0.5/day)</td>
<td>FREAER</td>
<td>4-25</td>
<td>10-30</td>
<td>4</td>
<td>4**</td>
<td>4</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>Sediment Oxygen Demand (gm/m²/day)</td>
<td>BENT</td>
<td>0.2-0.8</td>
<td>0.1-0.3</td>
<td>1.0-2.0</td>
<td>++</td>
<td>1.0</td>
<td>0.07-7.0</td>
<td>-</td>
</tr>
<tr>
<td>CBOD Oxidation Rate (1/day)</td>
<td>OXIDR</td>
<td>0.02</td>
<td>0.1</td>
<td>0.05</td>
<td>0.21</td>
<td>0.17</td>
<td>0.01-2.0</td>
<td>0.01*</td>
</tr>
</tbody>
</table>

Loss Rates 1/Day): (1/day)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mnemonic</th>
<th>Ches Bay</th>
<th>James River</th>
<th>This Study</th>
<th>COG</th>
<th>Clark + Jaworski</th>
<th>Zison et al.</th>
<th>DiToro + Thomann</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBOD</td>
<td>SETTL(9)</td>
<td>0.03-0.10</td>
<td>0.0-0.25</td>
<td>0.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DO Deficit</td>
<td>SETTL(10)</td>
<td>0.01-0.38</td>
<td>0.0</td>
<td>0.00-0.25</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Photosynthetic Coefficient</td>
<td>PHOTOQ</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Respiratory Quotient</td>
<td>RESPI</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

* = 1/day/deg. C
** = O'Connor-Dobbins formula plus wind reaeration
+ = various constructs discussed
++ = benthic layer flux modeled
CHAPTER III. DATA REQUIREMENTS

In previous sections it has been noted that this study involved a set of nine water quality parameters or constituents, that the simulation period encompassed eight months, and that the area of study included all of Chesapeake Bay and the James and Potomac rivers from their confluence with the bay to the fall line. The data requirements for this project were substantial given the desired water quality constituent, time and space coverage. The Bay Program wanted the data sets to be synoptic, that is, covering all areas more or less simultaneously. As a result, some data sets with good local coverage were bypassed in favor of data sets with lesser density but concurrent sampling.

Calibration Data Sets

During the early 1970's the U. S. Army Corps of Engineers sponsored bay-wide data collection efforts in support of the development of the Chesapeake Bay hydraulic model which was built on Kent Island, Maryland. These field efforts emphasized physical variables, namely tidal heights, currents, water temperature and salinity. However, additional measurements of water quality conditions were made in a number of areas during the same time frame. The data sets for 1970 and 1971 most closely provided the desired coverage. Therefore the Chesapeake Bay Program designated those years as the calibration years. In Table 5 are specified the years and sequence in which the hydrodynamics and water quality models were calibrated.
Table 5. Calibration Data Sheets

James River

Hydrodynamics and water quality models calibrated using 1971 data.

Both models were then run for 1970 to provide boundary conditions for the Chesapeake Bay water quality model.

Potomac River

Hydrodynamics model calibrated using 1971 data.

The calibrated hydrodynamics model was then run to simulate 1970 flow conditions and the water quality model was calibrated using 1970 water quality data.

Chesapeake Bay

Hydrodynamics model calibrated with 1971 data.

The calibrated hydrodynamics model was then run to simulate 1970 hydrographic conditions, as were the tributary models, so that the water quality model could be calibrated using 1970 field data.

Model Input Requirements

Although the calibration data set is large, the volume of data required to operate the models is larger still. Hydrodynamics models require information on tidal heights and freshwater inflows. The water quality models require information on pollutant loadings, environmental conditions, and rate constants for biological and chemical processes.

Tides: Time sequences of water elevation at the downstream limits of the hydrodynamics models are required. Field observations for the bay and the two tributaries were processed by Fourier analysis to determine the major constituents of the tides. Synthetic tide records were then constructed and used in the models, essentially eliminating the effects of meteorological events from the record but leaving the dominant astronomical features. For the James and Potomac models, the
25

M, N, S tidal constituents were used. For Chesapeake Bay, only the 
2 2 2
M_2 and N_2 constituents were used.

**Freshwater flows:** Recorded river flows above the fall line were 
obtained from the U. S. Geological Survey in terms of daily flows. 
These records were complete for the periods of interest. Data for many 
years in the past also are available.

**Point Source Loads:** Pollutant loadings from the industrial and 
municipal dischargers were estimated by the Bay Program staff using 
available information. The data include volume flows and mass loadings 
of BOD (biochemical oxygen demand), nitrogen and phosphorus. In 
general, the point source loadings were assumed time invariant during 
any given simulation.

In a few instances it was necessary to adjust the loads to reflect 
features which have been observed. Specifically, for the 1970–71 period 
nutrient loads entering the Patapsco River (Baltimore Harbor) reacted 
with both the natural environment and the wastewaters from the Bethlehem 
Steel plant at Sparrow's Point. Presumably iron from the industrial 
wastewaters and phosphorus from the municipal sources combined and 
precipitated out, thereby greatly reducing the amount of phosphorus 
which passed through the river and entered Chesapeake Bay. The 
reductions used in the model study are based, in large part, upon 
calculations made earlier by Hydroscience (1975).

**Fall Line Loadings:** For the 1970–71 calibration period, fall line 
loadings were estimated using measured daily flows and load-flow 
relationships which had been determined previously by Guide and Villa 
(1972). Regression equations for Conowingo Dam on the Susquehanna are 
given below and illustrate the general form of the equations used.
\[ T. \text{PO}_4 \text{ as } \text{PO}_4 \text{L} = 0.061Q^{1.261} \]
\[ P. (\text{inorganic}) \text{L} = 0.010Q^{1.381} \]
\[ \text{TKN as N} \text{L} = 16.410Q^{0.837} \]
\[ \text{NO}_2^+ \text{NO}_3 \text{ as N L} = 1.202Q^{1.128} \]
\[ \text{NH}_3 \text{ as N L} = 15.170Q^{0.733} \]
\[ \text{TOC L} = 31.050Q^{0.939} \]

where \( L \) = nutrient loadings (lbs/day)

\( Q \) = river discharge (cfs)

The data set resulting from these calculations were daily mass loadings of nutrient species. Daily loadings of BOD and chlorophyll were estimated by multiplying the flows by daily concentrations calculated in the watershed modelling (see following section).

It should be noted that the fall line loadings result from both point and nonpoint sources in the portion of the basin draining to that point. For the approach taken, regression relationships, there is no way to determine the relative importance of these two types of pollutant sources.

**Below-Fall-line Nonpoint Source Loads:** Pollutant loadings in streamflows and stormwater runoff from that portion of the basin lying below the fall line were estimated by the Northern Virginia Planning District Commission (NVPDC) using the watershed model of the Chesapeake Bay basin. That model was calibrated using river flow and quality records and the results of five intensive watershed studies conducted for the Bay Program. It has been used to provide both fall line loads and coastal plains nonpoint loads for use in projecting future conditions.
For calibration purposes, the watershed model was used to predict nonpoint loads for areas downriver of the fall-line. Model runs for 'existing conditions' used 1980 land use statistics and the rainfall records from 1974, a year of moderate or average rainfall and runoff. The daily nonpoint loads for 1974 were divided by the daily flows to get daily average concentrations of the water constituents. These concentrations were then multiplied by the 1970 and 1971 daily flows to estimate the nonpoint source loads for those two calibration years. It was assumed that land use changes within the 1970-1980 time frame did not significantly affect the coastal plains nonpoint loads.

Atmospheric Fallout: Nutrient loadings reaching the water bodies directly in precipitation were determined by the Bay Program staff and supplied to VIMS with the nonpoint source loadings. Loadings are proportional to both the amount of rainfall and the water surface area.

Benthic Releases: Release of ammonia and orthophosphate from the bottom sediments was included in the models. Benthic release rates per unit area were determined by Bay Program staff using data from other field studies under the Chesapeake Bay Program. (For details see EPA, 1982 - 'Technical Studies - A Synthesis.') The Potomac was divided into three sections having individual benthic release characteristics, while eight zones were identified for the Bay. In order to calculate the magnitude of the nutrient inputs, these release rates were multiplied by appropriate bottom areas. For ammonia, the bottom area used in the calculation was the area estimated to be covered by less than 60% sand and lying within the model element. For phosphorus, the area used was the bottom area which was both less than 60% sand and lying at a depth of more than 9.1 m (30 ft).
Distinct seasons were identified for these calculations. For ammonia, separate release rates were used for Spring, Summer and Fall (see Table 6). For phosphorus, it was assumed that P04 became available to the water column only under anaerobic (Summer) conditions. The phosphate ions released from the sediment under Fall, Winter and Spring conditions were assumed to be locked up in complex iron precipitates under aerobic conditions. This accumulated store of nutrient was released to the water column at the onset of anaerobic conditions at the beginning of June. This 'burst' release of nutrient spanned three weeks in the water quality model.

**Solar Radiation:** For short term simulations, solar radiation can be taken as a constant. Over an eight month period, however, both the length of the daylight period and the intensity of the light vary considerably. In Figure 7 it can be observed that the maximum values increase from around 400 to 450 langleyes per day (Ly/d) at the beginning of March to nearly 750 Ly/d in June (around 2600 hours), with decreasing levels thereafter. In addition it can be seen that the radiation is highly erratic with minimum values on the order of 100 Ly/d occurring on numerous days during that period. Presumably these represent periods of intense cloud cover.

Radiation records for two locations (an up-Bay site and a down-bay site) were supplied to VIMS by the Chesapeake Bay Program. Values for intermediate locations were determined by interpolation assuming a linear variation with distance.
Table 6. Benthic Flux Release Rates

(10^{-6} \text{kg/m}^2/\text{day})

<table>
<thead>
<tr>
<th></th>
<th>Spring (Mar-April)</th>
<th>Spring Burst (June 1-21)</th>
<th>Summer (June 22-Aug)</th>
<th>Fall (Sept-Oct)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>James River</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH$_4$</td>
<td>13.7</td>
<td>15.6</td>
<td>15.6</td>
<td>11.2</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>24.8</td>
<td>2.7</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Potomac River-Elements</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-15 NH$_4$</td>
<td>18.9</td>
<td>37.8</td>
<td>37.8</td>
<td>37.8</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>80.5</td>
<td>6.2</td>
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<tr>
<td>16-27 NH$_4$</td>
<td>4.9</td>
<td>9.8</td>
<td>9.8</td>
<td>9.8</td>
</tr>
<tr>
<td>PO$_4$</td>
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<td>28.2</td>
<td>2.2</td>
<td>0.0</td>
</tr>
<tr>
<td>28-48 NH$_4$</td>
<td>63.0</td>
<td>63.0</td>
<td>63.0</td>
<td>4.5</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>24.2</td>
<td>1.9</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Chesapeake Bay-Segments</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CB1 NH$_4$</td>
<td>22.0</td>
<td>6.8</td>
<td>6.8</td>
<td>30.8</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>6.2</td>
<td>2.7</td>
<td>0.0</td>
</tr>
<tr>
<td>CB2 NH$_4$</td>
<td>2.4</td>
<td>8.8</td>
<td>8.8</td>
<td>6.8</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>13.4</td>
<td>2.1</td>
<td>0.0</td>
</tr>
<tr>
<td>CB3 NH$_4$</td>
<td>7.8</td>
<td>17.1</td>
<td>17.1</td>
<td>7.8</td>
</tr>
<tr>
<td>PO$_4$</td>
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<td>43.0</td>
<td>3.8</td>
<td>0.0</td>
</tr>
<tr>
<td>CB4 NH$_4$</td>
<td>25.4</td>
<td>24.4</td>
<td>24.4</td>
<td>0.3</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>76.2</td>
<td>2.6</td>
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</tr>
<tr>
<td>CB5 NH$_4$</td>
<td>18.1</td>
<td>17.1</td>
<td>17.1</td>
<td>18.1</td>
</tr>
<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>68.4</td>
<td>4.2</td>
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</tr>
<tr>
<td>CB6 NH$_4$</td>
<td>13.7</td>
<td>15.6</td>
<td>15.6</td>
<td>17.6</td>
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<tr>
<td>PO$_4$</td>
<td>0.0</td>
<td>22.2</td>
<td>0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>CB7 NH$_4$</td>
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<td>21.0</td>
<td>21.0</td>
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</tr>
<tr>
<td>PO$_4$</td>
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<td>14.8</td>
<td>3.3</td>
<td>0.0</td>
</tr>
<tr>
<td>CB8 NH$_4$</td>
<td>13.7</td>
<td>15.6</td>
<td>15.6</td>
<td>11.2</td>
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<td>PO$_4$</td>
<td>0.0</td>
<td>24.8</td>
<td>2.7</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Figure 7. James River solar radiation from March 1, 1971 to October 31, 1971.

Figure 8. Water temperature variations from March 1, 1971 to October 31, 1971.
Water Temperature: Water temperatures exhibit a strong seasonal cycle in the Chesapeake Bay region and are influenced more by air temperatures than by incident radiation. Typically minimum readings occur in January and February and are in the range 0 to 5°C. Maximum values occur in late July and August and range between 25 and 30°C, although some locations routinely experience even higher temperatures.

Field data for the calibration period were examined by the Bay Program staff and simple sine curves fitted to the data. The values necessary to describe these sine curves were supplied to VIMS for two locations on each water body. Modellers then determined water temperatures for intermediate locations via linear interpolations. The records for the two control stations in the James River are shown in Figure 8.

Upstream Boundary Conditions: For the tributary estuaries and for Conowingo Dam at the head of the Bay, the upstream boundaries were such that material could enter the system but could not leave the system, except in the downstream direction. In other words conditions existing in the most upstream model segments were determined by the model, incorporating both prior and downstream conditions as well as the loadings crossing the fall line (so-called flux boundary condition). The daily flow records from the gaging stations maintained by the U.S. Geological Survey were obtained for all of the major tributaries. The 1971 hydrographs for the James River, both the portion of the basin above the fall line and the portion lying in the coastal plain, and two of its tributaries, the Chickahominy River and the Appomattox River, are shown in Figure 9. Fall line loadings have been discussed further in an earlier section.
**Downstream Boundary Conditions:** At the downstream boundaries (the adjacent segment of Chesapeake Bay for the tributaries and the Atlantic Ocean for the Bay model) typical water characteristics were determined by examination of historical records. These values are listed in Table 7. Although these values were held constant during the simulations, the boundary values were not held constant. During flood tide the water entering the system has the characteristics just mentioned. During ebb tide, however, the water leaving the system has characteristics determined by the model (so-called dispersive boundary conditions.) and would reflect the collective effects of advective transport, mixing, biochemical transformations, high or low river flow and so on.

![Graph](image_url)

Figure 9. James River fresh water inflows from March 1, 1971 to October 31, 1971.
Table 7. Downstream Boundary Conditions*

<table>
<thead>
<tr>
<th></th>
<th>Potomac</th>
<th>James</th>
<th>Chesapeake Bay</th>
</tr>
</thead>
<tbody>
<tr>
<td>Salinity</td>
<td>18.2</td>
<td>21.41</td>
<td>32.0</td>
</tr>
<tr>
<td>Chlorophyll</td>
<td>20.0</td>
<td>5.1</td>
<td>2.6</td>
</tr>
<tr>
<td>Org-N</td>
<td>0.40</td>
<td>0.25</td>
<td>0.05</td>
</tr>
<tr>
<td>NH$_3$-N</td>
<td>0.10</td>
<td>0.12</td>
<td>0.022</td>
</tr>
<tr>
<td>NO$_2$+NO$_3$-N</td>
<td>0.10</td>
<td>0.06</td>
<td>0.02</td>
</tr>
<tr>
<td>Org-P</td>
<td>0.05</td>
<td>0.09</td>
<td>0.025</td>
</tr>
<tr>
<td>Inorg-P</td>
<td>0.08</td>
<td>0.03</td>
<td>0.012</td>
</tr>
<tr>
<td>CBOD</td>
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<td>1.0</td>
</tr>
<tr>
<td>DO deficit</td>
<td>2.0</td>
<td>0.72</td>
<td>0.2</td>
</tr>
</tbody>
</table>

* Salinity values in parts per thousand, chlorophyll in micrograms per liter, and all other values are in milligrams per liter.
CHAPTER IV. CALIBRATION RESULTS

Calibration Procedures

Calibration of the models occurred in a stepped fashion. Calibration of the hydrodynamics models preceded calibration of the water quality models, because adjustment of the biological and chemical coefficients would be meaningless if the underlying physical transport processes were not simulated properly. Similarly, calibration of the tributary models preceded that for the bay, because the tributaries export materials to the bay. Thus, calibration of the bay model had to await a stage when these inputs were well defined.

The appendices to this report contain many plots and tables showing the results of the calibration. The plots include both time histories for specific locations and longitudinal profiles for given times or time periods. Statistical information is summarized in tables and illustrated graphically as well. Readers interested in the details of the calibration are referred to materials in the appendices.

In this chapter the calibration results will be summarized and discussed. The emphasis will be on assessing the success of the calibration and noting information that has been gained through the process.

James and Potomac - Hydrodynamics

The primary inputs to the hydrodynamics models are the tidal forcing functions at the downstream boundaries and freshwater inputs at upstream locations. Initial efforts to calibrate the hydrodynamics models focused on tidal elevations and currents with appropriate
adjustments to the friction coefficients. The goal was to reproduce tide ranges and maximum currents that were roughly equal to those given in the Tide Tables. Once that had been achieved, 'fine tuning' of the hydrodynamics model emphasized adjustments to the dispersion coefficients to reproduce observed salinity distributions. Because salt is neither produced nor destroyed within the rivers, it provides a conservative tracer with a single downstream source. If the salinity distribution is reproduced by the model, that suggests that the model coefficients are reasonable ones. If the predictions are accurate for a variety of freshwater flows and for a number of simulation periods, then confidence in the model increases.

Typical results are shown in Figures 10 and 11. It should be noted that often the model predictions show up as thick lines in the figures. The thickness of the line represents the differences occurring within the tidal cycle. If the horizontal scale were made much longer, the variations due to tides would become apparent. When the horizontal scale is compressed, the lines overlap and form a band. Field observations are indicated in two ways: mean values for the observations taken over depth at a station are plotted as circles while the vertical lines indicate the range of values for that set of observations.

Tidal elevations and currents for the James River are shown in Figure 10 for Upper Brandon, about halfway between the bay and the fall-line, and Richmond, just below the falls. In mid-estuary, both the elevations and the currents are dominated by the semidiurnal tides and are relatively well behaved, but near the fall line the effect of the semi-diurnal tides is strong only during periods of low flow (2500 hours
Figure 10(a). Time variation of current and tidal elevation at Node 21, Upper Brandon, J7.)
Figure 10(b). Time variation of current and tidal elevation at node 40, Richmond H015.
Figure 11. Time variation of salinity in the James River: 
(a) node 1, river mouth, J1, (b) node 4, Newport News Point, J2, (c) node 7, Joel Point, J3. 
(see Figure 2b for node locations).
Figure 11 (Cont'd). Time variation of salinity in the James River: (d) node 11, Hog Point, J4, (e) node 15, Swanns Point, J5. (see Figure 2b for node locations).
to 5500 hours in Figure 10b). The influence of the river is strong during periods of high runoff and is clearly indicated in the plots (e.g. elevation of 4m and downstream current of 2.5 m/sec about 2200 hours). At intermediate locations, the effects of high river flow are reduced but still are apparent in the plots (Figure 10a, 2200 hours). Typical plots of salinity over the eight month simulation period are shown for five locations in the James in Figure 11.

Calibration of both the James and the Potomac hydrodynamics models appears satisfactory, given the ability of the models to reproduce observed time variations in salinity at various points in the river, as illustrated by plots for the Potomac River shown in Figure 12. Unfortunately the limited number of data points for the calibration period make more substantive and quantitative statements impossible. When one examines time variations over the eight month simulation period, the best temporal coverage of the field data is about monthly — normally the spacing is greater still. In particular, none of the data sets covers a period when salinity values were changing, so there is no way one can evaluate how well the model reproduces system responses to short term or transient events. When longitudinal profiles of monthly averages are compared, only four to six data pairs are available per month. Statistics for such limited data sets are not particularly informative or reliable.

It appears that the tributary models reproduce physical transport processes and have been calibrated to the greatest extent possible within the limitations of the data for the chosen calibration period. Confidence in the model would be greatly improved if additional efforts
Figure 12. Time variation of salinity at three locations in the Potomac River: (a) node 7, Ragged Point, (b) node 16, Potomac River Bridge, and (c) node 19, Mathias Point. (see Figure 2c for node locations).
were made using other data sets, especially those with good spatial coverage and data sets encompassing varying flow conditions.

Potomac and James - Water Quality

It is important to note the range of environmental conditions encompassed in the simulations. Water temperatures in March were below 5°C, but rose to above 26°C in August before falling back to about 18°C at the end of October. Freshwater inflows also varied greatly. For example, flows to the Potomac in March and April averaged about 600 cubic meters per second (cms) with transient events producing flows as high as 2,700 cms. In contrast to these high flows, in late September the freshwater flow over the falls had dropped to less than 40 cms. Another seasonal variable is the duration of daylight, which is less than twelve hours per day at both the beginning and the end of the simulation period, but reaches a maximum of 14.7 hours per day at solstice. Each of these three factors reaches its critical stage at a different point in the simulation, day length in late June, water temperature in late August, and freshwater inflow in late September.

Calibration results for the Potomac River suggest that the model reproduces observed seasonal trends. For example, chlorophyll levels are low in the spring when the days are short and water temperatures are low. Furthermore, the longitudinal concentration profile is flat due to strong downstream advection resulting from the high river flows. Profiles in late summer show much higher peak concentrations and greater spatial variation in concentrations, as would be expected.

Review of the data in Tables 1 through 4 indicates that the parameter values used in this study are generally comparable to those
used in other studies of the tidal Potomac River. One of three parameters overall which were varied spatially was the orthophosphate settling or loss rate. A constant rate of 0.15 per day was used for model elements 32 through 41, that is from the Blue Plains wastewater treatment plant downstream to about Hallowing Point. This loss rate corresponds to a settling velocity of about 0.75 m/day.

There is evidence that inorganic phosphorus becomes adsorbed to suspended sediments and thence removed from the water column (Veith and Sposito, 1977; Parfitt et al., 1975). Thomann and Fitzpatrick (1982) consider this loss mechanism to be particularly vigorous downstream of the Blue Plains facility. In earlier work, Clark and Jaworski (1972) asserted that phytoplankton uptake could account for only 10% to 20% of the phosphorus lost from the system. The results of the present study indicate similar behavior. For example, the predictions for the month of October show a rise in chlorophyll of about 40 μg/l below Blue Plains, the observations a rise of about 80 μg/l. For the assumed phosphorus to chlorophyll ratio (0.001 mg/μg), these changes would produce a phosphorus uptake of 0.04 or 0.08 mg/l, or a tenth or less of the observed and predicted reduction in inorganic phosphorus levels over that reach of the river.

One difference between phosphorus and nitrogen cycles is that it was found necessary to include a loss term for organic nitrogen, while none was necessary for organic phosphorus. This result may follow from the relatively rapid recycling of the latter.

Another spatially variable parameter was the chlorophyll loss rate. According to Lear and Smith (In Mason and Flynn, 1976, p. 70) Anacystis Cyanea cannot reproduce in salt water so they tend to die out between
Maryland Point and Morgantown. This change in phytoplankton populations was achieved in the model by the use of a loss rate of 0.08 per day in elements 15 through 24.

Model input values for sediment oxygen demand were kept within the range of 1 to 2 grams of oxygen per square meter of bottom per day, values typical of estuarine muds (Zison, et al., 1978). The highest values (1.9 gm/sq m/day at 20 C) were in the elements 14 through 28, which corresponds roughly to those reaches where the phytoplankton are dying off. It is plausible to attribute an enhanced sediment oxygen demand to bottom sediments enriched by dead phytoplankton.

The calibration coefficients used for the Potomac River give results that generally apply with a certain balance between overpredictions and underpredictions. The 'give and take' that accompanies any change in coefficients arises from limitations of the field and input data sets and approximations included in the model formulation. To illustrate this, the September and October simulations will be contrasted. In the plots which will be presented the data are monthly means. For the model predictions, the average of all predictions is shown by a solid line while the maximum and minimum values predicted are indicated by dashed lines. The field observations are represented by circles, which represent the monthly average values, and vertical lines, which represent the range of observations for that location.

In both September and October the model reproduces quite nicely the sharp changes in inorganic phosphorus levels occurring in proximity to the Blue Plains outfall (Figures 13 and 14). The October predictions for organic phosphorus generally reproduce the observed longitudinal
Figure 13. Longitudinal profiles of average water quality conditions in the Potomac River during September.
Figure 14. Longitudinal profiles of average water quality conditions in the Potomac River during October.
profile, but the peak concentrations are overpredicted. In September, however, the model not only overpredicts the peak concentrations of organic-P, but also the observed peak appears to be about 20 km downriver from the predicted peak. The September predictions for nitrogen species, on the other hand, generally reproduce the observed distributions and peak concentrations, with the exception that the model predicts an organic-N peak near Blue Plains and that peak is not apparent in the field data (Figure 15). Perhaps it should not be surprising that the September prediction for chlorophyll generally conforms to observed patterns, given that the predictions for inorganic nutrients were reasonably good.

Chlorophyll levels for October were underpredicted although the general shape of the distribution was simulated. The October predictions for organic nitrogen and ammonia nitrogen are good, except that the model shows a more gradual decline of ammonia-N than was observed in the field (Figure 16). Predictions for nitrate and nitrite nitrogen were good throughout much of the estuary and the location of the peak was simulated but peak concentrations were nearly double those predicted by the model. Noting that the previous month's predictions were good, this discrepancy suggests that perhaps the Blue Plains facility produced an effluent that was partially nitrified during October. Whether that happened or not, it is very likely that variations in the characteristics of the Blue Plains effluent and other point sources varied, whereas the model loadings are held constant. It also should be noted that the field observation were made on a single day, October 20th.
Figure 15. Longitudinal profiles of average water quality conditions in the Potomac River during September.
Figure 16. Longitudinal profiles of average water quality conditions in the Potomac River during October.
Review of all eight month's simulations indicates that BOD patterns were poorly reproduced with predictions typically below observed levels. No reason for this discrepancy is readily apparent. Resuspension of bottom sediments and other processes which have not been included in the model could be at work, or nonpoint source loadings might be in error. To further illustrate the latter point, we note that during April, nitrate plus nitrite nitrogen predictions are too high in the upper estuary. When the regression equation for nitrate and nitrite is used to determine the fall line load, a concentration of more than 2.5 mg/l is calculated for a flow of 2,200 cms. In contrast the nonpoint source loadings generated by NVPDC using the watershed model (for use in the so-called production runs) never had nitrate plus nitrite nitrogen concentrations exceeding 1.9 mg/l and that result was obtained only at low flows.

In a more quantitative assessment, the comparison of predictions and observations for each of the eight months of the simulation period suggests that the relationships were strong for several of the water quality measures. Correlation coefficients were greater than 0.8 seven of the eight months for salinity and nitrate plus nitrite nitrogen. For inorganic phosphorus, the correlation coefficient was greater than 0.8 in five months and greater than 0.6 in all months. Correlation coefficients for organic phosphorus and ammonia nitrogen were greater than 0.6 for five and six of the eight months respectively. Values of the correlation coefficient for BOD and chlorophyll were highly variable, but most of the values for organic nitrogen and dissolved oxygen were less than 0.4.
The calibration results for the James River are similar except that the spatial, temporal, and parameter coverage is less for field observations in those systems. As a result calibration has been achieved in a qualitative sense only. The statistics comparing model predictions and field observations, along with the time histories at specific locations and the longitudinal profiles for each month for each system are included in the appendices.

Chesapeake Bay - Hydrodynamics

Examination of the calibration results for the Chesapeake Bay hydrodynamics model indicates that it does simulate the longitudinal variation in salinity over the longer term (8-month averages shown in Figure 17). When similar longitudinal plots were made on a monthly basis, thirty seven of forty eight times the monthly means fell within the range of model predictions for that same month and station. Closer examination suggests the differences between predictions and observations are not random. First it should be noted that these comparisons are far from perfect in that the model averages are based on evenly spaced predictions throughout the month, whereas the observation means are based on available data, often only the values for a single day. Nonetheless, it appears that the model underpredicts salinities during high flow periods and slightly overpredicts salinities during low flow periods, as shown in the April and July profiles in Figure 18. Time variations for specific model elements show similar behavior, as illustrated by the plots for elements 105 and 116, located in the bay just downstream and upstream of Baltimore (Figure 19). It is interesting to note that the range of salinity values at around 1,000
Figure 17. Longitudinal variation of salinity (eight month average) in Chesapeake Bay.

Figure 18. Longitudinal variation of salinity in Chesapeake Bay, monthly average conditions for April and July.
Figure 19. Time variation of salinity in Chesapeake Bay at model elements 105 and 116.
hours was on the order of 15 parts per thousand, which represents extremely strong stratification. Furthermore the salinity range for any given date can be large or small with no obvious seasonal trend.

The conclusion which must be drawn is that the parameterization of dispersion processes in the 2-D model works over the longer term, but is less successful for the shorter term. This could be improved by additional calibration efforts or by modification of the model structure, but neither of these approaches will be particularly successful unless the calibration exercise includes simulation of a variety of flow conditions for which there is good temporal and spatial coverage in the field data. It should be noted that the field observations in 1970-71 for model elements 105 and 116 are much more closely spaced in time than those for most other bay areas.

Chesapeake Bay - Water Quality

The time plots and longitudinal profiles of the water quality constituents in the appendix indicate that the Chesapeake Bay water quality model has been calibrated in a qualitative sense. Seasonal trends and general spatial patterns have been reproduced. However, because the temporal, spatial and parameter coverage is sparse, it would be possible to achieve other equally good calibration results using different sets of values for the transformation rates. Verification of the model with a more robust data set, such as that resulting from the Bay Program's survey in 1980, would add greatly to the study.

It has been suggested that the results for the three systems be compared and differences between systems noted. No striking differences are apparent and given the qualitative nature of the calibration for the
Bay and the James, and the uncertainties associated with coefficient values, it is not clear that this would be particularly productive. Differences could be due to a number of factors and not be caused by any fundamental difference in character or process. A more useful exercise, it is believed, would be to examine the work that has been completed and to critically evaluate it. Accordingly, in the following chapter that will be done.
CHAPTER V. DISCUSSION

'Physicists know that their methods of analysis and logical reasoning can never explain the whole realm of natural phenomena at once, and so they single out a certain group of phenomena and try to build a model to describe this group. In doing so, they neglect other phenomena, and the model will therefore not give a complete description of the real situation. The phenomena which are not taken into account may either have such a small effect that their inclusion would not alter the theory significantly, or they may be left out simply because they are not known at the time when the theory is built.

All these models are approximations which are valid for a certain range of phenomena. Beyond this range, they no longer give a satisfactory description of nature, and new models have to be found to replace the old ones—or, better, to extend them by improving the approximation. To specify the limitations of a given model is often one of the most difficult, and yet one of the most important tasks in its construction. According to Geoffrey Chew, it is essential that one should always ask, as soon as a certain model or theory is found to work: Why does it work? What are the model's limits? In what way, exactly, is it an approximation? These questions are seen by Chew as the first step toward further progress.' (from 'The Tao of Physics', Capra).

The initial phases of the EPA–Chesapeake Bay Program culminated in the publication of 'A Profile of Environmental Change' (EPA, 1983) and the Program's recommendations to management, 'A Framework for Action' (EPA, 1983). The actions of the federal government and the several states suggest that there will be continued study and analysis of water quality problems in Chesapeake Bay as well as efforts to implement the management recommendations. For that reason, the Bay Program requested that the shortcomings and limitations of the present effort be described and discussed, so that in the future persons who undertake similar modelling studies can avoid some of the pitfalls we have encountered.
Accordingly, in the following sections, the discussion will address technical, data, and resource limitations.

Technical Limitations of the Present Study

Mathematical models are useful to water quality managers because they allow hypothetical cases to be tested, such as the effects of extreme flows or temperatures, or various combinations of nutrient loads. Models also are relatively inexpensive because they are simplified versions of the real world. Although recent advances in computer technology have allowed for better and better representations, all models incorporate a number of assumptions, simplifications, and omissions in order for the computations to be tractable. The key to a successful study then depends on the selection of the appropriate set of simplifications. For this to occur, (1) the managers must define the problems with great care and detail, (2) they and the modelers must evaluate the models that are available and select the one(s) most appropriate for the problems being addressed, and (3) the two groups must communicate. In retrospect it appears that we could have done better in all of these areas.

1) Problem Definition

In large part because the relationships between nutrients and water quality in estuaries are not well-defined, the intended uses of the model were initially stated in general terms. For example, the 'Research Summary' (EPA, 1980) states that '...the models will be used to determine likely trouble spots and to project future water quality conditions under various management situations.' During the course of the Bay Program, as more information became available from other
research efforts, the direction of the model study changed. For example, bottom water anoxia was given much attention in the latter stages of the Bay Program, but was infrequently mentioned in the earlier periods. Generally speaking, it is a good thing to revise work plans and to utilize new information, but some changes can be accommodated more easily than others.

The change from short-term model simulations (i.e. two weeks) to long term (i.e. eight months) simulations had important ramifications. Because computational costs would have been great for that simulation period and the original model grid, the grid was made coarse. That modification did reduce the time for computations, and thereby the costs, but it also delayed the project and greatly reduced the spatial resolution. Several trial grids were developed during this period, each taking a considerable amount of effort to develop and evaluate. This was perhaps the biggest change in the modelling approach, but there were many other smaller modifications as well, and each caused some delay, duplication of effort, and/or often wasted effort.

Failure to define the precise uses of a model may seem like a small mistake to non-modellers, but this misconception probably arises from a perception that models are active agents that solve problems. Nothing could be further from the truth. Models are simply tools to answer questions. For this particular case, a variety of environmental conditions and waste loadings must be specified before the model will provide predictions of water quality conditions. It is only through analysis and interpretation of a number of model simulations that modelers, engineers, scientists, and managers can generalize on causes of problems and system responses, and through that process management
directions evolve. Thus a successful program includes specification in advance of both the general direction of the modelling effort and the details of the simulations to be made. For the case at hand, the direction was stated in vague terms and the details of the desired simulations changed repeatedly. Better definition of project goals and model uses should be attempted in all future efforts. If achieved, model studies should be more fruitful.

2) Model Selection

Selection of the 'best' math model involves both technical and practical considerations. In fact two rather exhaustive studies were made to determine what models were available and which of those were suitable for the project at hand (Najarian, 1979, and Ambrose, 1980). Various classes of models are available. With regard to spatial resolution, the Chesapeake Bay Program opted for a 3-dimensional representation of the bay proper and contracted for a hydrodynamic model to be developed. Subsequently, it appeared that the hydrodynamics model would not be available much before the Bay Program was scheduled to end, and that development of a 3-D water quality model would take even longer yet. Thus, this research effort was not expected to provide a tool for use by water quality managers within the original five year duration of the Chesapeake Bay Program. Another model was needed to fill that gap.

Subsequent evaluations by Bay Program managers appear to have been limited to 2-dimensional models, with two choices available - 2-D in the vertical plane (laterally averaged) or 2-D in the horizontal plane (vertically averaged). Each has its strengths and weaknesses, and these are important or not important depending on the intended use of the model. Given that the technical aspects of the project were defined in
only general terms, it is not surprising that practical considerations carried the day. Specifically, a vertically averaged, 2-D hydrodynamics model had been applied to Chesapeake Bay to study storm surge elevations and that same hydrodynamics model had been linked to a water quality model in another application. Thus both hydrodynamics and water quality models of the vertically averaged type were 'on the shelf' and ready to be used. Although 2-D vertical plane (longitudinal and vertical variations simulated) hydrodynamics models had been applied to the Potomac River and to Chesapeake Bay, (for example, by Wang) no water quality model had been coupled to those circulation and stratification models. Indeed, we know of no such water quality models even today.

In other words, when the 3-dimensional approach appeared to require a time frame greater than could be accommodated in the original Bay Program schedule, the available 2-D models were assessed. Vertical plane hydrodynamics models were available, but no water quality routine was extant. Both hydrodynamic and water quality models were available with the horizontal plane representation and that approach was chosen.

In retrospect, perhaps the one-dimensional approach should have been selected. Although this would mean a rather gross spatial representation of the bay, it would have been relatively simple to achieve and it would have been possible to link the bay directly with the major tributaries in a single, branched model. To the extent that one-dimensional models can capture the dominant circulation patterns of broad, partially-stratified estuaries, the transport processes would have been simulated for the entire system as an integral whole. The obvious limitations of a 1-D representation apparently were considered to outweigh the advantages of that approach.
Whatever the correctness of the decision, a cooperative agreement between the EPA and the VIMS was signed in 1980 and work initiated to calibrate the vertically averaged, 2-dimensional models of water movement and water quality in Chesapeake Bay. Subsequently, the project was amended and 1-dimensional models of the Potomac River and the James River were added. Although direct linkage of these models was proposed, the Chesapeake Bay Program chose not to pursue that objective. The selection of the vertical-average models meant that certain classes of problems could not be addressed directly. More specifically, once the vertically integrated model had been chosen, it was not possible to examine directly the causes and mechanisms of bottom water anoxia or any other stratification induced phenomenon. That fact may not have been communicated forcefully to the persons who approved the model choice, perhaps because bottom water anoxia had not yet been noted as a critical and worsening problem. Or perhaps they intended to use correlations between various observed features to estimate the vertical variations in water quality.

In closing we would note that some have concluded that the 'best' model was not selected. (e.g. EPA, 1980b.) However, those individuals typically have very clear and strong beliefs as to the critical problems existing in Chesapeake Bay and, as a result, can determine with equal clarity which models can or cannot address those problems. We believe that disagreements resulted in large part because the requirements to be imposed on the model(s) were not well-defined in advance of model selection. In all future studies, model requirements (for example, steady state versus 'real time', one-dimensional versus three-dimensional, etc) should be specified before any models are selected.
3. **Communications**

Effective communications is an objective for all projects, but that goal is especially elusive when the work encompasses both highly technical matters and diffuse, societal goals. For the case at hand, the general goal of improved water quality and a 'healthy' bay were apparent and widely accepted. Translating those general goals into specific water quality objectives involves interactions among the diverse set of bay user groups and managers. Few of those individuals will have had much direct experience with or knowledge and understanding of mathematical models, and consequently it is difficult to adequately relate the technical problems and difficulties to the less technically trained members of the group. Given that difficult and challenging task, it is not surprising that some misunderstandings occurred. For example, one report noted that: 'Low levels of dissolved oxygen have been apparently characteristic of the deep channels as a consequence of natural processes and OUR WATER QUALITY MODEL WILL HELP US TO ASSESS WHETHER INCREASED NUTRIENTS WILL EXACERBATE THE PROBLEM'. (DeMoss et al., 1980. Capitalization added for emphasis.) Although the water quality model can provide a framework for assessing water quality trends, it should have been apparent to all involved that a vertically averaged model was inappropriate for the study of a problem arising from vertical variations of water density. It is apparent that good communications between the modelers and the managers were lacking in this instance.

In addition to the difficulty inherent in technical communications, it also should be remembered that the project was extremely ambitious and that the time constraints were severe. Once the work had been
initiated, the modelers were urged to complete a prodigious amount of work in rapid order. They had a myriad of details to attend to and were required to work diligently. Little time was available to philosophize about the program direction or to consider alternative routes. Once the project had been initiated the scientists focused their energies on completing the tasks at hand. Perhaps more effort should have been devoted to status reports to the managers explaining progress, difficulties and anticipated problems.

To summarize, it is a good thing for the project managers to seek to accomplish as much as possible with the funding appropriated. However, the complexity of the technical issues, the broad geographical scope of the study, and the time constraints imposed upon the Bay Program all complicated matters and made it especially important that there be good communications among participants.

In future studies more time and attention should be given to interactions between the modellers (and other technically oriented persons) and the managers and users. The complexity of the issues and the trade-offs which must inevitably be accommodated should be discussed until it is clear that each side understands the other and a mutually acceptable direction is selected.

Present Study - Data Limitations

Once a modelling approach has been stated, the data required to carry out the program can be identified relatively easily. For the present study, the approach selected used 'real time' (intra-tidal) models with 1-D representations of the tributaries and 2-D (longitudinal-lateral) representation of Chesapeake Bay. Furthermore
the models simulated nutrient transformations, phytoplankton growth and nutrient uptake, and the dissolved oxygen cycle. An additional constraint placed on the data set by the Bay Program was that the entire system should be covered in a more or less synoptic fashion for the calibration period. A piecewise calibration of the models was not desired.

Field data: Review of available data demonstrates that the requisite parameters have not been measured except in very recent years (Mc'Erlean and Reed). Furthermore the size of the bay makes synoptic surveys difficult and costly, requiring a large number of instruments and vessels, (e.g. 1980 Bay Program survey). The period selected for calibration, 1970 and 1971, was characterized by a large scale field effort supported by the U.S. Army Corps of Engineers to gather data for the hydraulic model of the bay system. Even so, coverage is often sparse in both the temporal and spatial domains, and some parameters are measured only sporadically. Only for the Potomac River is the data set relatively dense. For the Chesapeake Bay proper and for the James River, the 1970-71 water quality data are insufficient for a true or definitive model calibration. That is, a number of sets of model coefficients could be prepared each of which would 'fit' the field observations. Only additional data would allow one to narrow the field and select the calibration coefficients in a strict quantitative fashion. Some specific limitations will be noted in the following paragraphs.

Calibration of the hydrodynamics model would be improved if there were tidal height measurements at more locations and tidal currents measurements for more than a few tidal cycles at a number of stations.
Existing current measurements either provide reasonably good spatial coverage but last only a few tidal cycles, for example the Corps of Engineers hydraulic model data set, or provide long term measurements but at a very small number of stations, for example measurements made by Pritchard near Calvert Cliffs. In fact, the data set generated by the Bay Program in 1980 should be very useful for future model studies, as will the results of the NOS 'Chesapeake Bay Circulatory Study'.

There has been much discussion concerning the limitations of vertically averaged models and the ability/inability of that formulation to capture the dominant circulation features. Some of those concerns could be allayed if it could be demonstrated that the model predicts salinities well for a variety of flow conditions. Although the 1971 hydrograph includes one very high flow event, field measurements of salinity in much of the bay occur at roughly monthly intervals, a spacing too great to characterize and understand the system response and insure that model behavior is similar. Noting that freshwater flows can vary by several orders of magnitude, it is a difficult task to determine the appropriate coefficients when the forcing function varies to that degree. Therefore, it is preferable to have data for a number of these transient events and for the peak flows to be of differing magnitudes. It is unlikely that the data set for any one year will meet all of these criteria, but there is no reason that one should be restricted to a single year, especially for calibration of the hydrodynamics model. Perhaps measurements made in the Corps of Engineers hydraulic model could fill the data gap: that possibility should be investigated.

Both the hydrodynamics and the water quality submodels are 'real time'. That is, the time step for integration is much smaller than
either the daily cycle or the tidal cycle. Few data sets document
changes in ambient conditions at this time scale, especially in
Chesapeake Bay. Thus the ability of the model to reproduce these
fluctuations is largely untested. A combination of seasonal
observations with intensive measurements is useful for determining
values for model coefficients. Recent model studies in the Potomac
embayments suggest that some of the rates used in daily average or tidal
average model studies may be inappropriate for certain real time
simulations (Cerco, personal communication, 1983). Although average
conditions may be reproduced using traditional values, shorter term
fluctuations may or may not be simulated well. The only way to see if
the model reproduces diurnal and tidal variations is to compare the
predictions with field observations. Although these data sets are not
common and will be limited to small portions of the system, future
efforts must include assessment of the real time capabilities of the
models.

In even shorter supply are measurements of rates, such as nutrient
remineralization rates, phytoplankton growth rates and so on. First,
these transfer processes are extremely important to the health of the
bay and warrant measurement from scientific considerations alone. In
addition, each time one of these rates is specified, the range over
which other coefficients can vary is narrowed. Measurement of more
rates would improve the reliability of the water quality models and
probably would indicate how model formulations could be improved. An
important aspect of this is the specification of how the rates vary as a
function of water temperature. Present formulations are often based on
very limited field data. Variations with salinity and other factors also might warrant study.

Spatial coverage of the system is not uniform - the upper bay has been studied much more than the lower bay, and many studies of the Potomac terminated at about the freshwater-saltwater interface. But perhaps the areas most lacking in observations are the junctions. These are important because values in the bay determine the boundary conditions for the tributary models, and conditions in the tributary determine the fluxes to the bay. In fact, little is known about the exchange of materials between the tributaries and the bay. The work of Wang (1983) indicates that the exchange can be affected greatly by winds and other meteorological events. Studies of these interactions would provide important information for both modelers and managers.

Input data sets: The model calibration depends not only on adequate field observations of water quality, but also on the availability of good input data sets, in particular point and nonpoint source pollutant loadings. The calibration period, 1970-71, predates the 1972 Clean Water Act Amendments and therefore also the NPDES permit monitoring program. What data was available was used to characterize point source loads, with the loading rates being held constant for the eight month simulation period. Data from sewage treatment plants show that effluent characteristics vary in response to air temperatures, rainfall, and events occurring at the treatment plant and that neither the flow rate nor the quality of the effluent are truly constant. Clearly variations of this type will be important in the vicinity of major discharges, and some unknown amount of uncertainty will be added to the model
predictions away from the outfall because the model does not include those variations.

The calibration period is unusual in that field sampling of the water quality at the fall line of the major tributaries of Chesapeake Bay was underway. Typically four or five samples were taken each month. From that data set regression relationships were derived between loading rates and flows (Guide and Villa, 1972). Comparison of loading rates calculated first from flow and concentration measurements and then from the regression relationship show general agreement, but with large differences occurring for specific dates. Guide and Villa used the relationships to determine nutrient loadings to the bay system, but instead of daily flows, they used mean monthly flows to 'reduce the biased nature of a limited sampling program'.

For the present study, however, the Bay Program opted to use daily means flows and to derive daily loading rates using the regression equations. Because the original data set is based on roughly weekly observations, there is no obvious way to evaluate that decision. Perhaps it would have been better to use seasonal relationships rather than lumping all data together, or in some other way to have modified the approach taken. What we can see is that some of the estimated loading rates do 'drive' the models. For example, nitrate plus nitrite nitrogen loads to the Potomac River are sensitive to flow rates, and concentrations in the uppermost element show distinct peaks at times of high flow. Those peak concentrations are advected downstream and are apparent in the time histories for downriver stations (Figure 20).

The use of the previously developed regression relationships is difficult to understand in general, because the Chesapeake Bay Program
Figure 20. Time variation of nitrite-plus-nitrate-nitrogen at nodes 44, 36, and 27 in the Potomac River, showing how fall line loads influence conditions at downstream stations.
devoted a significant portion of its efforts to the application of a watershed model to the entire Chesapeake Bay drainage basin. The calibrated watershed model was to be used to generate fall line loads for future conditions and to test management alternatives, but not for the calibration of the estuary models. Although it is beyond the scope of this report to compare and contrast deterministic and statistical models, we would note in passing that the data set used for the watershed model calibration probably was much more extensive than those used for the development of the statistical relationships a decade ago.

Other nonpoint sources loads were estimated using the best information available. For example, the results of sediment-water column exchange studies conducted in 1980 were used to develop the benthic nutrient release rates. While the data generated through the Bay Program represents a major step forward, it should be recognized that these exchanges have not been measured in many locations and the relationships have not been developed which would allow the rates to be predicted accurately. In particular, the variation of flux rates with water temperature needs further study.

In summary, a large data set was prepared to estimate the loading rates of nutrients and BOD from wastewater treatment plants, the free-flowing rivers, and nonpoint sources of pollution. Uncertainty exists with regard to each type of input for a variety of reasons. If, at some future date, it is determined that a major water quality field effort should be undertaken, that effort should include elements to measure the pollutant inputs as well as ambient water quality. The familiar old adage about a chain being only as strong as its weakest link applies in this instance.
Present Study - Resource Limitations

The modelling efforts undertaken by the Chesapeake Bay Program were very ambitious, certainly the present study was ambitious. Much was accomplished even if all the objectives were not met. Models of water movement and water quality were applied to the bay system using the 1970 and 1971 data sets. Much more could be done.

Many of the shortcomings of the present study derive from limited time and limited manpower (or dollars to pay salaries) to accomplish the work. Simply stated, the resources allocated were insufficient for the needs, and midcourse changes to the program only exacerbated that condition. The most important point is that any future efforts should provide a greater level of support and that more realistic objectives should be pursued. Time should be allowed not only for model calibration, but also to examine the behavior of the modelled system. Subsequently, management alternatives could be evaluated more critically and perhaps new alternatives proposed.
CHAPTER VI. CONCLUSIONS AND RECOMMENDATIONS

The mathematical model studies which were undertaken had ambitious goals. Much has been accomplished but not all of the objectives have been achieved. Hydrodynamics and water quality models have been applied to the Potomac River, the James River, and Chesapeake Bay. They have been calibrated in a qualitative sense, that is, they reproduce general water quality trends. For these models, future work that would result in improved predictive capabilities includes:

- Use the data resulting from the Bay Program's 1980 survey to improve model calibration.
- Use other tidal height, current, and salinity records to improve the calibration of the hydrodynamics models, in particular, to improve the parameterization of mixing processes through verification of salinity distributions for a number of transient flow events.
- Use other data sets, especially ones providing intensive temporal sampling, to refine and verify the water quality models. For example, the data for 1977 in the Potomac could be useful.
- Use the watershed model to generate the fall line loadings for all calibration and verification periods.
- Re-examine the use of constant flow and constant effluent quality for large (say greater than 10 mgd) municipal and industrial discharges.
- Re-examine the formulations for temperature induced variations in biochemical transformation rates and modify as appropriate.

Managers could decide to embark on new water quality modelling studies in order to address different problem areas. For such a program to be successful, the managers must first determine the water quality objectives, and state what type of math model predictions are needed. The simulation period, the geographical coverage, the temporal and
spatial resolution, the measures and aspects of water quality to be simulated, and so on must be stated. Then one can determine which models are appropriate for those needs and evaluate the feasibility of employing those models within the existing time and budgetary constraints. If more time or greater funding is required, then the objectives must be revised until there are strong reasons to believe that the desired work can be accomplished with the available funds and in the desired time frame.

A number of studies could be undertaken to improve our understanding of Chesapeake Bay and the processes at work, thereby increasing the ability of scientists to advise managers and to predict system responses. Some of these studies would provide immediate benefits, while others would be relevant over longer time frames or to only a few specific aspects of water quality.

- Analyze field data to determine relationships among environmental conditions and water quality. For example, vertical salinity gradients and longitudinal salinity gradients should be coupled in some sense. If that relationship were strong, then predictions from the vertically-averaged model could be used to estimate the vertical structure. Other correlations might exist which would extend the usefulness of these models.

- Use existing laterally averaged 2-D models to examine density stratification to determine whether the representation they provide is adequate for study of water quality in the deep channels. It may be necessary to modify those models to account for lateral variations in currents and salinity.

- Continue development of a 3-D hydrodynamics model so that circulation processes can be studied without neglecting either lateral or vertical variations in salinity, tidal heights, and tidal currents.

- Study the effects of meteorological events on the circulation patterns in Chesapeake Bay, assess the impact of those events, and incorporate important processes in new hydrodynamics models. For example, little information is
available to show how wind and waves affect circulation patterns and dispersion. If data were available that allowed these factors to be included in the formulation of the dispersion terms, then the models would be improved.

- Study bay-tributary exchanges to better understand how the tributaries affect each other and the bay. For example, one might attempt to determine the portion of the pollutant loads introduced near Washington, D. C. that is trapped in the Potomac River estuary and the portion that passes through the Potomac and into Chesapeake Bay. Additionally, one might ask whether the pollutants entering the bay from the Potomac affect the Rappahannock or other down-bay tributaries.

- Measure, when possible, biochemical transformation rates employed in the models, including the effect of temperature and other important environmental factors on those rates. This would include remineralization rates, phytoplankton growth and respiration rates, sediment-water column exchange rates, and so on.

- Increase the data available to document short-term changes in water quality, such as the system response to freshets (say daily sampling for a week or two) and sunlight/darkness (diurnal studies with sampling every few hours or more frequently).

- Improve the characterization of major pollutant inputs, such as determining any seasonal variations in effluent quality or shorter term changes in effluent flow rates in response to rainfall. Continue fall-line monitoring and upgrade watershed model to include in-stream phytoplankton growth and water-column-sediment exchanges.
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APPENDIX A

ONE-DIMENSIONAL HYDRODYNAMIC AND WATER QUALITY MODEL
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ONE-DIMENSIONAL HYDRODYNAMIC AND WATER QUALITY MODEL

1. HYDRODYNAMIC MODEL

The hydrodynamic model is based on the cross-sectional area-integrated continuity and momentum equations. These equations have been previously derived by several authors such as Harleman and Lee (1969). The governing equations for the one-dimensional unsteady flow in variable area tidal channels are the continuity equation,

\[ \frac{\partial \eta}{\partial t} + \frac{\partial Q}{\partial x} = q \quad (A1) \]

and the momentum equation,

\[ \frac{\partial Q}{\partial t} + \frac{\partial QU}{\partial x} + gA \frac{\partial \eta}{\partial x} + gQ \frac{\partial Q}{\partial x} + \frac{\partial W_x}{\partial x} \frac{\partial x}{\partial x} + \frac{\partial Adc}{\partial x} \frac{\partial \rho}{\partial x} = 0 \quad (A2) \]

where

- \( B \) = channel top width,
- \( \eta \) = elevation of water surface with respect to a horizontal datum,
- \( Q \) = cross-sectionally averaged discharge, \( Q = AU \),
- \( x \) = distance along the channel,
- \( t \) = time,
- \( q \) = fresh water inflow per unit length,
- \( U \) = cross-sectionally averaged velocity,
- \( g \) = gravitational acceleration,
- \( A \) = cross-sectional area,
- \( C_c \) = Chezy coefficient,
$R_h$ = hydraulic radius of the channel,
$\beta$ = wind shear stress coefficient,
$W_x$ = wind velocity along the channel,
$\rho$ = water density,
$\rho_a$ = air density,
d$_c$ = distance from water surface to centroid or cross-section,

The last term in equation (A2) represents the effects of a longitudinal density gradient. The relationship between density of water and salinity is approximated by

$$\rho = 1000 + 0.75s \quad \text{(A2)}$$

where

$s$ = average salinity (ppt) and
$\rho$ = water density (kg/m$^3$).

(a) Initial and Boundary Conditions

The solution of equations (A1) and (A2) requires the specification of initial and boundary conditions. Initial conditions are specified for water surface elevation, $\eta_0$, and velocity, $U_0$, at the start time, say, $t = 0$

$$\eta(x,0) = \eta_0 \quad \text{(A4a)}$$
$$U(x,0) = U_0 \quad \text{(A4b)}$$

There are normally two types of boundary conditions; one specifies flow velocity and the other specifies elevation. At the ocean boundary, $x = x_a$, where most tide measurements exist, the surface elevation is prescribed
\[ \eta(x_a, t) = \eta_a \]  

(A4c)

where

\[ \eta_a = \text{the astronomical tide.} \]

At the upstream end, \( x = x_s \), either a free surface or velocity can be prescribed. In case of a land boundary the velocity is normally assumed to be zero.

\[ U(x_s, t) = 0 \]  

(A4d)

Equations (A1), (A2) and (A4) constitute the hydrodynamic model. These will be solved using the finite element method described in Section 4 of this Appendix.

2. BIOCHEMICAL WATER QUALITY MODEL

The biochemical water quality model is based on the one-dimensional conservation of mass equation. This equation has been previously derived by several authors such as Harleman (1971). In

(1) Chlorophyll 'a',

(2) Organic nitrogen,

(3) Ammonia nitrogen,

(4) Nitrite-nitrate nitrogen,

(5) Organic phosphorus,

(6) Inorganic phosphorus,

(7) CBOD,

(8) Dissolved oxygen deficit,

(9) Salinity and

(10) Coliform bacteria.
The schematic diagram of the ten interacting constituents is shown in Figure A1. Each constituent in the model is represented by a box; the arrows between the boxes show the assumed relationships and the directions of transfer of material. The modeling domain is inscribed in the big circle. The external influences such as waste inputs and solar radiation are indicated outside the big circle. The notation for each constituent is represented by \( C_i \), where the subscript \( i \) \((i = 1,2,3,\ldots,9,0)\) is used to represent the ten constituents above respectively.

The one-dimensional conservation of mass equation for each water quality constituent is

\[
\frac{\partial}{\partial t} (AC_i) + \frac{\partial}{\partial x} (QC_i) = \frac{\partial}{\partial x} (AE\frac{\partial C_i}{\partial x}) + AR_i - Ak_{si} C_i + W_i \tag{A5}
\]

where

\( C_i \) = concentration of the \( i \)th water quality constituent \((M/L^3)\),
\( R_i \) = time rate of sources or sinks due to biochemical reactions \((M/TL^3)\),
\( E \) = dispersion coefficient \((M^2/L)\),
\( k_{si} \) = loss rate \((1/T)\),
\( W_i \) = external waste input loads \((M/LT)\).

\( M,L,T \) = mass, length and time scales.

The loss rate \( k_{si} \) is the loss out of the system either by settling or by other mechanisms which cannot be easily modeled, for example, the exchange of nutrients between the water column and the river bottom. The magnitude of the loss rate has to be determined against observed data during model calibration. The term \( W_i \) represents external waste inputs into the model and includes waste loads from point and nonpoint-sources.
The dispersion coefficient is calculated from
\[ E = m(x) E_T + E_2(x) \]
where
\[ E_T = 63 \mu U R^{5/6} \]
m = a coefficient to account for channel irregularities, and

\[ E_2 = \text{a spatially varying constant which takes into account} \]
the increased dispersion towards the downstream end.

The values of \( m \) and \( E_2 \) have to be adjusted against field observations during model calibration.

(a) Initial and Boundary Conditions

Equation (A5) requires the specification of initial and boundary conditions. Initial conditions specify the water quality concentrations at the model start time, say at \( t = 0 \).

\[ C_i(x,0) = C^0_i \]
where
\[ C^0_i = \text{the given initial concentrations}. \]

There are two types of boundary conditions (Christodoulou, 1976)

(i) Concentration boundary conditions and

(ii) Dispersive boundary conditions.

These correspond to the essential and the natural boundary conditions respectively. The concentration boundary conditions specify concentrations \( C_i(x_B, t) \) at the boundaries \( x = x_B \). The dispersive boundary conditions specifies \( AE \partial C / \partial x \) at the boundaries \( x = x_D \). The choice of boundary conditions depends on the behavior and the availability of field data for a specific problem.

It must be emphasized that a one dimensional model limits the results to quantities which are averaged over a channel.
cross-section. This assumption may not be appropriate if the water body is wide, or if there is pronounced stratification. Also the waste discharge at a point is assumed to be completely mixed over the cross-section. This assumption may not be valid at the point of discharge, but will be reasonable at some distance away from the point of discharge.

3. BIOCHEMICAL PROCESSES

The various biochemical processes are incorporated into equation (A5) through the term $R_i$. The reactions occurring in estuarine waters are very complex and involve feed forward mechanisms which produce pronounced non-linearities. In general our knowledge of reactions in natural waters is not well advanced. Consequently reaction rates are commonly represented by simplified mathematical expressions. The reaction kinetics used in this study are of two types, namely; (1) First order reactions and (2) Michaelis-Menton reactions. These reaction forms are empirical, they usually are adopted because of mathematical tractability. The kinetic term $R_i$ in equation (A5) for each constituent is formulated as follows:

(a) Chlorophyll`a`, $C_1$

The biomass of phytoplankton in the estuary is represented by the concentration of chlorophyll`a`. A relatively homogeneous layer of phytoplankton is assumed, so that the growth and death rates are average values for the entire phytoplankton community. The basic kinetics governing the amount of chlorophyll`a` in the water body is the growth, death and zooplankton predation as expressed by the equation
\[ R_1 = (G - D - Z)C_1 \] \hspace{1cm} (A6)

where

\[ C_1 = \text{chlorophyll'a' (\mu g/l)}, \]
\[ G = \text{growth rate of phytoplankton (1/day)}, \]
\[ D = \text{endogenous respiration rate of phytoplankton (1/day)} \] and
\[ Z = \text{zooplankton grazing rate (1/day)}. \]

Phytoplankton grow by assimilating inorganic nutrients in the presence of light. The growth rate is assumed to be a direct function of temperature when under optimal light and nutrient conditions; non-optimal light and nutrient conditions will reduce this growth rate. The equation for growth of phytoplankton can therefore be written as a temperature dependent growth rate modulated by the light and nutrient effects

\[ G = k_T F N \] \hspace{1cm} (A7)

where

\[ k_g = \text{optimum growth rate coefficient (1/day/°C)}, \]
\[ T = \text{temperature, °C}, \]
\[ F = \text{attenuation of growth due to non-optimal light and} \]
\[ N = \text{attenuation of growth due to nutrient limitation}. \]

The effect of non-optimal light intensity is to reduce the growth rate. Steele (1962) proposed that the reduction in growth rate be represented by

\[ F = \frac{I}{I_s} e^{(1 - \frac{I}{I_s})} \] \hspace{1cm} (A8)
where

\[ I = \text{light intensity in the water column (angleys)}, \]
\[ I_s = \text{saturating or optimal light intensity (angleys)} \] and
\[ e = 2.1718. \]

In the water column, light intensity decreases exponentially with depth. For a given value of surface light intensity, the light intensity at any depth can be calculated by

\[ I = I_o e^{-k_e z} \] (A9)

where

\[ I_0 = \text{surface light intensity}, \]
\[ z = \text{depth} \] and
\[ k_e = \text{light extinction coefficient}. \]

In order to obtain the average light intensity in the water column, equation (A8) is integrated over the depth. The resultant expression for depth averaged light is

\[ F = \frac{e^{I_0}}{k_e H (1 - e^{-I_s})} \] (A10)

where

\[ H = \text{water depth}. \]

The surface light intensity, \( I_o \), varies diurnally following a sine curve peaking at midday, such that

\[ I = \begin{cases} \frac{I_o \pi}{2L_d} \sin \left( \frac{(t_d - t_s)}{L_d} \right) & \text{for } t_s < t_d < (t_s + t_d) \\ 0 & \text{otherwise} \end{cases} \] (A11)
where
\[ L_d = 12 + 2.7 \sin \left( \frac{2\pi (t_y - 20)}{365} \right) \] is the day length (hours),
\[ t_s = 12 - \frac{L_d}{2} \] is the sunrise time (hours),
\[ I_m = \text{total daily solar radiation (langleys)}, \]
\[ t_y = \text{days since January 1st}, \]
\[ t_d = \text{time of the day (hours) and} \]
\[ \pi = 3.14159. \]

As the phytoplankton concentration increases, the absorption of light by the cells themselves reduces the solar energy available at deeper levels. The reduction, known as the self shading effect, is modeled by increasing the light extinction in proportion to the concentration of phytoplankton. The empirical equation of Riley (1956) is used in this model

\[ k_e = k_e^0 + 0.054C_a^{0.66} + 0.0088C_a \]  
\[ (A12) \]

\[ k_e^0 = \text{light extinction coefficient at zero chlorophyll' a' concentration (m}^{-1}). \]

The attenuation of light is chiefly caused by the suspended matter in the water (Colijn, 1982). The value of the extinction coefficient can be estimated from the formula \( k_e^0 = 1.7/D_s \), where \( D_s \) is the Secchi disk visibility reading (Sverdrup, 1970). The reported range of the extinction coefficient is 0.4 to 8 m\(^{-1}\).

The optimum light level for photosynthesis has been found to vary over short spans of time and space. It has been established that
under certain conditions the photosynthetic capacity reflects to some degree the past light history (Kremer and Nixon, 1978). The basic assumption is that the optimum light for growth tracks the light history to which the algae has been exposed. Based on these conditions, the optimum light in this study is determined as a weighted moving average of the light intensity at the 1 meter depth for the previous three days.

\[ I_s = (0.7I_1 + 0.2I_2 + 0.1I_3)e^{-ke} \]

(A13)

where

\[ I_j \] = the average surface light \( j \) days earlier, \( j = 1, 2 \) and 3.

This equation clearly has no limit to acclimation, however. It may be necessary to include light thresholds above and below which acclimation may not occur, such as the low radiation levels in winter. The nutrient limitation on chlorophyll growth rate due to the inorganic nitrogen and inorganic phosphorous in this model is expressed by

\[ N = \left( \frac{C_3 + C_4}{C_3 + C_4 + k_{mn}} \right) \left( \frac{C_6}{C_6 + k_{mp}} \right) \]

where

\[ k_{mn} = \text{Michaelis-Menton constant for inorganic nitrogen (mg/1)}, \]
\[ k_{mp} = \text{Michaelis-Menton constant for inorganic phosphorous (mg/1)}, \]
\[ C_3 = \text{ammonia nitrogen (mg/1)}, \]
\[ C_4 = \text{nitrite-nitrate nitrogen (mg/1)} \text{ and} \]
\[ C_6 = \text{inorganic phosphorous (mg/1)} \].

The endogenous respiration rate, \( D \), and the zooplankton grazing rate, \( Z \), are assumed to be temperature dependent, thus
\[ D = k_r'T \]  
\[ Z = k'_zT \]  

where

\[ k_r' = \text{endogenous respiration coefficient (1/day} \cdot ^\circ \text{C}) \text{ and} \]
\[ k'_z = \text{zooplankton grazing coefficient (1/day} \cdot ^\circ \text{C}). \]

b. Organic Nitrogen, \( C_2 \)

In natural waters organic nitrogen undergoes a series of transformations mediated by bacteria. Organic nitrogen is transformed into ammonia nitrogen which itself is subsequently transformed to nitrite and then to nitrate nitrogen. In this model, the internal sources of organic nitrogen are considered to be phytoplankton and zooplankton endogenous respiration. The sink of organic nitrogen is the hydrolysis of organic nitrogen to nitrite and nitrate. The kinetics is of the first order type

\[ R_2 = r_n(D_2 + f_zZ)C - k_2C_2 \]  
\[ k_2 = k'_2T \]

where

\[ C_2 = \text{organic nitrogen (mg/1)}, \]
\[ r_n = \text{nitrogen-chlorophyll ratio (mg-N/\mu g-chlorophyll)}, \]
\[ k_2 = \text{organic nitrogen to ammonia nitrogen hydrolysis rate (1/day)}, \]
\[ k'_2 = \text{organic nitrogen to ammonia nitrogen hydrolysis coefficient (1/day} \cdot ^\circ \text{C}) \text{ and} \]
\[ f_z = \text{assimilation efficiency, value ranges from 0.4 to 0.8}. \]
c. **Ammonia Nitrogen, \( c_3 \)**

The kinetics for ammonia nitrogen is

\[
R_3 = k_2 C_2 - k_3 c_3 - r_n (1 - P)C_1 , \quad \text{where}
\]

\[
P = \frac{C_4}{C_4 + k_{mn}} \quad \text{for nitrate preference} \tag{A18a}
\]

\[
P = 1 - \frac{C_3}{C_3 + k_{mn}} \quad \text{for ammonia preference} \tag{A18b}
\]

\[
k_3 = k_3' T
\]

where

\[
C_3 = \text{ammonia nitrogen (mg/l)},
\]
\[
C_4 = \text{nitrite-nitrate nitrogen (mg/l)},
\]
\[
k_3 = \text{ammonia to nitrate nitrification rate (1/day)},
\]
\[
k_3' = \text{ammonia to nitrate nitrification coefficient (1/day/°C)}\]
\[
P = \text{nitrate or ammonia nitrogen preference.}
\]

The first term on the right hand side of equation (A17) represents the hydrolysis from organic nitrogen, the second term is the loss of ammonia nitrogen due to nitrification, the third term represents the uptake by phytoplankton, and the factor \( P \) represents the nitrate nitrogen or ammonia nitrogen preference.

d. **Nitrite-Nitrate nitrogen, \( c_4 \)**

In this model nitrite and nitrate nitrogen are combined as one
variable, because in natural estuarine waters, the concentration of nitrate nitrogen is normally at an order of magnitude larger than the concentration of nitrite nitrogen. The combined variable simplifies the model yet retains the effects of nitrite nitrogen.

The kinetics for nitrite-nitrate nitrogen is

\[ R_4 = -Pr_nGCl + k_3C_3 \]  \hspace{1cm} (A19)

The first term on the right hand side is the uptake by phytoplankton, the second is the source of nitrite-nitrate nitrogen from nitrification of ammonia nitrogen.

e. Organic Phosphorus, C_5

The biochemical kinetics of organic phosphorus consists of hydrolysis of organic phosphorous to inorganic phosphorous, and the release of organic phosphorous from death of phytoplankton and zooplankton. The kinetic expression for organic phosphorous is

\[ R_5 = r_p(D + f_zZ)C_1 - k_5C_5 \] \hspace{1cm} (A20)

where

\[ C_5 = \text{organic phosphorous (mg/l)}, \]
\[ k_5 = \text{organic phosphorous to inorganic phosphorous conversion rate (1/day)}, \]
\[ k'_5 = \text{organic phosphorous to inorganic phosphorus conversion coefficient (1/day/°C)} \text{ and} \]
\[ r_p = \text{phosphorus-chlorophyll ratio (mg-P/μg-chlorophyll)}. \]
f. Inorganic Phosphorus, $C_6$

Only the inorganic phosphorous fraction of the total phosphorous is considered to be taken up by phytoplankton. The internal source of inorganic phosphorous is the hydrolysis of organic phosphorous, such that

$$R_6 = -r_p C_1 + k_5 C_5$$  \hspace{1cm} (A21)

\[g. \text{ CBOD, } C_7\]

CBOD is handled as a first order decaying substance in a classical manner. The sink of CBOD is the oxidation by bacteria and the internal sources are the die off of phytoplankton and zooplankton.

$$R_7 = 2.67 r_c (f_2 Z) C_1 - k_7 C_7$$  \hspace{1cm} (A22)

\[k_7 = k'_7 (1.047)\]

where

$$C_7 = \text{CBOD (mg/l)},$$
$$k_7 = \text{CBOD oxidation rate (1/day)},$$
$$k'_7 = \text{CBOD oxidation rate at } 20^\circ \text{C and}$$
$$r_c = \text{carbon-chlorophyll ratio (mg-C/\mu g-chlorophyll)}$$

The factor 2.67 arises from the fact that the complete oxidation of one gram of carbon to carbon dioxide requires 2.67 grams of oxygen.

\[h. \text{ DO Deficit, } C_8\]

DO is coupled to CBOD, nitrogen and phytoplankton. The external source of DO is atmospheric reaeration; the sinks are oxidation of CBOD, oxidation of ammonia nitrogen and nitrite nitrogen, and the
respiration of zooplankton and phytoplankton. The equation is written in terms of DO deficit

\[ B_8 = k_7 C_7 + 4.57 k_3 C_3 - a_p C_1 + a_r C_{12} + b_8 - k_8 C_8 \]  

(A23)

\[ a_p = 2.67 r_c k_{op} \]
\[ a_r = 2.67 r_c / k_{or} \]
\[ k_8 = k_8'(1.024) \quad H \quad U \]
\[ b_8 = b_8'(1.065) \]

where

- \( C_8 \) = dissolved oxygen deficit (mg/l),
- \( a_p \) = rate of oxygen production from photosynthesis (1/day),
- \( a_r \) = rate of oxygen depletion by respiration (1/day),
- \( k_{op} \) = photosynthetic quotient,
- \( k_{or} \) = respiration ratio,
- \( k_8 \) = reaeration rate (1/day),
- \( k_8' \) = reaeration coefficient at 20°C,
- \( b_8 \) = benthic oxygen demand (gm-O_2/m^2/day) and
- \( b_8' \) = benthic oxygen demand at 20°C.

DO is calculated by subtracting the DO deficit from the saturation values of DO. The saturation DO depends on temperature and salinity of the water, \( C_9 \), and is determined by the empirical formula

\[ DO = 9.0806 - (0.18725 - 0.0044972(T-20) - 0.00205C_9)(T-20) \]
\[ - (0.0556 - 0.0002739C_9)C_9 \]  

(A24)
1. Salinity, $C_s$

Salinity is treated as a conservative substance without source/sink term, since there are no biochemical reactions.

$$R_s = 0$$  \hspace{1cm} (A25)$$

where

$$C_s = \text{salinity (ppt)}.$$  

j. Coliform Bacteria, $C_o$

Coliform bacteria die off rate is handled as a first order decay process

$$R_o = -k_o C_o$$  \hspace{1cm} (A26)$$

$$T-20$$

$$k_o = k'_o (1.040)$$

where

$C_o = \text{coliform bacteria (number/100 ml)},$

$k_o = \text{coliform bacteria die off rate (1/day)}$ and

$k'_o = \text{coliform bacteria die off rate at 20°C}$. 
4. FINITE ELEMENT FORMULATION

4.1 Introduction

Equations (A1), (A2), (A5) and their associated initial and boundary conditions are the governing equations for the biochemical water quality model. The model constitutes an initial-boundary value problem with twelve equations for twelve unknowns \( n, Q \) and \( C_i \) (\( i = 1, 2, 3, \ldots, 9, 0 \)) and uses the finite element method (FEM) for the numerical solution. For practical and economic reasons equation (A2) was linearized by using the value of \( Q \) from the previous integration time step and equation (A5) solved successively for each water quality constituent.

The FEM is a numerical technique for obtaining approximate solutions to mathematical problems defined by differential equations. The theory of FEM is quite well known, and is described in a number of excellent text books written on this subject, e.g. Zienkiewicz (1977) or Huebner (1975).

The FEM discretizes the solution domain into a number of subregions called elements with each element represented by a number of points called the nodes where the dependent variables are determined. The unknown variable is approximated within each element by an interpolation function expressed in terms of the values at the nodes. The system equations for the entire solution domain are obtained by assembling the contributions from the individual elements.
4.2 Variational Statements and the Finite Element Approximation

Using the Galerkin weighted residual method, the variational statements for equations (A1), (A2) and (A5) are obtained by multiplying the equations with arbitrary weighting functions $\delta \eta$, $\delta Q$ and $\delta C$ respectively, integrating over the length of the estuary $L$ and requiring the resulting expression to vanish

$$
\int_{L} \left( \frac{\partial \eta}{\partial t} + \frac{\partial Q}{\partial x} - q \right) \delta \eta \, dx = 0 \quad (A27)
$$

$$
\int_{L} \left( \frac{\partial Q}{\partial t} + \frac{\partial QU}{\partial x} + g \frac{\partial \eta}{\partial x} + g \frac{Q}{AC_{R}^2} + g \frac{\partial^2 \rho}{\partial x} \right) \delta Q \, dx = 0 \quad (A28)
$$

$$
\int_{L} \left( \frac{\partial AC}{\partial t} + \frac{\partial QC}{\partial x} - \frac{\partial}{\partial x} \left( AE \frac{\partial C}{\partial x} \right) - AR + Ak C - W \right) \delta C \, dx + \int_{x}^{*} F \, \delta C \, dx = 0 \quad (A29)
$$

where

$$
F_{x}^{*} = AE \frac{\partial C}{\partial x} \bigg|_{x = x_{B}}
$$

is the prescribed dispersive flux boundary condition at $x = x_{B}$.

For clarity the surface wind term in equation (A2) and the subscript $i$ in equation (A5) have been omitted. An additional step is performed to reduce the order of the derivative in equation (A29) by integrating the dispersive term by parts, the equation becomes

$$
\int_{L} \left\{ \left( \frac{\partial AC}{\partial t} + \frac{\partial QC}{\partial x} - AR + Ak C - W \right) \delta C + AE \frac{\partial^2 C}{\partial x^2} \right\} dx + F_{x}^{*} \delta C - F_{L}^{*} \delta C = 0 \quad (A30)
$$

where

$$
F_{x}^{*} = AE \frac{\partial C}{\partial x} \bigg|_{x = 0}
$$
and

\[ P^*_x = AE \frac{\partial C}{\partial x}, x = \ell \]

are the given dispersive boundary conditions at the downstream end, \( x = 0 \), and at the upstream end, \( x = \ell \), respectively.

For convenience the first two terms in equation (A30) can be written as

\[
\frac{\partial AC}{\partial t} + \frac{\partial QC}{\partial x} = A \frac{\partial AC}{\partial t} + Q \frac{\partial AC}{\partial x} + C \left( \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} \right)
\]

\[ = A \frac{\partial AC}{\partial t} + Q \frac{\partial AC}{\partial x} + Cq \]

In the finite element method the solution domain is divided into a number of elements and the field variables \( \eta, Q \) and \( C \) in each element are approximated by trial functions

\[ \eta = \hat{\eta} = \{N\}^T \{\eta\} \quad (A31a) \]
\[ Q = \hat{Q} = \{N\}^T \{Q\} \quad (A31b) \]
\[ C = \hat{C} = \{N\}^T \{C\} \quad (A31c) \]

where

\[ \hat{\eta}, \hat{Q}, \hat{C} \quad = \text{approximate solutions in an element,} \]
\[ \{N\}^T \quad = \text{a row vector of the interpolation function and} \]
\[ \{\eta\}, \{Q\}, \{C\} = \text{the vectors of the unknown nodal variables to be determined.} \]

The interpolations are usually defined locally for elements or subdomains. In a one dimensional problem, such as the present study, the elements will be line segments along the \( x \)-axis. Using a local coordinate system as shown in Figure A2, the linear variation of
The interpolations are usually defined locally for elements or subdomains. In a one-dimensional problem, the elements will be line segments along the x-axis. The simplest line element is a line segment with two nodes. This is the type of element used in the present study. Higher polynomials can be used, but a linear variation is preferred because it is simple to use and simple to interpret physically. Using a local coordinate system as shown in Figure 4.1, the linear variation of the field variable such as the concentration \( C \) in equation (A31c) can be written as

\[
C = \hat{C} = N_1 C_1 + N_2 C_2
\]

Figure A2. Finite element approximation to the exact solution.

where

\[
N_1 = \frac{(x_2-x)}{(x_2-x_1)}, \quad N_2 = \frac{(x-x_2)}{(x_2-x_1)},
\]
\( x_1, x_2 \) = coordinates of the two ends of the element and 
\( C_1, C_2 \) = the nodal values at \( x_1 \) and \( x_2 \) respectively.

Equation (A32) can also be written in matrix form as

\[
\dot{\mathbf{c}} = \{N\}^T \{c\}
\]  
(A33)

where

\[
\{c\} = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}
\]

\[
\{N\}^T = \{N_1 \ N_2\}
\]

The weighting functions \( \delta \eta, \delta Q, \text{ and } \delta C \) also have the same form as the trial functions as in equations (A31a to c). All the other variables such as \( A \) and \( B \) are expressed in a similar fashion.

Substituting the trial functions (A31a, b and c) and the similar weighting functions into equations (A27), (A28) and (A30). The resulting element integrals can be evaluated explicitly for every element. The global equations are obtained by assembling the individual element equations. After cancelling the terms \( \{\delta \eta\}^T, \{\delta Q\}^T \text{ and } \{\delta C\}^T \), the results can be written as

\[
[M_\eta] \frac{d\{\eta\}}{dt} + [K_\eta]\{Q\} = \{F_\eta\}
\]  
(A34)

\[
[M_Q] \frac{d\{Q\}}{dt} + [K_Q]\{Q\} = \{F_Q\}
\]  
(A35)

\[
[M_C] \frac{d\{C\}}{dt} + [K_C]\{C\} = \{F_C\}
\]  
(A36)

Where the matrices are obtained from the assemblage of all the elements. The details of the integration and the matrices are given in section 6 of this Appendix.
5. TIME INTEGRATION

The FEM reduces the original set of partial differential equations in space and time into a set of ordinary differential equations in time. Several integration methods can be used to advance the solution in time from a given initial condition. The choice of time integration schemes has been discussed by Wang (1975) and by Roache (1972). In this study, the hydrodynamic and water quality equations are solved separately in two sub-models; and the trapezoidal rule with split time scheme (Wang, 1975) is used to advance the solution in time.

A. Hydrodynamic Model

Equations (A34) and (A35) are used to solve for $\eta$ and $Q$ respectively. In the split time scheme, these two equations are staggered in time such that $\eta$ is evaluated at times $t_{n+\frac{1}{2}}$ and $Q$ at times $t_n$ ($n = 1, 2, 3, \ldots$). Equations (A34) and (A35) can be written as

\begin{align*}
[M_\eta]\{(\eta)_{n+\frac{1}{2}} - (\eta)_{n-\frac{1}{2}}\} &= \{(F_\eta) - [K_\eta](Q)_n\} \Delta t \quad \text{(A37)} \\
[M_Q]\{(Q)_{n+1} - (Q)_n\} + [K_Q]\{(Q)_{n+\frac{1}{2}} + (Q)_n\} \Delta t/2 &= \Delta t\{F_Q\} \quad \text{(A38)}
\end{align*}

where

$\Delta t =$ the size of the integration time step.

Using given initial values $\{\eta\}_{n-\frac{1}{2}}$ and $\{Q\}_n$, the solution proceeds by first solving equation (A37) for $\{\eta\}_{n+\frac{1}{2}}$; and then solving equation (A38) for $\{Q\}_{n+1}$ using initial values $\{Q\}_n$ and $\{\eta\}_{n+\frac{1}{2}}$ from the previous half time step. The process is then repeated for the subsequent time steps.
B. Water Quality Model

The ten water quality constituents $C_1$ are obtained by solving equation (A36) successively for each water quality constituent. Employing the trapezoidal rule of integration, the finite difference form of equation (A36) can be written as

$$[M_C]\{C\}_{n+\frac{1}{2}} - \{C\}_{n-\frac{1}{2}} + [K_C]\{C\}_{n+\frac{1}{2}} + \{C\}_{n-\frac{1}{2}} \Delta t/2 = \Delta t\{F_C\} \quad (A39)$$

Equation (A39) is used to solve for $C_1$ at times $t_{n+\frac{1}{2}}$ from the given initial values $\{C\}_{n-\frac{1}{2}}$ and the values of $\{\eta\}_{n+\frac{1}{2}}$ and $\{Q\}_{n+\frac{1}{2}}$ from the hydrodynamic model. The process is then repeated for the subsequent time steps.

As mentioned in section (a) of this Appendix there are two types of boundary conditions, corresponding to the essential and the natural boundary conditions. The essential boundary conditions are imposed by modifying the final system equations; the natural boundary conditions are imposed by evaluating the dispersive flux (Harleman, 1972). For the water quality model, the ocean boundary condition is handled by checking the discharge at each time step. If the discharge is into the boundary, the concentration of the incoming water is specified. If discharge is out of the boundary, the dispersive flux is specified.

C. Stability Conditions

The stability criteria for a given set of equations are commonly determined by the method of von Neumann (Roache, 1972) in order to determine whether the spurious errors introduced in the numerical method will amplify. The stability criteria in the present study are
difficult to obtain analytically, but guidelines for stability criteria for the hydrodynamic model can be obtained using the Courant condition

\[ \Delta t_{cr} < \frac{\Delta x}{\sqrt{2gh}} \]  \hspace{1cm} (A40)

where

\[ \Delta t_{cr} = \text{critical time step for the onset of instability}, \]
\[ \Delta x = \text{typical grid size}, \]
\[ H = \text{typical water depth and} \]
\[ g = \text{gravitational acceleration}. \]

For the convective-diffusion equation, Roache (1972) has shown that using the explicit integration scheme when the grid Reynolds number

\[ \frac{u\Delta x}{E} < 2 \]  \hspace{1cm} (A41)

the diffusion restrictions

\[ \frac{E\Delta t}{\Delta x^2} < 0.5 \]  \hspace{1cm} (A42)

and

\[ \Delta t < \frac{2E}{U^2} \]  \hspace{1cm} (A43)

are necessary and sufficient for the stability of the linear and constant \( U \) case. The effects of spatially varying \( U \) can not be ascertained, however. Similarly the implicit integration scheme using the trapezoidal rule has been found to be unconditionally stable.
In practice the stability criteria vary from problem to problem, since the stability of the numerical solution is governed by a number of factors such as the particular way of formulating the equations and the truncation errors of the computer. Guidelines can be established by using equation (A40) for the hydrodynamic model and equations (A42) and (A43) for the water quality model. It is interesting to note that the stability criteria for hydrodynamic models are much more stringent than the water quality counterparts. Therefore it is more efficient to separate the hydrodynamic and water quality systems into two sub-models as has done in the present study.

Another problem that may occur with the numerical solution of the conservation of mass equation is the presence of spatial oscillations. Spatial oscillatory solutions generally occur in a node to node manner, hence called 2x oscillations. The occurrence of spatial oscillation is not a true stability problem because it is not unbounded, but the result oscillates about the correct solution. Lee and Harleman (1971) found that the solution tended to oscillate in the vicinity of steep concentration gradients. If the oscillations can be tolerated, a smoothing technique can be used to suppress the oscillations; since this is done on output only, it has no internal effect on the solution.

The oscillations also can be suppressed by damping mechanisms such as by adding artificial dispersion terms to the equation or by using numerical schemes such as the upwind differencing method which introduces artificial dispersion into the equation (Chow, 1979). The best approach, however, is to make judicious mesh refinements and to reexamine the specification of boundary conditions (Gresho and Lee, 1981).
6. EVALUATION OF THE ELEMENT INTEGRALS

The integrals in equations (A27), (A28) and (A30) are evaluated term by term. In this formulation the superscript $e$ is used to denote element properties and the symbol $\Sigma$ is used to denote summation over all the elements. For brevity the symbols $dx$ is omitted in all the integrals; and the superscript $e$ is also omitted when not ambiguous.

The subscripts 1 and 2 are used to denote values at the two end nodes of an element (see Figure A2).

The integrals in equation (A27) are

\[
\int \frac{\partial}{\partial t} \delta \eta = \sum_e \int \frac{\partial}{\partial t} \delta \eta \\
= \sum_e \{\delta \eta\}^T \{N\} \{N\}^T \{B\} \{\eta\}^T \frac{\partial \{\eta\}}{\partial t} \\
= \sum_e \{\delta \eta\}^T \{M_e\} \frac{\partial \{\eta\}}{\partial t}
\]

\[
\int \frac{\partial Q}{\partial x} \delta \eta = \sum_e \int \frac{\partial Q}{\partial x} \delta \eta \\
= \sum_e \{\delta \eta\}^T \{N\} \frac{\partial \{N\}}{\partial x} \{Q\} \\
= \sum_e \{\delta \eta\}^T \{K_n^e\} \{Q^e\}
\]

\[
\int q \delta \eta = \sum_e \int q^e \delta \eta \\
= \sum_e \{\delta \eta\}^T \{N\} q^e
\]
where the matrices

\[ [M^e] = \int_e \{N\} \{N\}^T \{B\} \{N\}^T \]

\[ = \frac{L^e}{12} \begin{bmatrix} 3B_1 + B_2 & B_1 + B_2 \\ B_1 + B_2 & B_1 + 3B_2 \end{bmatrix} \]

where \( L^e = x_2 - x_1 \) is the length of an element (see Figure A2).

\[ [K^e] = \int_e \{N\} \frac{\partial \{N\}}{\partial x} \]

\[ = \frac{1}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \]

\[ \{F^e\} = \int_e \{N\} q^e \]

\[ = \frac{q^e L^e}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \]

Equation (A27) is reduced to

\( \{\delta\eta\}^T \left( [M^e] \frac{d\{\delta\eta\}}{dt} + [K^e] \{\eta\} - \{F^e\} \right) = 0 \) \hspace{1cm} (A44)

Next we define the global vector arrays as follows

\( \{\delta\eta\} = \text{union of all} \{\delta\eta^e\} \)

\( \{\eta\} = \text{union of all} \{\eta^e\} \)

\( \{Q\} = \text{union of all} \{Q^e\} \)

Equation (A44) can be assembled into a single equation in matrix
form

\[ \{ \delta \eta \}^T \{ [M_{n}] \frac{d }{dt} [\delta \eta] + [K_{n}] \{ Q \} - \{ F_{n} \} \} = 0 \]  \hspace{1cm} (A45)

where the global matrices \([M_{n}]\), \([K_{n}]\) and \(\{ F_{n} \}\) are obtained from the assemblage of the element matrices. Since \(\{ \delta \eta \}\) is an arbitrary function, the terms within the brackets in equation (A45) must vanish, i.e.

\[ [M_{n}] \frac{d }{dt} [\delta \eta] + [K_{n}] \{ Q \} - \{ F_{n} \} = 0 \]  \hspace{1cm} (A46)

Evaluation of equation (A28) for each element \(e\)

\[ \int_{e} \frac{\partial}{\partial t} \delta Q = \{ \delta Q \}^T \int_{e} \{ N \} \{ N \}^T \frac{\partial \{ Q \}}{\partial t} \]

\[ = \{ \delta Q \}^T \left[ M_{Q}^{\epsilon} \right] \frac{\partial \{ Q \}}{\partial t} \]

\[ \int_{e} \frac{\partial}{\partial x} \delta Q = \int_{e} \left( U \frac{\partial Q}{\partial x} + \frac{\partial U}{\partial x} \right) \delta Q \]

\[ = \{ \delta Q \}^T \int_{e} \left( \{ N \} \left( \{ N \}^T \frac{\partial \{ Q \}}{\partial x} \right) + \{ N \} \left( \{ N \}^T \frac{\partial \{ Q \}}{\partial x} \right) \right) \]

\[ = \{ \delta Q \}^T \left[ K_{Q}^{\epsilon} \right] \{ Q^{\epsilon} \} \]

where \(U\) is taken to be the velocity from the previous integration time step.

\[ \int_{e} \left( gA \frac{\partial n}{\partial x} + gA \frac{\partial |Q|}{\partial x} \right) \delta Q = - \{ \delta Q \}^T \int_{e} \left( g \{ N \} \{ N \}^T \{ A \} \frac{\partial \{ N \}}{\partial x} \right) \]

\[ + f_1 \{ N \} \{ N \}^T \{ Q \} + f_2 \{ N \} \{ N \}^T \{ A \} \frac{\partial \{ N \}}{\partial x} \]

\[ = \{ \delta Q \}^T \{ F_{Q}^{\epsilon} \} \]
defining:

\[ f_1 = \frac{g \cdot \overline{\Omega}}{AC_e^2 R_h} \]
\[ f_2 = \frac{d_c}{\rho} \]

where the overbar denotes the average values of the two end nodes, for example \( \overline{A} = (A_1 + A_2)/2 \).

The matrices are

\[ [M_e] = \int_e \{N\} \{N\}^T \]
\[ = \frac{L_e}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \]

\[ [K_e] = \int_e \{N\} \{N\}^T \frac{\partial \{N\}}{\partial x} + \int_e \{N\} \frac{\partial \{N\}}{\partial x} \{U\} \{N\}^T \]
\[ = \frac{1}{6} \begin{bmatrix} -2U_1 - U_2 & -2U_1 + U_2 \\ -U_1 - 2U_2 & U_1 + 2U_2 \end{bmatrix} + \frac{1}{6} \begin{bmatrix} -2U_1 + 2U_2 & -U_1 + U_2 \\ -U_1 + U_2 & -2U_1 + 2U_2 \end{bmatrix} \]

\[ \{F_e\} = -\int_e (g\{N\} \{N\}^T \{A\} \frac{\partial \{N\}}{\partial x} + f_1 \{N\} \{N\}^T \{Q\} + f_2 \{N\} \{N\}^T \{A\} \frac{\partial \{N\}}{\partial x} \{\rho\}) \]
\[ = \frac{g}{6} \begin{bmatrix} -2A_1 - A_2 & -2A_1 + A_2 \\ -A_1 - 2A_2 & A_1 + 2A_2 \end{bmatrix} \{n_e\} - \frac{f_1 L_e}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \{Q_e\} - f_2 \begin{bmatrix} -2A_1 - A_2 & -2A_1 + A_2 \\ -A_1 - 2A_2 & A_1 + 2A_2 \end{bmatrix} \{\rho_e\} \]

Substituting all the integrals into equation (A28) and performing the global assembly of all the elements, the resultant equation can be expressed in matrix form as

\[ \left[ M_e \right] \frac{d\{Q\}}{dt} + [K_e] \{Q\} - \{F_e\} = 0 \]
Where \([M_Q], [K_Q]\) and \(\{F_Q\}\) are obtained from the global assembly of all the elements in the domain \(L\).

Evaluation of equation (A30) for each element \(e\)

\[
\int_{e} A^C_{\delta t} \delta C = \{\delta C\}^T \{N\} \{N\}^T \{A\} \frac{\delta \{N\}}{\delta t} \frac{\delta \{C\}}{\delta t}
\]

\[
= \{\delta C\}^T \left[ M^C_e \right] \frac{\delta \{C\}}{\delta t}
\]

\[
\int_{e} (Q^C_{\delta x} + k_s A C + Cq) \delta C + \int_{e} A \frac{\partial \delta C}{\partial x} = \{\delta C\}^T \left( \{N\} \{N\}^T \{Q\} \frac{\partial \{N\}}{\partial x} \frac{\partial \{C\}}{\partial x} \right)
\]

\[
+ k_s \{N\} \{N\}^T \{A\} \{N\}^T \{C\} + q^e \{N\} \{N\}^T \{C\} + E^e \{N\} \{N\}^T \{A\} \frac{\partial \{N\}}{\partial x} \frac{\partial \{C\}}{\partial x}
\]

\[
= \{\delta C\}^T \left[ K^C_e \right] \{C^e\}
\]

\[
\int_{e} W \delta C = \{\delta C\}^T \left( \{N\} \right) \{W^e\}
\]

\[
= \{\delta C\}^T \left[ F^e_C \right]
\]

where the matrices

\[
[M^C_e] = \int_{e} \{N\} \{N\}^T \{A\} \{N\}^T
\]

\[
= \frac{L^e}{12} \begin{bmatrix}
3A_1 + A_2 & A_1 + A_2 \\
A_1 + A_2 & A_1 + 3A_2
\end{bmatrix}
\]

\[
[F^e_C] = \int_{e} \left( \{N\} \{N\}^T \{Q\} \frac{\partial \{N\}}{\partial x} \frac{\partial \{C\}}{\partial x} + k_s \{N\} \{N\}^T \{A\} \{N\}^T \{C\} + q^e \{N\} \{N\}^T \{C\} + E^e \{N\} \{N\}^T \{A\} \frac{\partial \{N\}}{\partial x} \frac{\partial \{C\}}{\partial x} \right)
\]

\[
= \int_{e} \left( \{N\} \{N\}^T \{Q\} \frac{\partial \{N\}}{\partial x} \frac{\partial \{C\}}{\partial x} + k_s \{N\} \{N\}^T \{A\} \{N\}^T \{C\} + q^e \{N\} \{N\}^T \{C\} + E^e \{N\} \{N\}^T \{A\} \frac{\partial \{N\}}{\partial x} \frac{\partial \{C\}}{\partial x} \right)
\]
Substituting all the integrals into equation (A30) and performing the global assemblage, again the resultant equation can be written in matrix form as

\[ [M_C] \frac{d\{C\}}{dt} + [K_C]\{C\} - \{F_C\} = 0 \]

where the matrices \([M_C]\), \([K_C]\) and \([F_C]\) are obtained from the assemblage of all the elements in the domain \(L\).
APPENDIX B. Calibration Figures and Statistics for the James River Model

1 - Map showing model segments

2 - Time variation of the nine water quality constituents for selected model nodes

3 - Longitudinal profiles of monthly average water quality constituent concentrations

4 - Statistical summary
Model segments for the James River estuary.
NODE 40.
NO3+NO2-N (µg/L)

NOD (100 HOURS)

 NODE 32.
1.2

0.8

0.4

0.0

-2

0.8

0.4

0.0

-2

0.8

0.4

0.0

-2

11 12 20 24 32 40 44 48 52 56 60

0 4 8 12 16 20 24 28 32 36 40 44 48 52 56 60

0 4 8 12 16 20 24 28 32 36 40 44 48 52 56 60

0 4 8 12 16 20 24 28 32 36 40 44 48 52 56 60

NODE 28.
The image contains several graphs showing data over time. The top graph appears to be a plot of dissolved oxygen (DO) concentration over time, with data points plotted at various time intervals (100 hours). The bottom two graphs seem to be related to different measurements, possibly DO decay and another parameter, with similar time intervals (100 hours) for data collection. Each graph shows fluctuations and trends that indicate changes in the measured variables over time.
NODE 19.
NODE 18.
NODE 10.
NODE 4.
B3.11

Graphs showing the concentration of various substances (INORG-P, ORG-P, DO, BODU) as a function of distance from the mouth of a river or stream, with data points and lines indicating trends over August.
JAMES RIVER WATER QUALITY MODEL STATISTICS

JAMES RIVER WATER QUALITY MODEL STATISTICS
N = NO. OF DATA POINTS,
E = AVERAGE ERROR,
RE = RELATIVE ERROR,
SE = STANDARD ERROR,
CV = COEFFICIENT OF VARIATION,
A = SLOPE,
B = INTERCEPT,
R = CORRELATION COEFFICIENT.
(999.999 IS MEANINGLESS)

MARCH

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### JAMES RIVER WATER QUALITY MODEL STATISTICS

#### MAY

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### JAMES RIVER WATER QUALITY MODEL STATISTICS (ALL POINTS)

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Observed versus model predicted salinity values for the James River, 1 March through 31 October, 1971.
APPENDIX C. Calibration Figures and Statistics for the Potomac River Model

1 - Map showing model segments

2 - Time variation of the nine water quality constituents for selected model nodes

3 - Longitudinal profiles of monthly average water quality constituents concentrations

4 - Statistical summary
Model segments for the Potomac River estuary.
The image contains several graphs showing data over time. The x-axis represents time in hours, while the y-axis represents various measurements in milligrams per liter (mg/L). The graphs illustrate trends and changes over the specified time periods.
DO (mg/L)

DO DEF. (mg/L)

CBOD (mg/L)
OCTOBER
**ORG-N (MG/L)**

- Distance from mouth (KM)
- May

**CHLOROPHYLL A (UC/L)**

- Distance from mouth (KM)
- May
April
## POTOMAC RIVER WATER QUALITY MODEL
### SUMMARY OF CALIBRATION STATISTICS

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N = NO. OF DATA POINTS,  
E = AVERAGE ERROR,  
RE = RELATIVE ERROR,  
SE = STANDARD ERROR,  
CV = COEFFICIENT OF VARIATION,  
A = INTERCEPT,  
B = SLOPE,  
R = CORRELATION COEFFICIENT.  
(999.999 IS MEANINGLESS)
APPENDIX D. Calibration Results for the Chesapeake Bay Model

1 - Model elements and nodes

2 - Time variation of the water quality constituents for selected elements

3 - Longitudinal profiles of monthly mean water quality constituent concentrations
Numbering of model nodes for Chesapeake Bay.
Numbering of model elements for Chesapeake Bay.
The diagram shows the concentration of DO (DO) and DO deficit (DO DEF) over time. The concentration of DO decreases from 12 mg/L to 8 mg/L over a period of 60 hours, while the DO deficit remains relatively constant at 2 mg/L.
CHLOROPHYLL A (MG/CU.M) vs. TIME (HOURS) * 10^2

SALINITY (PPT) vs. TIME (HOURS) * 10^2

ELEV 92
NO2+NO3-N (mg/L)

NH3-N (mg/L)