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A Modeling Study of Hypoxia and Eutrophication in the Tidal Rappahannock River, Virginia

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Kyeong Park, Albert Y. Kuo and Bruce J. Neilson

Special Report in Applied Marine Science and Ocean Engineering No. 322

School of Marine Science
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College of William and Mary
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ABSTRACT

A laterally integrated, two-dimensional, real-time model, consisting of linked hydrodynamic and water quality models, is applied to the tidal Rappahannock River, Virginia. The hydrodynamic model, based on the principles of conservation of volume, momentum and mass, predicts surface elevation, current velocity and salinity. The water quality model, based on the conservation of mass alone, predicts eight parameters; dissolved oxygen (DO), chlorophyll 'a', carbonaceous biochemical oxygen demand (CBOD), organic nitrogen, ammonia nitrogen, nitrite-nitrate nitrogen, organic phosphorus and inorganic phosphorus.

The hydrodynamic model was calibrated and verified using field data collected in 1987 and 1990, and was used to study hydrodynamic processes. A reverse longitudinal salinity gradient, that has been frequently observed in the Rappahannock, was explained in terms of bottom topography and vertical mixing. This argument was further supported by the salinity data from 1981-1990 slackwater surveys. The often confusing usage of the phrase "limit of salt intrusion" in place of "limit of gravitational circulation" was clarified.

The water quality model was calibrated and verified using field data from 1990 surveys, and was used to study water quality conditions. Hypoxia, even anoxia, persists during summer in the bottom water of the lower portion of the tidal Rappahannock. Sensitivity analysis shows that the bottom water becomes hypoxic regardless of DO and CBOD in the incoming bay water. Hypoxia can be relieved more by eliminating CBOD than by increasing DO in the incoming bay water. An increase in either residual velocity or vertical mixing also can relieve the hypoxic condition. Water column respiration, including CBOD decay, nitrification and algal respiration, is as important as sediment oxygen demand, and the CBOD decay is the most important of the water column processes.

High chlorophyll concentrations in the lower portion of tidal freshwater have been observed in many estuaries. Sensitivity analysis indicated that the high chlorophyll concentrations in the Rappahannock cannot be maintained without an external input of nutrients. A hypothesis was proposed to account for the nutrient source and the downriver limit of high chlorophyll concentrations.
ACKNOWLEDGEMENTS

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Dissolved oxygen (DO) deficiency, as an index of deteriorated water quality, has been widely observed in estuarine and coastal waters such as the New York Bight (Falkowski et al. 1980), the New Jersey coast (Swanson & Sindermann 1979) and Chesapeake Bay (Officer et al. 1984). In Chesapeake Bay, anoxia (no dissolved oxygen) has been documented since the 1930’s (Newcombe & Horne 1938). It has been more widespread and of longer duration during recent times (Flemer et al. 1983), and appears to have had significant ecological effects (Seliger et al. 1985). All major subestuaries on the western side of Chesapeake Bay have deep basins near their mouths. Hypoxia (deficient dissolved oxygen) has been observed frequently in the deep basin of the Patuxent River, Maryland (Laubach & Summers 1987) and the Rappahannock and York rivers in Virginia (D’Elia et al. 1981; Phoel et al. 1981; Kuo & Neilson 1987; Kuo et al. 1991a; Kuo & Park 1992; Llansó 1992).

The mid-reach of the tidal Rappahannock River between km 80-145 (distance measured from river mouth) is bounded by shallow regions at the up- and down-river boundaries (see Fig. 3-2). The upper limit of salt intrusion occurs between km 70-120 depending upon the freshwater discharge. The tidal freshwater portion just upriver of the limit of salt intrusion is characterized by a chlorophyll maximum (Anderson 1986). He suggested the hydrodynamic trapping of phytoplankton biomass in the region of the turbidity maximum, rapid internal cycling of essential nutrients such as silica, demise of freshwater phytoplankton during transport to the saline part of the river, and light limitation in the oligohaline reach of the river as controlling factors. These high phytoplankton concentrations in the tidal freshwater reaches and the low salinity transition regions of estuaries have been observed frequently in many other estuarine environments (Haertel et al. 1969; Lipson et al. 1979; Cloern et al. 1983; Pennock
1985; Relexans et al. 1988; Schuchardt & Schirmer 1991). Key mechanisms suggested by these investigators are river discharge, water residence time, solar radiation and nutrients.

This report documents the application of a laterally integrated two-dimensional model of hydrodynamics and water quality to study the observed phenomena of hypoxia and eutrophication in the tidal Rappahannock River, Virginia. The mathematical model, explained in detail in Park & Kuo (1993), is briefly described in Chapter II. The characteristics of the study area, the tidal Rappahannock River, are described in Chapter III. The calibration and verification of the hydrodynamic model using field data collected in 1987 and 1990 is discussed in Chapter IV. The water quality model was calibrated and verified using field data collected during summer of 1990 (Chapter V).

Once calibrated and verified, the model is a powerful tool that can be used to study the characteristic behavior of the prototype. Sensitivity analysis was performed to study the hydrodynamic and water quality characteristics of the tidal Rappahannock River. The hydrodynamic responses of the prototype are included in Chapter IV. The sensitivity analysis of the water quality model (Chapter VI) emphasized the lower part of the estuary where hypoxia, or even anoxia, has persisted during summer in the bottom water and the middle part of the tidal river, which was characterized with high chlorophyll concentration. The summary of this study with recommendations for future study is presented in Chapter VII.
II. DESCRIPTION OF THE MODEL

2-1. Hydrodynamic Model

The laterally integrated two-dimensional hydrodynamic model developed by Kuo et al. (1978) was extensively modified and used to calculate the flow field and salinity. With a right-handed Cartesian coordinate system with the x-axis directed seaward and the z-axis directed upward, the governing equations are,

\[
\frac{\partial (uB)}{\partial x} + \frac{\partial (wB)}{\partial z} = q_p \tag{2-1}
\]

\[
\frac{\partial}{\partial t} (B, \eta) + \frac{\partial}{\partial x} \int_{H}^{b} (uB) dz = q \tag{2-2}
\]

\[
\frac{\partial (uB)}{\partial t} + \frac{\partial (uBu)}{\partial x} + \frac{\partial (uBw)}{\partial z} = -\frac{B}{\rho} \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (A_B \frac{\partial u}{\partial x}) + \frac{\partial}{\partial z} (A_B \frac{\partial u}{\partial z}) \tag{2-3}
\]

\[
\frac{\partial p}{\partial z} = -\rho g \tag{2-4}
\]

\[
\frac{\partial (sB)}{\partial t} + \frac{\partial (sBu)}{\partial x} + \frac{\partial (sBw)}{\partial z} = \frac{\partial}{\partial x} (K_B \frac{\partial s}{\partial x}) + \frac{\partial}{\partial z} (K_B \frac{\partial s}{\partial z}) + S_p \tag{2-5}
\]

\[
\rho = \rho_o (1 + ks) \tag{2-6}
\]

\[
A_z = \alpha Z^2 \left(1 - \frac{Z}{h}\right)^2 \left| \frac{\partial u}{\partial z} \right| (1 + \beta R_l)^{-\frac{1}{2}} + \alpha_w \frac{H_w^2}{T} \exp\left(-\frac{2\pi Z}{L}\right) \tag{2-7}
\]

\[
K_z = \alpha Z^2 \left(1 - \frac{Z}{h}\right)^2 \left| \frac{\partial u}{\partial z} \right| (1 + \beta R_l)^{-\frac{3}{2}} + \alpha_w \frac{H_w^2}{T} \exp\left(-\frac{2\pi Z}{L}\right) \tag{2-8}
\]

where

- \( t = \) time,
- \( \eta = \) position of the free surface above mean sea level,
- \( u \& w = \) laterally averaged velocities in the x and z directions, respectively,
s = laterally averaged salinity,
B & B = river width and width at the free surface including side storage area,
H = total depth below mean sea level,
q_p = point source discharge,
q = lateral inflow including q_p,
p & ρ = pressure and water density,
g = gravitational acceleration,
A_x & A_z = turbulent viscosities in the x and z directions, respectively,
K_x & K_z = turbulent diffusivities in the x and z directions, respectively,
S_0 = source or sink of salt,
ρ_o & k = density of freshwater and a constant (7.5 × 10^4 ppt^-1),
Z & h = distance from the surface and total depth (h = η + H),
R_i = local Richardson number,
H_w, T & L = height, period and length, respectively, of wind-induced waves, and
α, β & α_w = constants.

Equations 2-1 and 2-2 are the laterally and sectionally, respectively, integrated continuity equations for an incompressible flow. Equation 2-3 is the laterally integrated equation of motion for an incompressible but non-homogeneous flow, and represents the momentum balance along the longitudinal axis of an estuary. When the hydrostatic approximation, i.e., gravity is the dominant force in the vertical direction, is applied to the equation of motion in the z direction, the result is the hydrostatic equation (Eq. 2-4). Equation 2-5 is the laterally integrated mass-balance equation for salt. The density is related to the salinity by the simplified equation of state (Eq. 2-6), which is usually regarded as a satisfactory approximation because of the large horizontal gradients of salinity in estuaries (Hamilton 1977). Munk-Anderson type formulations are used to specify the turbulent mixing coefficients (Equations 2-7 and 2-8).
Equations 2-1 through 2-3 are solved by a finite difference method to obtain the time-varying solution of the free surface elevation ($\eta$) and the laterally averaged velocity fields ($u$ and $w$). The pressure term ($p$) is evaluated using Eq. 2-4 with the water density ($\rho$) from Eq. 2-6, and salinity ($s$) using Eq. 2-5. The detailed description of the method of solution including boundary conditions, turbulence closure model and stability criteria can be found in Park & Kuo (1993).

2-2. Water Quality Model

The water quality model is based on the equation describing the mass-balance of eight interlinked water quality parameters (Fig. 2-1): phytoplankton population (Chl), organic nitrogen (N1), ammonia nitrogen (N2), nitrite-nitrate nitrogen (N3), organic phosphorus (P1), inorganic (ortho) phosphorus (P2), carbonaceous biochemical oxygen demand (CBOD) and dissolved oxygen (DO). For each parameter, the following equation that is solved by the finite difference method:

$$\frac{\partial (cB)}{\partial t} + \frac{\partial (cBu)}{\partial x} + \frac{\partial (cBw)}{\partial z} = \frac{\partial}{\partial x}(K_x B \frac{\partial c}{\partial x}) + \frac{\partial}{\partial z}(K_z B \frac{\partial c}{\partial z}) + BS_e + BS_i$$  (2-9)

where

- $c =$ laterally averaged concentration of any parameter,
- $S_e =$ time rate of external addition (or withdrawal) of any parameter across the boundaries, and
- $S_i =$ time rate of internal increase (or decrease) of any parameter by biochemical reaction processes.

Equation 2-9 gives the distribution of any parameter using the physical parameters ($u$, $w$, $\eta$, $K_x$, and $K_z$) determined from the hydrodynamic model. The physical transport terms, both advective and diffusive, are treated in the same manner as those in the mass balance equation for salt (Eq. 2-5).
The last two terms of Eq. 2-9 represent, respectively, the external and internal sources (or sinks). The latter are due primarily to biochemical reactions. The processes included in the model are shown in a schematic diagram in Fig. 2-1. Each rectangular box in Fig. 2-1 represents one parameter being simulated by the model. The arrows between parameters represent the biochemical transformation of one substance into the other. An arrow with one end unattached to a parameter (rectangular box) represents an internal source (or sink) due to the biochemical reaction or an external source (or sink).

The mathematical expressions used in this study for the terms, $S_e$ and $S_i$, for each of the eight parameters are the extension of the one-dimensional water quality model described in Kuo et al. (1991b). Detailed description of the model including the method of solution can be found in Park & Kuo (1993), and the following sections list the model formulations of $S_e$ and $S_i$.

2-2-1. Phytoplankton population

\[ S_i = (G - R - P) \text{Chl} \]  
\[ S_e = \frac{K_{\text{Chl}}}{\Delta z} (\lambda_1 \text{Chl}_{k-1} - \text{Chl}_i) + \frac{W\text{Chl}}{V} \]

\[ G = k_{g1} \theta_1^{T-20} L(I_a, I_s, k_e, \text{Chl}, \Delta z) \cdot N(N_2, N_3, P_2) \]

\[ L = \frac{e}{K_e \Delta z} \left[ \exp \left( -\frac{I}{I_s} \exp(-K_e[H_s+\Delta z]) \right) - \exp \left( -\frac{I}{I_s} \exp(-K_e[H_s]) \right) \right] \]

\[ K_e = k_e + K_{e, \text{Chl}} \text{Chl} \]

\[ I_1 = I_a \left( \frac{24}{r_d + r_u} \right) \frac{\pi}{2} \sin \left( \pi \frac{r - r_u}{r_d - r_u} \right) \quad \text{if} \quad r_u < r < r_d \]

\[ = 0 \quad \text{if} \quad r < r_u \quad \text{or} \quad r > r_d \]

\[ N = \min \left\{ \frac{N_2 + N_3}{K_{mn} + N_2 + N_3}, \frac{P_2}{K_{mp} + P_2} \right\} \]

\[ R = R(20) \theta_2^{T-20} \]
\[ P = P(20) \cdot \theta_1^{T-20} \]  
(2-10i)

where

\[ \lambda_1 = \begin{cases} 0 & \text{for } k = 1 \text{ (at top layer)}, \\
1 & \text{for } 2 \leq k \leq N, \text{ and } N \text{ is the number of layers at each segment}, 
\end{cases} \]

Chi = concentration of chlorophyll 'a' (µg l⁻¹),

G & R = growth and respiration rate of phytoplankton (day⁻¹), respectively,
P = mortality rate due to predation and other factors (day⁻¹),

K_{cchl} = settling rate of phytoplankton (cm day⁻¹),

Δz & V = layer thickness (cm) and layer volume (liter), respectively,

WChl = external loading of Chl (µg day⁻¹) including nonpoint source,

k_{gr} = optimum growth rate at 20°C (day⁻¹),

\[ \theta_1 = \text{constant for temperature adjustment of growth rate}, \]

T = temperature (°C),

L = attenuation of growth due to suboptimal lighting,

N = attenuation of growth due to nutrient limitations,

e = constant = 2.7183,

Hₘ = depth from the free surface to the top of the layer (cm),

K_c = light extinction coefficient (cm⁻¹) corrected for self-shading of plankton,

k_c = light extinction coefficient (cm⁻¹) at zero chlorophyll concentration,

K_{c, Chl} = light extinction due to self-shading of plankton (cm⁻¹ per µg l⁻¹),

I_{opt} = optimum solar radiation rate (angleys day⁻¹),

I_t = solar radiation at time t (angleys day⁻¹),

I_s = total daily solar radiation (angleys day⁻¹),

\[ t = \text{time of day (in hours)}, \]

t_u & t_d = times (in hours) of sunrise and sunset, respectively,
N2, N3 & P2 = concentrations (mg l\(^{-1}\)) of ammonia nitrogen, nitrite-nitrate nitrogen and inorganic phosphorus, respectively,

\(K_m\) & \(K_p\) = half-saturation concentrations (mg l\(^{-1}\)) for uptake of inorganic nitrogen and inorganic phosphorus, respectively,

\(R(20)\) & \(P(20)\) = respiration and mortality rate at 20°C (day\(^{-1}\)), respectively,

\(\theta_2\) = constant for temperature adjustment of respiration rate, and

\(\theta_3\) = constant for temperature adjustment of mortality rate.

2-2-2. Organic nitrogen

\[
S_i = -\frac{K_{n_{12}}N1}{K_{n_{12}} + N1} + a_n(R + a_pP)F_nChl
\]  
\(S_e = \frac{K_{n_{11}}}{\Delta Z} (\lambda_1N1_{k-1} - N1_k) + \frac{BenN1}{\Delta Z} \frac{B_k - \lambda_2B_{k+1}}{B_k} + \frac{WNI}{V} \)

where

\(\lambda_2 = 1\) for \(1 \leq k \leq N-1,\)

\(0\) for \(k = N\) (at bottom layer),

\(N1\) = concentration of organic nitrogen (mg l\(^{-1}\)),

\(K_{n_{12}}\) = ammonification rate of N1 to N2 (mg l\(^{-1}\) day\(^{-1}\)) = \(K_{n_{12}}(20) \cdot \theta_4^{T-20}\),

\(K_{n_{12}}(20)\) = ammonification rate at 20°C,

\(\theta_4\) = constant for temperature adjustment of ammonification rate,

\(K_{n_{11}}\) = half-saturation concentration for ammonification (mg l\(^{-1}\)),

\(a_n\) = ratio of nitrogen to chlorophyll in phytoplankton (mg N per \(\mu g\) Chl),

\(a_p\) = fraction of consumed phytoplankton recycled by zooplankton,

\(K_{n_{11}}\) = settling rate of N1 (cm day\(^{-1}\)),

\(F_n\) = fraction of metabolically produced nitrogen recycled to the organic pool,

\(BenN1\) = benthic flux of N1 (g m\(^{-2}\) day\(^{-1}\)), and
WN1 = external loading of N1 (mg day\(^{-1}\)) including point and nonpoint sources.

### 2-2-3. Ammonia nitrogen

\[
\frac{S_i}{K_{h2} + N2} = \frac{N1}{K_{h1} + N1} + \frac{K_{ni} N1}{K_{h1} + N1} + a_n (R + a_P (1 - F) Chl) - a_n G \cdot PR \cdot Chl \quad (2-12a)
\]

\[
S_e = \frac{\text{BenN2} B_k - \lambda_2 B_{k+1}}{\Delta z} + \frac{WN2}{V} \quad (2-12b)
\]

\[
PR = \frac{N2 N3}{(K_{mn} + N2) (K_{mn} + N3)} + \frac{N2 K_{mn}}{(N2 + N3) (K_{mn} + N3)} \quad (2-12c)
\]

where

- \(K_{n23}\) = nitrification rate of N2 to N3 (mg l\(^{-1}\) day\(^{-1}\)) = \(K_{n23}(20) \cdot \theta_5^{T-20}\),
- \(K_{n23}(20)\) = nitrification rate at 20°C,
- \(\theta_5\) = constant for temperature adjustment of nitrification rate,
- \(K_{n23}\) = half-saturation concentration for nitrification (mg l\(^{-1}\)),
- \(K_{n1}\) = half-saturation concentration for oxygen limitation of nitrification (mg l\(^{-1}\)),
- \(PR\) = preference of phytoplankton for N2 uptake,
- \(\text{BenN2}\) = benthic flux of N2 (g m\(^{-2}\) day\(^{-1}\)), and
- \(WN2\) = external loading of N2 (mg day\(^{-1}\)) including point and nonpoint sources.

### 2-2-4. Nitrite-nitrate nitrogen

\[
\frac{S_i}{K_{h3} + N2} = \frac{N2}{K_{h1} + N1} + \frac{K_{ni} N1}{K_{h1} + N1} + a_n G (1 - PR) Chl \quad (2-13a)
\]

\[
S_e = -K_{h3} + DO \frac{N3}{K_{h3} + DO} + \frac{\text{BenN3} B_k - \lambda_2 B_{k+1}}{\Delta z} + \frac{WN3}{V} \quad (2-13b)
\]

where

- \(K_{n33}\) = denitrification rate (day\(^{-1}\)) = \(K_{n33}(20) \cdot \theta_6^{T-20}\),
- \(K_{n33}(20)\) = denitrification rate at 20°C,
- \(\theta_6\) = constant for temperature adjustment of denitrification rate,
$K_{h33} =$ half-saturation concentration for denitrification (mg l$^{-1}$),

$BenN3 =$ benthic flux of N3 (g m$^{-2}$ day$^{-1}$), and

$WN3 =$ external loading of N3 (mg day$^{-1}$) including point and nonpoint sources.

2-2-5. Organic phosphorus

\[
S_i = -\frac{K_{p12} P_1}{K_{hp12} + P_1} + a_p (R + a_P) F_p \text{Chl} \\
S_e = \frac{K_{p11}}{\Delta z} (\lambda_1 P_{1_k-1} - P_{1_k}) + \frac{BenP1}{\Delta z} \frac{B_k - \lambda_2 B_{k+1}}{B_k} + \frac{WP1}{V}
\]

where

$P_1 =$ concentration of organic phosphorus (mg l$^{-1}$),

$K_{p12} =$ mineralization rate of P1 to P2 (mg l$^{-1}$ day$^{-1}$) = $K_{p12}(20) \cdot \theta_p^{T-20}$,

$K_{hp12} =$ half-saturation concentration for mineralization (mg l$^{-1}$),

$a_p =$ ratio of phosphorus to chlorophyll in phytoplankton (mg P per µg Chl),

$K_{p11} =$ settling rate of P1 (cm day$^{-1}$),

$F_p =$ fraction of metabolically produced phosphorus recycled to the organic pool,

$BenP1 =$ benthic flux of P1 (g m$^{-2}$ day$^{-1}$), and

$WP1 =$ external loading of P1 (mg day$^{-1}$) including point and nonpoint sources.

2-2-6. Inorganic (or ortho) phosphorus

\[
S_i = \frac{K_{p12} P_1}{K_{hp12} + P_1} + a_p (R + a_P)(1 - F_p) \text{Chl} - a_p G \cdot \text{Chl} \\
S_e = \frac{K_{p22}}{\Delta z} (\lambda_1 P_{2_k-1} - P_{2_k}) + \frac{BenP2}{\Delta z} \frac{B_k - \lambda_2 B_{k+1}}{B_k} + \frac{WP2}{V}
\]

where
\[ K_{p2} = \text{settling rate of P2 (cm day}^-1), \]
\[ \text{BenP2} = \text{benthic flux of P2 (g m}^-2\text{ day}^-1), \] and
\[ \text{WP2} = \text{external loading of P2 (mg day}^-1) \text{ including point and nonpoint sources.} \]

2-2-7. Carbonaceous biochemical oxygen demand

\[
S_i = -K_c \text{CBOD} + a_c a_{co} (a_r P) \text{Chl} \tag{2-16a}
\]
\[
S_e = \frac{K_{BOD}}{\Delta z} (\lambda_1 \text{CBOD}_{t-1} - \text{CBOD}_t) + \frac{SOD}{K_{DO} + DO} \frac{B_k - \lambda_2 B_{k+1}}{B_k} + \frac{WBOD}{V} \tag{2-16b}
\]

where

CBOD = concentration of carbonaceous biochemical oxygen demand (mg l\(^{-1}\)),

\[ K_c = \text{first-order decay rate of CBOD (day}^-1) = K_c(20) \cdot \theta_8 \cdot 20, \]

\[ K_c(20) = \text{CBOD decay rate at 20°C}, \]

\[ \theta_8 = \text{constant for temperature adjustment of CBOD decay rate}, \]

\[ a_c = \text{ratio of carbon to chlorophyll in phytoplankton (mg C per µg Chl)}, \]

\[ a_{co} = \text{ratio of oxygen demand to organic carbon recycled} = 2.67, \]

\[ K_{BOD} = \text{settling rate of CBOD (cm day}^-1), \]

SOD = sediment oxygen demand (g m\(^{-2}\) day\(^{-1}\)),

\[ K_{DO} = \text{half-saturation concentration for benthic flux of CBOD}, \]

\[ WBOD = \text{external loading of CBOD (mg day}^-1) \text{ including point and nonpoint sources.} \]

2-2-8. Dissolved oxygen

\[
S_i = -K_c \text{CBOD} - a_{no} \frac{K_{h23} N2}{K_{h23} + N2 K_{nit} + DO} \frac{DO}{DO} + a_c a_{co} (PQ \cdot G - \frac{R}{RQ}) \text{Chl} \tag{2-17a}
\]
\[
S_e = (1 - \lambda_1) K_r (\text{DO}_z - \text{DO}) - \frac{SOD}{\Delta z} \frac{DO}{K_{DO} + DO} \frac{B_k - \lambda_2 B_{k+1}}{B_k} + \frac{WDO}{V} \tag{2-17b}
\]
\[ K_r(20) = \left( K_r \frac{u_{eq}}{h_{eq}} + W_{rea} \right) \frac{1}{\Delta z} \]  

\[ W_{rea} = 72.8 U_w^{0.6} - 31.7 U_w + 3.72 U_w^2 \]  

\[ K_r = K_r(20) \cdot \theta_s^{T-20} \]  

\[ DO_s = 0.146244 \cdot 10^2 - 0.367134 T + 0.4497 \cdot 10^{-2} T^2 \]  

\[- (0.966 \cdot 10^{-1} - 0.205 \cdot 10^{-2} T - 0.2739 \cdot 10^{-3} S) S \]  

Where

\[ DO = \text{concentration of dissolved oxygen (mg l}^{-1}), \]
\[ a_{no} = \text{ratio of oxygen consumed per unit of ammonia nitrogen nitrified} = 4.57, \]
\[ PQ = \text{photosynthesis quotient (moles O}_2 \text{ per mole C)}, \]
\[ RQ = \text{respiration quotient (moles CO}_2 \text{ per mole O}_2), \]
\[ K_r = \text{reaeration rate (day}^{-1}), \]
\[ K_r(20) = \text{reaeration rate at 20°C (day}^{-1}), \]
\[ DO_s = \text{saturated DO concentration (mg l}^{-1}), \]
\[ WDO = \text{external loading of DO (mg day}^{-1}) \text{ including point and nonpoint sources}, \]
\[ K_r = \text{proportionality constant} = 393.3 \text{ in CGS unit}, \]
\[ u_{eq} = \text{weighted velocity over cross-section} = \Sigma(u_k B_k h_k) / \Sigma(B_k h_k), \]
\[ h_{eq} = \text{weighted depth over cross-section} = \Sigma(B_k h_k) / B_s, \]
\[ B_s = \text{width at the free surface}, \]
\[ W_{rea} = \text{wind-induced reaeration (cm day}^{-1}), \]
\[ U_w = \text{wind speed (in m sec}^{-1}) \text{ at the height of 10 m above surface, and} \]
\[ \theta_s = \text{constant for temperature adjustment of DO reaeration rate}. \]
Figure 2-1. Schematic diagram of interacting water quality parameters.
III. DESCRIPTION OF THE STUDY AREA, THE TIDAL RAPPAHANNOCK RIVER IN VIRGINIA

The hydrodynamic and water quality models were applied to the tidal portion of the Rappahannock River, Virginia to simulate the conditions in the summers of 1987 and 1990. This chapter describes the characteristics, both hydrodynamic and water quality, of the study area.

3-1. Hydrodynamic Characteristics

The Rappahannock River, one of the western shore tributaries of Chesapeake Bay, is located between the Potomac and York rivers. Figure 3-1 shows the map of the tidal Rappahannock River with sampling locations and geographic features mentioned in the text, and Fig. 3-2 shows the longitudinal bathymetry, both field survey data and model input. From the mouth at Windmill Point (km 0) to the fall line at Fredericksburg (km 172), the tidal river extends in a generally northwest direction (Division of Water Resources 1970). Being relatively narrow and straight, the river is suitable for the laterally integrated two-dimensional model.

The drainage area above the fall line gauging station is 4,132 km² (USGS 1992). Over the 85 years between 1907 and 1991, the discharge ranged from 0.14 to 3,964 m³ sec⁻¹ (ems) with a mean of 46.8 cms. The annual mean discharges were 39.8 and 46.2 cms for the water years 1987 and 1990 respectively (USGS 1988 and 1991).

The tidal wave takes about 9 hours to propagate from the river mouth to the fall line, the principal tidal component being the lunar semi-diurnal tide with a period of 12.42 hours. The mean tidal range increases from 37 cm near the mouth to 55 cm between Bowlers Wharf (km 52) and Wares Wharf (km 58), then decreases slightly to 46 cm at Leedstown (km 95), and increases again to 85 cm at Fredericksburg (National
The lower portion of the tidal Rappahannock River, like other western shore tributaries of Chesapeake Bay, is a partially mixed estuary. Net water movement follows a two-layered gravitational circulation, in which the longitudinal density (salinity) gradient pushes the saltier bay water upriver along the bottom and gravity moves the fresher surface water downriver.

The mixing of fresh and salt water, primarily caused by the action of tides and winds, occurs over a broad transition zone. The upper extent of salt water intrusion varies in response to the freshwater flow. Since 1971, the Virginia Institute of Marine Science (VIMS) has been conducting slackwater surveys in three major estuaries in Virginia (James, York and Rappahannock rivers). The salinity, temperature and DO data for the tidal Rappahannock River between 1970 and 1980 can be found in Brooks (1983). The salinity data in the Rappahannock River show that the salt water generally intrudes to around km 120 (near Nanzatico Bay) during low flow and around km 70 (near Tappahannock) during high flow. Conditions range from well mixed to strongly stratified, depending upon the tide and wind energy available for mixing as well as amount of freshwater discharge, in the region from the mouth to km 42 (near Tarpley Point) where the water depth ranges from 15 to 20 m. The water in the shallow reach between km 48 (near Sharps) and km 80 (near Blandfield Point) is usually well mixed, which suggests that the shallow depth (6 to 8 m) makes the region more susceptible to tidal as well as wind mixing. The sloping bottom between km 42-48 connects the deeper, lower part to the shallower, upper part of the river (Fig. 3-2).

Since the estuary empties into Chesapeake Bay, salinity in the estuary is moderated by distance from the ocean and the effect of freshwater flow from other tributaries to the bay, especially the Susquehanna River. A large portion of the estuary and its tidal tributaries is favorable for growing oysters since salinity is high enough to allow oysters
to grow, but low enough to discourage the most serious predators and diseases such as oyster drills and MSX (Kuo et al. 1975).

3-2. Water Quality Characteristics

The tidal portion of the Rappahannock River has three distinct sections, each of which exhibits characteristic water quality conditions (Figures 3-1 and 3-2); the lower (between the mouth and km 50), the middle (between km 80 and km 145) and the upper (between km 155 and the fall line) reaches. The 20 km reach immediately downriver of the fall line and the deep water in the lower part of the river have been identified as critical regions for DO (Kuo et al. 1975).

The upper 60 km of the tidal portion of the river, being very narrow, shallow and straight, is suitable for sectionally integrated one-dimensional model. There are four sewage treatment plants discharging waste water to the upper portion of this reach of the river. A prior modeling study has shown that both point and nonpoint source loadings have significant impacts on water quality there, and the relative importance of the two sources depends on the magnitude of the river discharge (Kuo et al. 1991b).

The lower portion of the Rappahannock River between the river mouth and km 50 is characterized by persistent hypoxic conditions in the bottom water during the summer. Kuo & Neilson (1987) made a qualitative investigation of the bottom DO in the three Virginia estuaries. They reported that hypoxia has been observed most frequently in the deep water of the Rappahannock River, but it occurs rarely in the James River though it receives the heaviest wastewater loadings among three estuaries. This difference has been attributed in part to the relatively strong gravitational circulation in the James River. Due to these circulation differences, the impact of increased urbanization may be more severe in the Rappahannock River than it has been in the James River.

Development of the Rappahannock River, therefore, should be preceded by a better
understanding of the water quality processes there.

The temporal and spatial variability of hypoxia in the lower portion of the Rappahannock River was studied by Kuo et al. (1991a). They observed a periodic reoxygenation of bottom water that was closely related to spring tide mixing. The destratification-stratification cycles caused by spring-neap tidal cycles has been documented in the Rappahannock Estuary as well as other Virginia estuaries (Haas 1977; D’Elia et al. 1981; Ruzecki & Evans 1986). A characteristic longitudinal pattern of bottom water DO also was observed. The bottom DO concentration decreased upriver from the river mouth, reaching a minimum at approximately km 42, upriver of the deepest point of the river, and then increasing as the water became shallower further upriver. A model for the bottom water DO concentration was formulated based on a simple DO budget consisting of only one source term (vertical mixing) and one sink term (including both benthic and water column oxygen demand), using a Lagrangian concept (Kuo et al. 1991a). Although this diagnostic study enabled them to investigate cause-effect relationships, the predictive application of the model was not always satisfactory due to the lack of complete information for input parameters, vertical mixing and oxygen demand. Spatially and temporally varying values for input parameters were required to improve the predictive capability of the model, which served as one impetus of the present study.

Another common feature shared by western shore tributaries of Chesapeake Bay is the presence of a sill at the river mouth, which restricts water exchange with the bay. The sill at the mouth of the Rappahannock River plays an important role in the estuary-subestuary exchange. Using the field data near the river mouth, Kuo & Park (1992) calculated that the mass exchange due to the tidal component was at least an order of magnitude smaller than that resulting from the subtidal component. The presence of the sill, the shoreline configuration and the pycnocline oscillation due to the winds combined
to affect the quality of incoming bay water along the bottom at the mouth.

The mid-reach of the river between km 80-145 is bounded by shallow regions at the up- and down-river boundaries (Fig. 3-2). The upper limit of salt intrusion, which moves up and down the river in response to the freshwater discharge, is located approximately at km 80. Just upriver of the limit of salt intrusion, there is a chlorophyll maximum (Anderson 1986). He suggested the hydrodynamic trapping of phytoplankton biomass in the region of the turbidity maximum, rapid internal cycling of essential nutrients such as silica, demise of freshwater phytoplankton during transport to the saline part of the river, and light limitation in the oligohaline reach of the river as controlling factors. These high phytoplankton concentrations in the tidal freshwater and low salinity transition regions of estuaries have been observed frequently in many other estuarine environments (Haertel et al. 1969; Lippson et al. 1979; Cloern et al. 1983; Pennock 1985; Relexans et al. 1988; Schuchardt & Schirmer 1991). Key mechanisms suggested by these investigators are river discharge, water residence time, solar radiation and nutrients. A part of the present study is to investigate the controlling mechanism(s) for the high chlorophyll concentration in the mid-part of the Rappahannock River, which is described in Section 6-2.
Figure 3-1. The tidal Rappahannock River in Virginia with sampling locations and geographic features mentioned in the text.
Hypoxic region (I-I)
High chlorophyll region (II-II)
STP dominant region (III-III)

Figure 3-2. Longitudinal bathymetry of the tidal Rappahannock River: solid line is the field survey data and dashed line is the model input.
IV. APPLICATION OF THE HYDRODYNAMIC MODEL

The steps in the application of the hydrodynamic model to the Rappahannock River are discussed in this chapter. First, the geometry was specified and the data files prepared (Section 4-1). Second, the model was calibrated such that it reproduced the tidal characteristics of the prototype. This calibration of the barotropic mode of the flow was achieved by adjusting Manning’s friction coefficient (Section 4-2). Third, the constants in the turbulent mixing terms, both viscous and diffusive, were adjusted such that the model reproduced the salinity structure (Section 4-3). Finally, the model’s ability to predict the surface elevation, current velocity and salinity distribution was verified through comparison of model predictions and field measurements of these parameters (Section 4-4).

The field data used for the above procedures were collected in 1987 and 1990 by VIMS. The full description of field measurements can be found in Kuo & Moustafa (1989) and Kuo et al. (1991b), respectively, for the 1987 and 1990 surveys; the station locations are shown in Fig. 3-1.

4-1. Geometrical Data

The hydrodynamic model was supplied with data describing the geometry of the tidal Rappahannock River. The geometry in the vertical two-dimensional model is represented by the width at each depth at the center of each grid cell. A bathymetric survey in 1973 made by the U.S. Army Corps of Engineers collected 102 bottom profiles along the tidal portion of the river (Kuo et al. 1975). These profiles were used to schematize the river with $\Delta x = 2.5$ km and $\Delta z = 2$ m. The river was divided into 71 segments with up to 10 layers vertically (Figures 3-2 and 4-1). The geometric data used in the model are listed in Table 4-1. The side storage area was defined to include
shallow (< 2 m) regions and tributaries (Fig. 4-1). The surface area of the side storage area was taken from nautical charts (National Ocean Survey). The center of the most downriver segment is located 1.1 km upriver from the river mouth. A time step increment (Δt) of 108 seconds, which guaranteed stability, was used for all the model runs.

4-2. Mean Tide Calibration

Manning’s friction coefficient, which is virtually the only calibration parameter affecting the calculation of surface elevation, was adjusted by simulating the equilibrium-state conditions. Freshwater inflow equal to the long-term mean at the fall line (46.8 cms), and a simple sinusoidal (M2) tide with an amplitude equal to the mean at the river mouth (18.3 cm) were used to force the hydrodynamic model. The initial condition was a level surface at mean-sea level. The longitudinal velocity was initially set to be vertically uniform and equal to the mean velocity, i.e., the freshwater discharge divided by cross-sectional area. The vertical velocity was initially zero. The effect of salt on the mean tidal range was negligible. Constant density (zero salinity everywhere) and variable density model simulations produced no practical difference in the mean tidal range. Mean conditions, that were obtained by running the model for a long time with constant boundary conditions, were used for the boundary and initial conditions for salinity. The model required 12 tidal cycles to reach an equilibrium state, i.e., the surface elevation and velocity throughout the estuary repeated from tidal cycle to tidal cycle.

The model results during the last tidal cycle were compared with predicted mean tide characteristics in Tide Tables (National Ocean Survey 1989). Manning’s coefficient was adjusted, within the commonly accepted range, until the model calculation of tidal range agreed with that from the Tide Tables. The times of high and low tides were then
used to fine tune the coefficient (Fig. 4-2). The calibrated model has a Manning’s friction coefficient of 0.018 between km 0-126, and 0.021 upriver of km 126.

Figure 4-2 shows the standing wave characteristics, which result from superposition of two progressive waves traveling in opposite directions. The phase difference between the outgoing reflected wave and the incident wave creates a nodal point of minimum tidal range at a distance of one quarter wave length from the head of the tidal river (near Leedstown). The model could reproduce this feature very well. As the tidal wave propagates upriver from the river mouth, the tidal range increases to a local maximum at km 58 (Wares Wharf), and then decreases to a local minimum around km 90 (near Leedstown). The maximum tidal range occurs near the head of the tidal river (Fredericksburg).

In the above mean tide calibration, Manning’s friction coefficient was not calibrated for the tidal current velocity because of the lack of velocity data at equilibrium state. However, since the model can reproduce the range and times of mean tide very well, as shown in Fig. 4-2, it also should be able to reproduce the transport well in order to maintain continuity relationship if the geometry used is correct. The model’s ability to reproduce the current velocity is verified in Section 4-4-1.

4-3. Calibration of Turbulent Mixing Terms

The constants ($\alpha$, $\beta$ and $\alpha_w$) in the expressions for the turbulent mixing coefficients (Equations 2-7 and 2-8) were calibrated with a simulation of salinity distributions from July 28 to August 24, 1987. Three time-varying boundary conditions, freshwater inflow through the upstream boundary and tide and salinity at the mouth, were specified for the model. The upstream boundary condition was specified with daily freshwater discharge measured at the Fredericksburg gauging station (USGS 1988). The model updated the freshwater discharge by linear interpolation over a 2 hour period from 0000 to 0200
hours, and then held it constant for the remaining 22 hours. Hourly tidal elevation measured at the mouth was used for the downstream boundary condition. The model linearly interpolated the hourly data to obtain the boundary conditions every time step. Four slackwater surveys at slack before ebb (SBE) flow were conducted on July 28 and August 4, 10 and 24. The salinity measurements at the mouth were linearly interpolated in time and used for the boundary condition.

To allow a "warming-up" time for the surface elevation and velocity, the model simulation started on July 23. The measured salinity distribution on July 28 was then inserted into the model to specify the initial condition. The constants in the turbulent mixing coefficients were evaluated by comparison of subsequent survey data and model results. The calibrated constants are $\alpha = 1.15 \times 10^2$, $\beta = 0.25$ and $A_x = K_x = 5 \times 10^5$ cm$^2$ sec$^{-1}$. The resulting salinity distributions are presented as plots of isohalines in a vertical plane containing the river axis in Figures 4-3 through 4-5. Only the salinity distributions between the river mouth and km 60 are presented in the figures because the most upriver station in the 1987 surveys was located at km 57.79. The tidally averaged values of $A_x$ on August 10 ranged from 0.46 to 26 cm$^2$ sec$^{-1}$ with the spatial mean of 6.5 cm$^2$ sec$^{-1}$. Those of $K_x$ ranged from 0.12 to 23 cm$^2$ sec$^{-1}$ with the spatial mean of 5.0 cm$^2$ sec$^{-1}$.

Two physical processes are involved in the mass transport, advection and turbulent diffusion. The advective mass transport is affected by the current velocity, which is determined by two modes of the flow, barotropic and baroclinic. The barotropic flow that is forced by the surface slope has been calibrated in the previous section (mean-tide calibration). The baroclinic flow that is driven by the density (salinity) structure is calibrated in this section through the adjustment of the momentum exchange coefficients ($A_x$ and $A_y$). They, in principle, should be calibrated by comparing the model results with the field measurements of current velocity. They, in practice, are usually calibrated.
with measurements of the salinity distribution because of the non-availability of velocity
data and the insensitivity of the velocity predictions to $A_x$ and $A_z$. Calibration of the
turbulent mixing coefficients, therefore, accounts for both the baroclinic mode of flow
and the turbulent diffusive mass transport.

The agreement in the location of the isohalines between the model results and field
measurements reflects that the model accurately simulated advective processes. The
agreement is more than satisfactory for August 10 (Fig. 4-4) and 24 (Fig. 4-5). The
model prediction of the salinity on August 4 (Fig. 4-3), however, is about 1 ppt higher,
over the region of salt intrusion, than the field measurement.

The diffusive mass transport is a measure of the turbulent exchange of mass. In
partially mixed estuaries, the horizontal advective transport of salt is balanced by the
vertical diffusive transport, which determines the stratification in the water column. For
discussion of the salinity structure in the Rappahannock River, the saline part of the river
is divided into three parts; the lower between km 0-42, the upper between km 48-80,
and the transitional between km 42-48.

4-3-1. Comparison of salinity distributions

In the lower part of the river (between km 0-42), the water depth ranges from 15
to 20 m (Fig. 3-2). Here, a well mixed condition was observed on August 10 (Fig. 4-4)
and 24 (Fig. 4-5), and a moderately stratified condition was observed on August 4 (Fig.
4-3). During this period, the successive spring tides alternated in strength between
strong and weak spring tides (Kuo et al. 1991a). Tidal mixing during the strong spring
tide, which occurs at roughly monthly intervals, caused the well mixed situation on
August 10 (Fig. 4-4). The neap tide on August 4 (Fig. 4-3) resulted in a more stratified
situation. The measurements taken at weak spring tide on August 24 (Fig. 4-5) show a
more mixed situation than August 4 between km 0-42. These features were very well
reproduced by the model (Figures 4-3 through 4-5).

Slackwater surveys in 1987, as well as those from other years (Brooks 1983), have shown that the water in the shallow reach between km 48-80 (Fig. 3-2) is often well mixed. This feature was not well reproduced by the model, especially for August 4 and 10. This discrepancy may be attributable to the shallow depth (6 to 8 m) and wind mixing. Wind data from the Norfolk airport, located 65 km to the south of the Rappahannock River mouth, were examined. Strong winds with peak gust speeds of 36 mph blew from the south-west on August 3; 26 mph winds blew from the south on August 9.

The effect of wind mixing was included in the simulation through the second term in Equations 2-7 and 2-8. The height, period and length of the wind-induced waves were evaluated using the Sverdrup-Munk-Bretschneider forecasting curves for deep water waves (U.S. Army Coastal Engineering Research Center 1973) and updated each day. The estimated wave lengths for the wind speeds of 26 and 36 mph indicate that the wind-induced waves are deep water waves. The salinity predictions that included wind mixing are shown in Figures 4-3 through 4-5 as dashed contours; the constant for wind mixing ($\alpha_w$) was calibrated to be $5 \times 10^{-3}$. The inclusion of wind mixing improves the agreement between the model predictions and field measurements, particularly over the top 6 to 7 meters of the water column. The inclusion of wind mixing in the model caused a more conspicuous change in salinity distribution on August 4 than on August 10; this occurred because the weaker tidal mixing due to neap tide on August 4 left more room for the wind mixing, and also because of the stronger winds on August 3 than on August 9. Since the wind was weak on August 23 and 24, no wind was included in model simulation for that period, and thus the change in the salinity distribution by including wind mixing was least on August 24 (Fig. 4-5).
4-3-2. Characteristic salinity distribution - negative, longitudinal salinity gradient

A conspicuous characteristic salinity distribution was often observed in the Rappahannock Estuary. Field measurements on August 4 (Fig. 4-3) and 24 (Fig. 4-5) showed a negative, longitudinal salinity gradient for some reaches of the river. The negative salinity gradient, which was quite distinct between km 40-50 on August 24, might be attributable to the bottom topography of the river (Fig. 3-2). The saline bay water, that enters the river through the mouth and moves upriver along the bottom, might be deflected upward in the presence of obstacles such as the sloping bottom, thereby reversing the longitudinal salinity gradient.

A model run with an ideal geometry (constant depth, and width varying in the vertical but not in the longitudinal direction) while keeping all other conditions the same, showed the absence of horizontal reversal in salinity gradient. Another model run with increased $K_z$ and real geometry showed that the increased vertical mixing could erase the reverse salinity gradient. These sensitivity model runs imply that the reverse salinity gradient can be expected to occur frequently in the Rappahannock Estuary, which has upriver-sloping bottom geometry, but that it may be erased by strong mixing associated with spring tides and/or strong winds.

This hypothesis is supported by the salinity data from 55 slackwater surveys for the Rappahannock River conducted by VIMS between 1981 and 1990. No reverse gradient was observed for 18 surveys characterized by strong spring tides. The data from the other 37 surveys showed the presence of the reverse salinity gradient. For 33 of these 37 surveys, the measurements were taken either at neap or at weak spring tides without strong winds. The remaining 4 surveys were conducted at strong spring tides with or without strong winds, so the presence of the reverse gradient in the latter 4 surveys might be due either to the insufficient mixing and/or to the salinity of the incoming water from the bay.
4-4. Model Verification

4-4-1. Surface elevation and longitudinal velocity in 1987

For the verification of the model with respect to surface elevation and horizontal velocity, a model simulation was conducted covering the period during which field measurements were taken in the summer of 1987. The same conditions described in Section 4-3 were used. Model predictions are compared with surface elevation measurements at Urbanna (Fig. 4-6) and Tappahannock (Fig. 4-7). To show the subtidal variations in surface elevation, both time series were subjected to a low-pass filter with a cut-off frequency of \((48 \text{ hr})^{-1}\), a modification of the low-pass filter designed by Groves (Thompson 1983). The filtered series that are considered as subtidal components are presented in Fig. 4-8. The excellent agreement demonstrates the model’s ability to reproduce the surface elevation in the prototype including both the semi-diurnal tidal fluctuations (Figures 4-6 and 4-7) and the subtidal (longer-term) variations (Fig. 4-8).

Figures 4-9 through 4-13 illustrate the comparisons of model predictions of horizontal velocity with current meter data taken at the river mouth and at km 16.6. The model can reproduce the velocity measurements at the mouth very accurately, at depths of 1.2 m (Fig. 4-9) and 9.7 m (Fig. 4-10). Considering that the model calculates the lateral average velocity while the current meter data are point measurements, the model predictions of velocity here are more than satisfactory. The field measurements at depths of 1.2 m (Fig. 4-11) and 10.0 m (Fig. 4-12) at km 16.6 are again well reproduced by the model. Near the bottom (18.7 m deep) at km 16.6, the model prediction is generally less than field data (Fig. 4-13). The current meter there (S4#747) showed some technical problems while deployed. The clock in the meter, that was set to record variables every 30 minutes, shifted slightly giving irregularly recorded signals. Examination of the data from S4#747 and S4#749 (10.0 m deep at the same location) indicates that there is no appreciable decrease in velocity with increasing depth from...
mid-depth toward the bottom. Considering this and the excellent model-field agreements elsewhere, the quality of the field data from S4#747 might be the cause of the discrepancy.

The current velocity in estuaries may be decomposed into two components, tidal and residual. The dominant residual velocity is characterized by the upriver movement of more saline water in the lower layer and the downriver movement of fresher water in the upper layer. Since the mass flux due to the residual component can be very important in the Rappahannock River (Kuo & Park 1992), the model’s ability to reproduce the average residual current correctly is essential.

A. Residual circulation: To eliminate the diurnal and semi-diurnal tidal constituents and fluctuations of higher frequencies, the velocity time series data were subjected to a low-pass filter with a cut-off frequency of (48 hr)^{-1}. The filtered series of predictions and measurements are presented in Figures 4-14b through 4-14f. The predicted residual currents (long dashed lines in Fig. 4-14) show the gravitational circulation with the downriver movement in the surface layer and the upriver movement in the bottom layer. Although the measured residual currents generally follow this pattern, they do show some variations with a dominant time scale of 4-to-6 days. This variability was attributed to local meteorological forcing and its effect on the salinity structure in the bay near the river mouth (Kuo & Park 1992). The wind affects the velocity field in the lower portion of the river both by transferring momentum through the surface and by changing the conditions in the bay. The momentum input from wind stress can be included in model calculations using a quadratic stress law (see Eq. 2-7 in Park & Kuo 1993). The model results (solid lines in Figures 4-8 and 4-14) using daily average wind speed and resultant wind direction from the Norfolk airport in Virginia show that inclusion of wind stress considerably improves the model-field agreement. The predicted residual currents with wind stress have the 4-to-6 day variations but they are not as large
as those in field measurements. This difference seems to be due to the bay conditions that are changed by wind events but have not been properly incorporated into model calculation.

Kuo & Park (1992) also analyzed the 1987 field data used in this study and showed that the density-driven current near the bottom at the river mouth was enhanced by the wind-driven circulation in the bay during periods of strong wind from the southwest quadrant. The time series plot of surface elevation at the river mouth (Fig. 4-14a) shows that the wind drove surface water out of the river, and thus lowered the surface elevation and caused a set-up in the bay that drove the bay water into the river along the bottom. This surface set-up in the bay favored the transport of the high salinity water into the river from the deep portion of the bay as a result of tilting of the pycnocline in the bay, and shoreline and bathymetric configurations around the bay-subestuary junction (Kuo & Park 1992). The present model simulates the processes occurring in the subestuary (Rappahannock Estuary) but not those occurring in the bay, such as surface set-up and tilting of the pycnocline. The model incorporates the effects of the bay conditions only through the downstream boundary conditions and thus needs detailed boundary conditions for surface elevation, current velocity and salinity to reproduce the effects of the processes occurring in the bay. Hourly measurements (Fig. 4-14a), which show the surface set-up at the mouth, were used for boundary conditions for surface elevation. In the present model, however, the downstream boundary conditions for velocity were estimated using the extrapolated values (see Section 2-2-4 in Park & Kuo 1993). This treatment is a reasonable method due to the lack of detailed current measurements in most of modeling efforts, but it cannot adequately reflect the processes such as the enhanced circulation due to the wind-driven surface set-up outside of the mouth. Furthermore, the Rappahannock model recognizes the effect of the transport of the high salinity water from the deep portion of the bay (as a result of pycnocline tilting
in the bay and geometric configurations around the bay-subestuary junction) only through the downstream boundary conditions for salinity. In the 1987 model simulation, the time-varying boundary conditions were constructed using the slackwater surveys conducted on July 28 and August 4, 10 and 24 (Section 4-3). This weekly-to-biweekly sampling cannot adequately reflect the conditions in the bay that vary in the time scale of 4-to-6 days. Therefore, the difference between the predicted residual currents with wind stress and field data may be attributable to the downstream boundary conditions. Accurate and detailed downstream boundary conditions for velocity and salinity are necessary to resolve the 4-to-6 day variations in the predicted residual currents. At the bottom of km 16.6, as mentioned earlier, the quality of the field data from S4#747 might be responsible, at least in part, for the variations in Fig. 4-14e.

The predicted residual velocities averaged over 58 tidal cycles (i.e., 2 spring-neap cycles) are presented as a vector plot in Fig. 4-15, in which every other point is omitted to enhance readability. The arrow length represents the magnitude and the arrow head indicates the direction of residual velocity no matter how small the magnitude is. The limit of salt intrusion, represented by the 1 ppt isohaline, also is included. In Fig. 4-15, the null point where the level of no-net-motion (LNNM) meets the estuary bottom, is located at the limit of salt intrusion (around km 95). Near the surface above LNNM, the seaward flowing velocity increases in a downriver direction despite the enlargement of the river cross-section in that direction. This augmented residual current is derived from the landward intrusion of bay water near the bottom below LNNM, which increases the flushing capacity of an estuary by an order of magnitude (Kuo et al. 1978). In the estuarine portion of the river, the maximum upriver velocity is -5.0 cm sec\(^{-1}\) in the lower layer, and the maximum downriver velocity is 3.9 cm sec\(^{-1}\) in the upper layer. Negative velocity indicates that the water flows in the upriver direction. This residual current is far smaller than the tidal current. The residual current can be decomposed into two
parts; baroclinic part due to the longitudinal density gradient and barotropic part due to the freshwater discharge. In the Rappahannock River, the baroclinic flow is small compared to the barotropic flow that includes both the tidal current and the freshwater-induced residual current.

B. Limit of gravitational circulation versus limit of salt intrusion: A model simulation using constant boundary conditions was performed to examine the response of residual velocity to the spring-neap cycle. A freshwater discharge of 10.0 cms at the fall line and a harmonic tide with M2 (17.2 cm) and S2 (2.53 cm) components at the mouth were used to force the model. A constant salinity profile at the mouth (18 and 20 ppt at the surface and bottom, respectively, with linear variation in the vertical) was used for the boundary condition. The average residual velocities over 2 spring-neap cycles are presented in Fig. 4-16. In the saline part of the river, the maximum residual velocities are -3.9 and 2.4 cm sec⁻¹ in the lower and upper layers, respectively. The null point is again located at the limit of salt intrusion. Figures 4-17 and 4-18 present the average residual velocities during spring and neap tides, respectively. The spring tide (Fig. 4-17) provides more mixing energy, and thus has weaker residual circulation than the neap tide (Fig. 4-18). In the saline part of the river, the maximum velocities in the lower and upper layers are -3.8 and 2.3 cm sec⁻¹, respectively, during spring tide and -4.2 and 2.8 cm sec⁻¹, respectively, during neap tide.

To study how the residual velocity responds to the freshwater discharge, another model simulation was conducted using the 1987 annual mean freshwater discharge of 39.8 cms (Fig. 4-19). All other conditions were kept the same as above. Figure 4-19, compared to Fig. 4-16, shows that when the increased freshwater discharge pushes the limit of salt intrusion farther downriver, the increased horizontal salinity gradient enhances the residual circulation. In the saline part of the river, the maximum bottom residual velocity is -4.6 cm sec⁻¹ and the maximum surface residual velocity is 3.3 cm
The null point also is pushed downriver, but it moves further than the limit of salt intrusion (Fig. 4-19).

The level of no-net-motion (LNNM) occurs where the longitudinal density gradient integrated over the water column above that depth (baroclinic) balances the mean surface slope due to the freshwater discharge (barotropic). The location of the null point, where LNNM meets the estuary bottom, depends upon the location of the limit of salt intrusion, the salinity gradient, geometry (total depth) and surface slope. Then, the location of null point relative to the limit of salt intrusion is a function of salinity gradient, geometry and surface slope. When the freshwater discharge increases from 10 cms (Fig. 4-16) to 39.8 cms (Fig. 4-19), the 1 ppt isohaline, which we are using as an indicator of the limit of salt intrusion, is pushed downriver to the top of the shallow region around km 80. Despite the augmented longitudinal salinity gradient, the reduced total depth makes the increase in baroclinic forcing not as large as that in barotropic forcing (surface slope). Then, the balance between baroclinic and barotropic forcing (i.e., null point) occurs downriver of the limit of salt intrusion. If the freshwater discharge is large enough to push the limit of salt intrusion downriver of the shallow region into the deep part, the null point will occur closer to the limit of salt intrusion. This is confirmed by the results from a model simulation with the freshwater discharge of 130 cms (Fig. 4-20). Therefore, the limit of salt intrusion should not be used to express, or to judge, the limit of gravitational circulation. For example, the expressions in the preceding paragraphs, "in the saline part of the river," need to be rephrased as "in the lower part of the river where the gravitational circulation exists."

4-4-2. Salinity distributions in 1990

The model’s ability to predict mass transport was verified with a simulation of salinity distributions from June 6 to August 7, 1990. Daily discharge from the fall line
gauging station (USGS 1991) and the hourly measurements of the surface elevation at the mouth were used for the upstream and downstream boundary conditions respectively. The same treatments, explained in Section 4-3, were applied to freshwater discharges and to tide measurements.

Three slackwater surveys were conducted at slack before flood (SBF) flow on June 6, July 5 and August 7. As in the calibration in Section 4-3, the salinity data at the mouth were linearly interpolated in time and used for the boundary condition. The model, however, requires the vertical salinity profile be specified at the mouth at SBE. This salinity profile at SBE was obtained by increasing the salt measurements at the mouth on three surveys until the model predictions at the mouth matched the field measurements. The model simulation started from June 4, and the measured salinity distribution on June 6 was used to specify the initial condition.

Using the same constants in the turbulent mixing coefficients used in Section 4-3 ($\alpha = 1.15 \times 10^{-2}$ and $\beta = 0.25$), the model predictions are compared with the field measurements on July 5 and August 7 in Figures 4-21 and 4-22, respectively. The boundary conditions at SBE were selected such that the model predictions at SBF matched the field observations at the mouth. Thus, the model-field agreement at the downstream boundary was forced by this method. Except at the mouth, the model predictions were generally lower by 2 to 3 ppt than the field measurements on both dates. The river contained less salt in the model predictions than in the field measurements. There are two possible explanations, the first of which is that advective mass transport in the model is too small and not able to transport enough salt upriver. The agreement, however, between the model and the field data in the model verification of current velocity was excellent in Section 4-4-1.

An alternative explanation is that the amount of salt coming into the river through the mouth may be responsible for the model-field discrepancy. That is, the lack of salt
within the river in the model might be due to the insufficient salt in the incoming water. The boundary condition, which specifies the salinity at the mouth, was evaluated by linear interpolation using the data from three slackwater surveys (June 6, July 5 and August 7) in 1990. This boundary condition might be too low for the model predictions to have as much salt as observed in the field data. This situation could happen if three surveys conducted at approximately monthly intervals would have missed event(s) of high salinity water intruding into the river. Data from the three surveys showed a monotonic increase in salinity at the mouth over the two month period. Since the intrusion of the high salinity water into the Rappahannock River has a time scale of 2 to 3 days (Kuo & Park 1992), it is highly probable that monthly sampling would miss such event(s). Thus, it was hypothesized that saltier water entered the river several days before each measurement on July 5 and August 7. Another boundary condition for salt at the mouth was constructed by assuming that the salinity at the bottom half of the water column was higher by 3 ppt on June 25 than the measurement on July 5, and by 3.5 ppt on August 2 than that on August 7. The model predictions with new boundary conditions (Fig. 4-23) show that the model-field agreement is much better than those in Figures 4-21 and 4-22.

Both July 5 and August 7 were near neap tides, and stratified conditions were observed from surface to bottom in the lower, deeper part of the river between km 0-42 (Fig. 3-2). In the shallower part of the river, upriver of km 48 to the limit of salt intrusion (around km 80), well-mixed conditions existed throughout the water column on both dates. As in the calibration, wind mixing was thought to be at least partly responsible for the observed salinity distributions. Wind data from the Norfolk airport in Virginia showed that wind with the peak gust speed of 26 mph blew from the southwest on July 4, and that with 25 mph blew from the south on August 6. The model predictions with the inclusion of the wind mixing (\(\alpha_w = 5 \times 10^{-3}\)) are also presented in
Fig. 4-23 as dashed contours. The inclusion of wind mixing improved the model-field agreement, particularly over the shallow region. The final calibrated model, therefore, includes the wind mixing.

The salinity measurements on both July 5 and August 7, 1990 show highly stratified conditions in the deeper, lower part of the river between km 0-42 and homogeneous conditions in the shallower part of the river between km 48-80 (Figures 4-21 and 4-22). The observed $\Delta s$ (vertical salinity difference between surface and bottom) around km 10 is approximately 4 and 6 ppt, respectively, on July 5 and on August 7. The observed $\Delta s$ around km 55 is approximately 1 ppt on both dates. Well-mixed conditions in the shallower part of the river between km 48-80, regardless of the conditions in the deeper, lower part of the Rappahannock River, have been frequently observed (Brooks 1983). These observations may indicate more vigorous vertical mixing in the shallower region than in the deeper region especially during sporadic wind events. Although this mechanism sounds physically reasonable in the prototype, the turbulence closure model based upon mixing length concept behaves in the different direction. In the mixing length theory, the turbulent mixing coefficients are affected by the mixing length and the velocity shear. The shape function, $Z(1-Z/h)$, in the mixing length part of Equations 2-7 and 2-8 will not allow more mixing in the shallower region. The shape function was not included in the formulation of the wind-induced mixing terms in Equations 2-7 and 2-8 to minimize this behavior. Although the model successfully described the general salinity distributions in the prototype, it could not always reproduce all the details observed. In Fig. 4-23, the verification results (dashed contours) are not as stratified as the observations between km 0-42 and at the same time not as homogeneous as the observations between km 48-80. The predicted $\Delta s$ around km 10 is approximately 3 and 4 ppt, respectively, on July 5 and August 7. Around km 55, the predicted $\Delta s$ is approximately 2 and 2.5 ppt, respectively, on July 5 and August
7. The model's predictive capability and thus applicability to other systems could be significantly improved with more understanding of the turbulent mixing processes.
Table 4-1. Geometric data for the model grid cells.

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* In the model, \( \Delta x = 2.5 \) km and \( \Delta z = 2 \) m (For the top layer, \( \Delta z \) is adjusted to account for the surface fluctuation).

b DIST = Distance (km) from the river mouth to the center of each segment.

c SST = Surface area of the side storage area \( (\text{km}^2) \) at mean tide.

d B = estuarine width (m); at the surface layer, it is width at mean tide.
Table 4-1. (continued).

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<td>4059.3</td>
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<td>63 23.6 1.157</td>
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<td>64 21.1 4.035</td>
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<td>65 18.6 24.015</td>
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<td>3109.0</td>
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<td>5486.4</td>
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For geometric data, see Table 4-1.

Figure 4-1. The model transects and side storage areas in the tidal Rappahannock River.
Figure 4-2. Mean tide calibration.
Figure 4-3. Model prediction and field measurement of salinity on 8/04/87: the most upriver station was at km 57.79 in 1987 surveys.
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Figure 4-5. Model prediction and field measurement of salinity on 8/24/87.
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Figure 4-8. Subtidal variations in surface elevation at Urbanna (a-b) and at Tappahannock (c).
Figure 4-9. Current simulation at the mouth, depth 1.2 m.
Figure 4-10. Current simulation at the mouth, depth 9.7 m.
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Figure 4-12. Current simulation at 16.6 km upriver from mouth, depth 10.0 m.
Figure 4-13. Current simulation at 16.6 km upriver from mouth, depth 18.7 m.
Figure 4-14. Surface elevation, both filtered and unfiltered, at river mouth (a), and subtidal variations in current velocity at river mouth (b-c) and at km 16.6 (d-f); arrows in (a) represent the events of strong southwest wind.
Figure 4-14. (continued).
Figure 4-15. Model prediction of residual velocity over 2 spring-neap cycles from 7/29/87 to 8/25/87.
Figure 4-16. Model prediction of residual velocity over 2 spring-neap cycles with constant freshwater flow of 10 cms.
Figure 4-17. Model prediction of residual velocity during spring tide with constant freshwater flow of 10 cms.
Figure 4-18. Model prediction of residual velocity during neap tide with constant freshwater flow of 10 cms.
Figure 4-19. Model prediction of residual velocity over 2 spring-neap cycles with constant freshwater flow of 39.8 cms.
Figure 4-20. Model prediction of residual velocity over 2 spring-neap cycles with constant freshwater flow of 130 cms.
Figure 4-21. Model prediction and field measurement of salinity on 7/05/90: see text for the boundary condition used.
Figure 4-22. Model prediction and field measurement of salinity on 8/07/90: see text for the boundary condition used.
Figure 4-23. Model prediction of salinity using new boundary condition: see text for the condition used.
V. APPLICATION OF THE WATER QUALITY MODEL

The water quality model also was applied to the tidal portion of the Rappahannock River. Emphasis was given to (1) the lower part of the river where hypoxia, or even anoxia, has persisted during summer in the bottom water and (2) the middle part of the river where a characteristic chlorophyll maximum has been frequently observed.

For each particular simulation run, appropriate input data must be determined. The water quality model is supplied with the information of the physical transport processes from the hydrodynamic model. The preparation of other input data related to the biochemical processes is discussed in Section 5-1. The water quality model was calibrated such that it reproduced the observed distributions of the water quality parameters on July 5, 1990 (Section 5-2). The model was then verified through comparisons of model predictions with two independently collected sets of field data in 1990 (Section 5-3). One is the data set from the August 7 slackwater survey by VIMS and the other is the data set on June 24, July 8 and August 5. The latter, hereafter referred to as the 'CBP data', was collected by the Virginia Water Control Board (VWCB) as a part of the Chesapeake Bay Fall Line and Tributary Water Quality Monitoring Program. Finally, quantitative assessments including scatterplots, the RMS error and the mean error are presented as a summary of model calibration and verification in Section 5-4.

5-1. Preparation of Input Data Set

Calibration and verification is far more difficult for the water quality model than for the hydrodynamic model, due to the large number of predicted water quality parameters to be calibrated and verified: DO, chlorophyll 'a' (Chl), CBOD, organic nitrogen (N1), ammonia nitrogen (N2), nitrite-nitrate nitrogen (N3), organic phosphorus...
(P1) and inorganic phosphorus (P2). It also is due to the large number of biochemical coefficients to be determined in the calibration. For a given condition, more than one set of calibration coefficients may provide roughly equivalent results, which means there are too many degrees of freedom to determine a unique set of coefficients. One way of avoiding this situation is to minimize the number of coefficients to be determined through comparison of model results and field conditions. This objective can be achieved by providing as many coefficients as possible either with the direct field measurements or with the literature values. The following principles were used: 1) utilize field measurements whenever available; 2) utilize literature values when measurements are not available; and 3) utilize calibration values only when no other sources are available or when other sources are shown to be unsuitable.

Since the model predictions will change depending upon the selection of biochemical coefficients, the water quality model should employ consistent coefficient values for different simulation runs. That is, the coefficient values should be transferable for the model predictions to compare with independent sets of field observations. The consistency must be so in the model, even though the biochemical coefficients need not be constant all the time in the prototype. Exceptions are field measurements such as light conditions, point source loadings, temperature, etc. This principle of consistency was observed wherever possible in the calibration and verification processes. The trade-off was that the model predictions did not always agree with the field observations as closely as they might if the model was adjusted to each survey individually. Therefore, discrepancies between model predictions and field observations must be understood as illustrative of the variability of natural processes rather than indicative solely of shortcomings in the model.
5-1-1. Literature values

Literature values are those that have been evaluated in published studies of similar systems. For the present study, the primary sources for literature values are:

1) the studies in the Potomac Estuary (Thomann & Fitzpatrick 1982), hereafter referred to as the 'PEM Report',
2) the studies in the Virginia Potomac Embayments (e.g., Cerco & Kuo 1983), referred to as the 'VPE Reports',
3) the EPA report on model rates, constants and formulation (Bowie et al. 1985), referred to as the 'EPA Report',
4) the book on surface water quality modeling by Thomann & Mueller (1987), referred to as the 'T&M Book', and
5) the studies in the upper tidal Rappahannock River (Kuo et al. 1991b), referred to as the 'UTR Report'.

5-1-2. Field measurements

The field data collected by VIMS during summer of 1990 were used for the calibration and a part of verification of the water quality model. They include the environmental conditions such as water temperature, downstream boundary conditions, sediment oxygen demand (SOD), benthic fluxes and light intensity related parameters, and loadings including nonpoint and point source loads. The full description of the field surveys and data are presented in Kuo et al. (1991b); the sampling locations are shown in Fig. 3-1.

A. Temperature: Slackwater survey data showed that spatial average temperature was 21.1°C on June 6 and 26.9°C on July 5 and August 7. Since the data to be compared with model predictions were collected in July and August, the temperature data at later dates were emphasized. A constant water temperature of 26.5°C was used for the
calibration and verification run, which covered the period from June 6 to August 7.

B. Downstream boundary conditions: Like salinity in Section 4-4-2, the water quality conditions at the mouth between the three slackwater surveys (June 6, July 5 and August 7) were linearly interpolated in time and used for the daily downstream boundary conditions for eight water quality parameters for both calibration and verification.

C. Nonpoint source loads: The nonpoint contribution from the watershed above the fall line was evaluated from freshwater discharge rates and concentrations of water quality parameters at the fall line. Daily discharge rates, those used for the hydrodynamic model, were obtained from USGS (1991). Results from a regression analysis were used for the concentrations of all nutrient forms including N1, N2, N3, P1 and P2 (Kuo et al. 1991b). Daily input for the concentrations of Chl, CBOD and DO was obtained from the linear interpolation of monitoring data. The distributed nonpoint source loading below the fall line was estimated by assuming constant nonpoint source load per unit drainage area. The load per unit area was calculated using the load at the fall line.

D. Point source loads: During the sampling period, four sewage treatment plants (Claiborne Run, FMC, Fredericksburg and Massaponax STP's) discharged waste water into the uppermost 10 km reach of the tidal river. The monitoring data from the STP's were linearly interpolated in time and used for the daily input of the point source loadings.

E. Benthic fluxes: Benthic nutrient fluxes and SOD were measured for the upper portion of the river between km 130-170 (see Fig. 3-1). The SOD ranged from 0.78 to 2.14 g m^{-2} day^{-1}, and the N2 flux from 0.03 to 0.12 g m^{-2} day^{-1}. The benthic flux of N3 and P2 was nearly zero. No measurements were made for organic matter. Since the field measurements covered only the upper 40 km of the river, SOD and benthic fluxes were considered to be calibration parameters for the remaining part of the river. They
were adjusted in the calibration within the measured ranges for SOD and N2 benthic flux. The estimated values were kept constant with respect to time for both calibration and verification.

F. Solar radiation and light extinction coefficient: Modeling of the growth of phytoplankton involves parameters related to the light intensity in Equations 2-10d through 2-10f; daily solar radiation ($I_d$), times of sunrise ($t_u$) and sunset ($t_d$), and light extinction coefficient ($K_e$). Daily inputs of $I_d$, $t_u$ and $t_d$ were obtained from the measurements at VIMS (Gloucester Point, VA). The light extinction coefficient as a measure of light attenuation in water is usually estimated using the secchi-depth (SD) measurement. The SD measurements in 1990 showed a good deal of scatter. The light extinction coefficients, which are derived using the assumed constancy of the product of SD and $K_e$, i.e., $SD \cdot K_e = 1.2$ and then corrected for self-shading of phytoplankton using Eq. 2-10e, are presented in Fig. 5-1.

Light in water is attenuated by two processes, absorption and scattering. Absorption refers to the attenuation due to the transformation of light into different forms of energy such as heat, and scattering refers to that due to the redirection of some of the light flux out of the main direction of travel (Tyler & Preisendorfer 1962). Effler (1985) recognized the variability in the product of SD and $K_e$ for any system, and showed that the constancy of $SD \cdot K_e$ should be expected only when the relative contributions of absorption and scattering to $K_e$ remain uniform. For example, since scattering affects SD more than $K_e$, the transparency (SD) in the scattering-dominant system is low but the light attenuation ($K_e$) may not be as high as that estimated from a constant $SD \cdot K_e$. Besides, there are measurement errors, mostly associated with the measurement of SD, which is highly sensitive to the ambient conditions such as light and water surface roughness, and is somewhat observer dependent. Therefore, field studies concerned with phytoplankton productivity should include routine measurement of $K_e$. 68
In the present study, the extinction coefficient was considered to be a calibration parameter. The coefficient was adjusted in the calibration, within the ranges estimated from SD measurements using the constancy of $SD \cdot K_c = 1.2$. Included in Fig. 5-1 are the values used for the model application, which were kept constant with respect to time in both calibration and verification.

5-2. Calibration

The water quality model was calibrated with a simulation of distributions of water quality parameters from June 6 to July 5, 1990. To allow a "warming-up" time for the physical parameters such as surface elevation and velocity, the model simulation started from June 4. The field data collected in the June 6 slackwater survey were then inserted into the model to specify the initial conditions, and the data from the July 5 slackwater survey were used for the calibration of the model. The range and mean over a day predicted by the model were compared with the observations collected on the same date.

The calibration was performed by adjusting the calibration parameters, most notably the biochemical rate constants described in Section 2-2 (see also Chapter 3 in Park & Kuo (1993) for more detailed description) until agreement was achieved between the model results and the field data. Kuo et al. (1991b) studied water quality conditions using one-dimensional water quality model in the upper 60 km reach of the tidal Rappahannock River. The calibration values from that study in the 'UTR Report' generally served as starting point in this model calibration. Since the way that these coefficients are obtained is as significant as the achievement of calibration itself, all model coefficients and their origins are presented before the calibration results.
5-2-1. Phytoplankton-related coefficients

The phytoplankton-related coefficients employed in the model calibration are listed in Table 5-1. The values in the 'VPE Reports' were adopted in this model application if all studies in the Virginia Potomac Embayments used the same values for those coefficients. For the temperature dependency of phytoplankton growth (θ₁), respiration (θ₂) and mortality (θ₃) rates, the 'T&M Book' provided definite values instead of ranges, and these values were used. The photosynthetic quotient (PQ) and respiration quotient (RQ) calculated from the data in the 'EPA Report' fall within very narrow ranges, and the mean values of these ranges were used. To conserve nitrogen and phosphorus within the system, 100% of phytoplankton consumed by zooplankton is assumed to be recycled within the system, i.e., a_r = 1. The other coefficients were either adopted from the 'PEM Report' or determined through calibration within the range of literature values.

5-2-2. Nitrogen-related coefficients

The nitrogen-related coefficients employed in the calibration are listed in Table 5-2. When coefficients had the same values in all the 'VPE Reports', those values were used. The values of other coefficients were determined either from the 'PEM Report' or through calibration within the range of literature values. Benthic flux measurements of N₂ ranged from 0.03 to 0.12 g m⁻² day⁻¹ over the upper 40 km reach of the river into which STP's discharge point source loads, mostly inorganic nutrients. In model calibration, a N₂ benthic flux of 0.05 g m⁻² day⁻¹ between km 80-175 was needed to maintain the model predictions of Chl, N₂ and total nitrogen as high as field measurements on July 5 (Figures 5-2, 5-3 and 6-16).
5-2-3. Phosphorus-related coefficients

The phosphorus-related coefficients employed in the calibration are listed in Table 5-3. Two parameters, settling rate \( (K_{\text{P2}}) \) and benthic flux \( (\text{BenP2}) \) of inorganic phosphorus \( (\text{P2}) \), are of particular interest.

A settling rate of \( \text{P2} \) higher than that of other parameters was required over the region upriver of km 147 to match the model results with field observations. The model simulation without settling resulted in \( \text{P2} \) concentrations much higher than field observations in all survey data used. Since the STP discharges are the primary source of phosphate in the river, this implies that some of phosphate from STP discharges was lost (settled) before being transported out of this reach of the river. Several studies have demonstrated a loss by adsorption of phosphate to sediment particles (Parfitt et al. 1975; Lake & MacIntyre 1977; Veith & Sposito 1977; Mayer & Gloss 1980). Experiments by Lake & MacIntyre (1977) showed that phosphate and tripolyphosphate were readily adsorbed to clay minerals and estuarine sediments.

In the tidal freshwater portion of the James and Potomac rivers, experiments using sediment cores indicated the existence of an equilibrium concentration of phosphate, which increases as DO decreases (Cerco 1985 and 1989). When the phosphate concentration in the water column is above the equilibrium concentration, the sediment takes up phosphate. When the phosphate concentration is below the equilibrium concentration, the sediment releases phosphate. When DO and P2 are higher than 5.0 and 0.02 mg l\(^{-1}\), respectively, almost all measurements in Cerco (1989) showed sediment uptake of phosphate. In 1990, the P2 concentration was higher than 0.02 mg l\(^{-1}\) near the STP discharges (Figures 5-2 and 5-3). This loss mechanism was incorporated into the model by introducing high settling rate near the STP discharges. A similar treatment was needed in the studies of the Potomac Estuary (Thomann & Fitzpatrick 1982), the Virginia Potomac Embayments (Kuo 1985) and the upper tidal Rappahannock River.
Over the mid-reach of the river, the Chl concentrations frequently have been observed to be high. In model calibration, a P2 benthic flux of 0.005 g m\(^{-2}\) day\(^{-1}\) between km 80-147 was needed to maintain the model predictions of Chl, P2 and total phosphorus as high as field measurements on July 5 (Figures 5-2, 5-3 and 6-15). This high Chl concentrations in the mid-reach are further discussed in Section 6-2.

5-2-4. CBOD- and DO-related coefficients

The coefficients related to CBOD and DO employed in the model calibration are listed in Table 5-4. The SOD of 2.0 g m\(^{-2}\) day\(^{-1}\), which is near the upper limit of the field measurements in the upper 40 km reach of the river (0.78 to 2.14 g m\(^{-2}\) day\(^{-1}\)), was used in model calibration. The coefficient \(K_{r_0} = 12.9\) for the English system of units in O'Connor & Dobbins (1958) was converted to \(K_{r_0} = 393\) for the CGS units. The definite values in the 'T&M Book' were used for the temperature dependency of CBOD decay rate \(\theta_a\) and DO reaeration \(\theta_o\).

5-2-5. Calibration results

The calibrated model results and field observations are shown in Figures 5-2 and 5-3, in which eight model parameters (DO, Chl, CBOD, N1, N2, N3, P1 and P2), total nitrogen and total phosphorus are presented. The daily averages of the model results, presented as plots of isopleths in a vertical-longitudinal plane along the river axis, are compared with the values from field observations in Fig. 5-2. Another view of the calibration results presented in Fig. 5-3 compares the ranges and averages over a day from the model at the surface and bottom layers with the field data along the distance from the river mouth. The field data were measured at the surface, mid-depth and bottom, the depths of which are shown in Fig. 5-2. This study presents the total
nitrogen and phosphorus, and their organic forms (N1 and P1) that include the portion in Chl, i.e., a_n-Chl and a_p-Chl, respectively, for nitrogen and phosphorus. To show the limit of salt intrusion as a reference, the tidal mean salinity distribution is also included in Figures 5-2 and 5-3.

Both figures show that model results and field measurements were in good agreement. Discrepancies were often attributable to observance of the consistency principle between calibration and verification rather than to failure to curve-fit the model results to the field data; some differences, however, did exist between the model results and the field measurements. The ranges of variations in the model results were generally smaller than those in the field data, because the model calculated the lateral average concentrations while the field data were point measurements, and also because of the random variability inherent to natural systems.

The model calibration run for Figures 5-2 and 5-3 included wind-driven reaeration using the expression (Eq. 2-17d) derived by Banks & Herrera (1977). The DO concentration when wind-driven reaeration was not included is presented in Fig. 5-4. To compare the model-field agreement with or without wind reaeration, two quantitative measures are used; the root-mean-square (RMS) error and the average. The RMS error, which is a measure of the absolute difference between predictions and observations, is defined as,

\[
RMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (P_i - O_i)^2}
\]

where \(P_i\) is the \(i^{th}\) prediction (daily average), \(O_i\) is the \(i^{th}\) observation and \(n\) is the number of observations. The RMS error estimated using all data points is 0.90 and 1.01, respectively, with and without wind reaeration. Since the primary objective of this model is to study hypoxia, which occurs in the lower part of the river, the model-field
agreement for DO in this part of the river is important. The RMS error at the surface between km 0-50, i.e., using 6 data points, is 0.84 and 1.42, respectively, with and without wind reaeration. At the surface between km 0-50, the average DO from the field data is 6.44 mg l⁻¹, and that from the model is 6.32 and 5.31 mg l⁻¹, respectively, with and without wind reaeration. Thus, the inclusion of wind-driven reaeration can improve the agreement between the model and the data by increasing the DO near the surface, most notably in the lower part of the river between km 0-50.

In the upper, freshwater portion of the river between km 90-175, which is mostly affected by the STP discharges, the total nitrogen from the model predictions was generally comparable to that from the field measurements except in the region between km 140-160 (Fig. 5-3). In this region (km 140-160), the model predictions of total nitrogen and N₂ was lower than the field data although the model results for other forms of nitrogen (N₁ and N₃) agreed well with the field data. The same discrepancy was encountered in the one-dimensional modeling study of the upper tidal Rappahannock River (Kuo et al. 1991b). The STP discharges are the primary source of inorganic nutrients including ammonia, and four STP’s discharged wastewater into the upper 10 km reach of the river. The monitoring data in 1990 showed that the N₂ loading into the river from 4 STP’s during one week before July 5 was approximately 80% of that during one week before August 7 (Kuo et al. 1991b). The Chl concentration between km 140-160 was higher on July 5 (Figures 5-2 and 5-3) than that on August 7 (Figures 5-5 and 5-6), which suggests that algae should uptake more nutrients, including N₂, for growth on July 5 than on August 7. Compared to the conditions on August 7, reduced input from STP’s and greater uptake by algae on July 5 should lead to lower N₂ concentration in this part of the river, which was shown in the model results but not in the field data. Therefore, it was suspected that there might be some errors in the measurements of either N₂ concentration between km 140-160 or point source loadings of N₂.
higher point source loads of N2, the model predictions of N2 would increase and thus those of DO would decrease over this region improving the model-field agreement for DO as well as N2 (see Figures 5-2 and 5-3). No attempt, however, was made to modify the point source loadings for N2 for July 5 because the model capability of reproducing N2 and DO distributions in this region was proved in the model verification for August 7 (Figures 5-5 and 5-6).

Another thing to be noted in Figures 5-2 and 5-3 is the P2 between km 80-140, where the P2 predictions are slightly lower than the field data. A P2 benthic release of 0.005 g m\(^{-2}\) day\(^{-1}\) was used in model calibration (Table 5-3), and an increase in the P2 release could take care of the model-field discrepancy. Increasing the P2 release, however, made the P2 predictions in the verification for August 7 too high compared to the field data (see Figures 5-5 and 5-6). To observe the principle of consistency (Section 5-1), the P2 release of 0.005 g m\(^{-2}\) day\(^{-1}\) was used in the calibration and verification, leaving the P2 predictions in the calibration slightly lower than the field data, which is further discussed in Section 5-3-1.

5-3. Verification

The model was calibrated with one set of field data collected on July 5, 1990. This calibration, however, does not guarantee that the validity of the model can be extended beyond the data set used in the calibration process. Verification is to test the validity of the model against an independent set of field data. That is, verification tests the adequacy and consistency of the previously evaluated coefficients using a different set of field data collected independently of the calibration survey and under different ambient conditions.

In the present study, the model run for calibration was extended through August 7, 1990 without changing the coefficient values determined in calibration. The predictive
capability of the model was tested through comparisons of model predictions with two independently collected data sets. One is the data from the August 7 slackwater survey by VIMS, and the other is the CBP data on June 24, July 8 and August 5. The range and mean over a day from the model were compared with the observations collected on the same date.

5-3-1. August 7 slackwater survey data by VIMS

The verification results for the August 7 data are presented in Figures 5-5 and 5-6 for eight model parameters plus total nitrogen and total phosphorus. The daily averages of the model predictions presented as plots of isopleths in a vertical-longitudinal plane along the river axis are compared with the values from field observations in Fig. 5-5. Figure 5-6 has plots of the ranges and averages over a day from the model at the surface and bottom layers, along with the field data, against distance from the river mouth. To show the limit of salt intrusion, the tidal mean salinity distribution is included in Figures 5-5 and 5-6.

The model predictions of DO in Figures 5-5 and 5-6 include wind-driven reaeration; DO distributions without wind-driven reaeration are presented in Fig. 5-7. Again, the RMS error and average are used as quantitative measures for the difference in model-field agreement. The RMS error using all data points is 1.07 and 1.19 with and without wind reaeration, respectively. The RMS error at the surface between km 0-50, is 0.60 and 0.80, respectively, with and without wind reaeration. At the surface between km 0-50, the average DO from the field data is 5.71 mg l⁻¹, and that from the model is 6.04 and 4.97 mg l⁻¹, respectively, with and without wind reaeration. As in the calibration, the inclusion of wind-driven reaeration improves the model-field agreement for DO, most notably near the surface between km 0-50. The final calibrated model, therefore, includes the wind-driven reaeration of DO.
In Figures 5-5 and 5-6, the P2 predictions between km 70-95 on August 7 are higher than the field data, while the Chl predictions are lower than the data. The P2 predictions in this region on July 5 in model calibration are lower than the field data (Figures 5-2 and 5-3). Comparison of the conditions on July 5 (Fig. 5-3) with those on August 10 (Fig. 5-6) shows that the measured P2 concentrations at the surface were approximately the same (0.01 mg l⁻¹) in this region, as was the water residence time; three day average freshwater discharge was 15.0 m³ sec⁻¹ (cms) from July 2 to 4 and 9.7 cms from August 4 to 6. However, total daily solar radiation (I₀) on July 5 was approximately twice that on August 7; three day average I₀ was 671 langleys day⁻¹ from July 3 to 5 and 373 langleys day⁻¹ from August 5 to 7. The secchi-depth (SD) measurements in Fig. 5-1 show that the light extinction coefficient (Kₑ) used in this region between km 70-95 is larger than those estimated from the SD measurements on August 7, especially that at km 90. Thus, it seems to be the light availability (too high Kₑ or too low I₀) that makes the predictions of P2 higher than the data and those of Chl lower than the data on August 7. With more light available, the Chl may take up more P2 leading to higher Chl and lower P2 predictions. This reasoning is confirmed by the results in Fig. 5-8 from a model simulation in which Kₑ in the mid-part was lowered from 0.019 to 0.014 cm⁻¹ (average of two Kₑ values at km 74 and 90 in Fig. 5-1) from August 3 to 7.

Most of the CBP data for N2, N3 and P2 are below detection limits (see the following section). Therefore, the current calibration and verification of the water quality model for nutrients were conducted using two sets of slackwater survey data for July 5 and August 7 by VIMS. These data along with other conditions used in calibration and verification such as light availability (Kₑ and I₀) do not result in the consistent model predictions of P2 in the mid-reach of the river. This will restrict the scope of model application in performing the sensitivity analysis regarding nutrient
limitation of the primary production. The present water quality model needs to be further calibrated with more thorough field data in order to conduct detailed study of nutrient limitation.

5-3-2. CBP data from VWCB

The verification results for the CBP data are presented in Figures 5-9, 5-10 and 5-11, respectively, for June 24, July 8 and August 5. Since the CBP data were collected only at two depths for DO, Chl, P2, N2, N3 and total nitrogen, Figures 5-9 through 5-11 compare the ranges and averages over a day from the model at the surface and bottom layers with field data for these 6 parameters. It should be noted in Figures 5-9 through 5-11 that many measurements of N2 (63%), N3 (60%) and P2 (92%) are below the detection limits, which are 0.04 mg l\(^{-1}\) for N2 and N3, and 0.01 mg l\(^{-1}\) for P2 (Chesapeake Bay Program 1992). For comparison, the slackwater survey data collected by VIMS have the detection limit of 0.005 mg l\(^{-1}\) for N2 and N3, and 0.003 mg l\(^{-1}\) for P2.

5-4. Calibration and Verification Summary

The figures in the preceding sections provide a qualitative comparison of model predictions and field observations. This traditional assessment of model accuracy, the perceived agreement between predictions and observations, depends upon the viewpoint and experience of the assessors. In order to render the evaluation of models less subjective, quantitative assessments of model accuracy are desirable. No single measure or set of measures is universally applicable for this purpose. The selection of appropriate measures is dependent upon the quantity and quality of the field data used and upon the nature of the model predictions. In the present study scatterplots, the RMS error, and the mean error are used.
Scatterplots for point-by-point comparison of predictions and observations are presented in Fig. 5-12 for eight model parameters plus total nitrogen and total phosphorus. A solid, diagonal line indicates the one-to-one correspondence. Magnitude of water quality parameters can range from zero (lower limit) to an unbounded value at the higher end. Because the scatterplot on a linear scale can be skewed by the presence of an unusually large value, all parameters except DO are plotted on a logarithmic scale.

Other measures included in Fig. 5-12 are the RMS and mean errors with \( n \) being the number of observations used to estimate them. The RMS error defined in Eq. 5-1 is a measure of the absolute difference between predictions and observations, and the RMS error of zero is ideal. Since the RMS error cannot discern the overprediction or underprediction, a second measure, the mean error, is desirable. The mean error \( (E) \) is defined as,

\[
E = \frac{1}{n} \sum_{i=1}^{n} (P_i - O_i) \tag{5-2}
\]

Positive \( E \) indicates that the model overpredicts the observations on the average and negative \( E \) indicates that the model underpredicts the observations on the average with zero \( E \) being ideal. Although the CBP data of N2, N3 and P2 from the VWCB are included in the scatterplots (Fig. 5-12), these were not used in estimating the RMS and mean errors because most of them are below the detection limits and model predictions are generally lower than the detection limits except near the STP discharges.
Table 5-1. Phytoplankton-related coefficients.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Equation</th>
<th>Value</th>
<th>Source*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_c$</td>
<td>2-16a</td>
<td>$0.05 \text{ mg C per } \mu g \text{ Chl}$</td>
<td>V</td>
</tr>
<tr>
<td>$a_n$</td>
<td>2-11a</td>
<td>$0.007 \text{ mg N per } \mu g \text{ Chl}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$a_p$</td>
<td>2-14a</td>
<td>$0.001 \text{ mg P per } \mu g \text{ Chl}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$a_r$</td>
<td>2-11a</td>
<td>$1.0$</td>
<td>Calibration</td>
</tr>
<tr>
<td>PQ</td>
<td>2-17a</td>
<td>$1.0 \text{ moles } O_2 \text{ per mole C}$</td>
<td>III, V</td>
</tr>
<tr>
<td>RQ</td>
<td>2-17a</td>
<td>$1.33 \text{ moles } CO_2 \text{ per mole } O_2$</td>
<td>III, V</td>
</tr>
<tr>
<td>$K_{mn}$</td>
<td>2-10g</td>
<td>$0.025 \text{ mg } l^{-1}$</td>
<td>I, II, III, V</td>
</tr>
<tr>
<td>$K_{mp}$</td>
<td>2-10g</td>
<td>$0.001 \text{ mg } l^{-1}$</td>
<td>I, II, III, V</td>
</tr>
<tr>
<td>$k_{gr}$</td>
<td>2-10c</td>
<td>$2.0 \text{ day}^{-1}$</td>
<td>I, V</td>
</tr>
<tr>
<td>$\theta_1$</td>
<td>2-10c</td>
<td>$1.066$</td>
<td>IV, V</td>
</tr>
<tr>
<td>$I_1$</td>
<td>2-10d</td>
<td>$250 \text{ langleys day}^{-1}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{c,Chl}$</td>
<td>2-10e</td>
<td>$0.00018 \text{ l } \mu g^{-1} \text{ cm}^{-1}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{Chl}$</td>
<td>2-10b</td>
<td>$10.0 \text{ cm day}^{-1}$</td>
<td>I, V</td>
</tr>
<tr>
<td>$R(20)$</td>
<td>2-10h</td>
<td>$0.17 \text{ day}^{-1}$</td>
<td>V</td>
</tr>
<tr>
<td>$\theta_2$</td>
<td>2-10h</td>
<td>$1.08$</td>
<td>IV, V</td>
</tr>
<tr>
<td>$P(20)$</td>
<td>2-10i</td>
<td>$0.02 \text{ day}^{-1}$</td>
<td>I, V</td>
</tr>
<tr>
<td>$\theta_3$</td>
<td>2-10i</td>
<td>$1.0$</td>
<td>IV, V</td>
</tr>
</tbody>
</table>

* I = PEM Report (Thomann & Fitzpatrick 1982)  
II = VPE Reports (e.g., Cerco & Kuo 1983)  
III = EPA Report (Bowie et al. 1985)  
IV = T&M Book (Thomann & Mueller 1987)  
V = UTR Report (Kuo et al. 1991b).
Table 5-2. Nitrogen-related coefficients.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Equation</th>
<th>Value</th>
<th>Source*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{u12}(20)$</td>
<td>2-11a</td>
<td>0.04 mg l$^{-1}$ day$^{-1}$</td>
<td>I/Calibration</td>
</tr>
<tr>
<td>$\theta_4$</td>
<td>2-11a</td>
<td>1.04</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{h12}$</td>
<td>2-11a</td>
<td>1.0 mg l$^{-1}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{u11}$</td>
<td>2-11b</td>
<td>8.0 cm day$^{-1}$</td>
<td>Calibration</td>
</tr>
<tr>
<td>$K_{n23}(20)$</td>
<td>2-12a</td>
<td>0.3 mg l$^{-1}$ day$^{-1}$</td>
<td>Calibration</td>
</tr>
<tr>
<td>$\theta_5$</td>
<td>2-12a</td>
<td>1.04</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{h23}$</td>
<td>2-12a</td>
<td>1.0 mg l$^{-1}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{nit}$</td>
<td>2-12a</td>
<td>2.0 mg l$^{-1}$</td>
<td>I</td>
</tr>
<tr>
<td>$K_{n33}(20)$</td>
<td>2-13b</td>
<td>0.35 day$^{-1}$</td>
<td>Calibration</td>
</tr>
<tr>
<td>$\theta_6$</td>
<td>2-13b</td>
<td>1.045</td>
<td>I</td>
</tr>
<tr>
<td>$K_{n33}$</td>
<td>2-13b</td>
<td>0.5 mg l$^{-1}$</td>
<td>Calibration</td>
</tr>
<tr>
<td>$F_n$</td>
<td>2-11a</td>
<td>0.75</td>
<td>II, V</td>
</tr>
<tr>
<td>BenN1</td>
<td>2-11b</td>
<td>0.0 g m$^{-2}$ day$^{-1}$</td>
<td>V</td>
</tr>
<tr>
<td>BenN2$^b$</td>
<td>2-12b</td>
<td>0.0 - 0.05 g m$^{-2}$ day$^{-1}$</td>
<td>Field Data/Calibration</td>
</tr>
<tr>
<td>BenN3</td>
<td>2-13b</td>
<td>0.0 g m$^{-2}$ day$^{-1}$</td>
<td>V</td>
</tr>
</tbody>
</table>

* see Table 5-1.

$^b$ 0.05 g m$^{-2}$ day$^{-1}$ upriver of km 80, and 0.0 elsewhere.
Table 5-3. Phosphorus-related coefficients.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Equation</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{p12}(20)$</td>
<td>2-14a</td>
<td>0.06 mg l$^{-1}$ day$^{-1}$</td>
<td>V</td>
</tr>
<tr>
<td>$\theta_7$</td>
<td>2-14a</td>
<td>1.04</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{bp12}$</td>
<td>2-14a</td>
<td>1.0 mg l$^{-1}$</td>
<td>II, V</td>
</tr>
<tr>
<td>$K_{p11}$</td>
<td>2-14b</td>
<td>10.0 cm day$^{-1}$</td>
<td>V</td>
</tr>
<tr>
<td>$F_p$</td>
<td>2-14a</td>
<td>0.55</td>
<td>Calibration</td>
</tr>
<tr>
<td>$K_{p22}$</td>
<td>2-14b</td>
<td>2-15b 0.0 - 20.0 cm day$^{-1}$</td>
<td>Calibration</td>
</tr>
<tr>
<td>BenP1</td>
<td>2-14b</td>
<td>0.0 g m$^{-2}$ day$^{-1}$</td>
<td>V</td>
</tr>
<tr>
<td>BenP2$^c$</td>
<td>2-15b</td>
<td>0.0 - 0.005 g m$^{-2}$ day$^{-1}$</td>
<td>Calibration</td>
</tr>
</tbody>
</table>

* see Table 5-1.

$^b$ 20.0 cm day$^{-1}$ upriver of km 147, and 0.0 elsewhere.

$^c$ 0.005 g m$^{-2}$ day$^{-1}$ between km 80-147, and 0.0 elsewhere

Table 5-4. CBOD- and DO-related coefficients.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Equation</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_c(20)$</td>
<td>2-16a</td>
<td>0.1 day$^{-1}$</td>
<td>III, IV</td>
</tr>
<tr>
<td>$\theta_8$</td>
<td>2-16a</td>
<td>1.047</td>
<td>I, IV</td>
</tr>
<tr>
<td>$K_{DO}$</td>
<td>2-16b</td>
<td>0.5 mg l$^{-1}$</td>
<td>Calibration</td>
</tr>
<tr>
<td>SOD</td>
<td>2-16b</td>
<td>2.0 g m$^{-2}$ day$^{-1}$</td>
<td>Field Data/Calibration</td>
</tr>
<tr>
<td>$K_{ro}$</td>
<td>2-17c</td>
<td>393</td>
<td>see text</td>
</tr>
<tr>
<td>$\theta_9$</td>
<td>2-17e</td>
<td>1.024</td>
<td>IV</td>
</tr>
</tbody>
</table>

* see Table 5-1.
Figure 5-1. Light extinction coefficients: the horizontal lines represent the values used in model calibration and verification.

\[
K_e = 1.2/SD - 0.00018 \text{ Chi}
\]

SD in cm and Chi in \( \mu g \text{ l}^{-1} \)

DISTANCE FROM MOUTH (km) vs. EXTINGUISH COEFFICIENT (cm\(^{-1}\))
Figure 5-2. Model calibration results and tidal mean salinity on 7/05/90: the isoconcentration contours are model results and the point values are field data.
Figure 5-2. (continued).
Figure 5-2. (continued).
Figure 5-3. Model calibration results (daily mean, maximum and minimum) and tidal mean salinity at surface and bottom on 7/5/90.
Figure 5-3. (continued).
Figure 5-3. (continued).
Figure 5-4. Model prediction of DO on 7/05/90 without wind reaeration.
Figure 5-5. Model verification results and tidal mean salinity on 8/07/90: the isoconcentration contours are model results and the point values are field data.
Figure 5-5. (continued).
Figure 5-5. (continued).
Figure 5-6. Model verification results (daily mean, maximum and minimum) and tidal mean salinity at surface and bottom on 8/07/90.
Figure 5-6. (continued).
Figure 5-6. (continued).
Figure 5-7. Model prediction of DO on 8/07/90 without wind reaeration.
Figure 5-8. Model prediction on 8/07/90 when increasing light availability between km 53-109.
Figure 5-9. Model verification results (daily mean, maximum and minimum) at surface and bottom on 6/24/90 using the field data from VWCB.
Figure 5-10. Model verification results (daily mean, maximum and minimum) at surface and bottom on 7/08/90 using the field data from VWCB.
Figure 5.10. (continued)
Figure 5-11. Model verification results (daily mean, maximum and minimum) at surface and bottom on 8/05/90 using the field data from VWCB.
Figure 5-11. (continued).
Figure 5-12. Scatterplots, RMS errors and mean errors for model calibration and verification: scatterplots include the data from VIMS and VSWCB, but error analysis for N2, N3 and P2 uses the VIMS data only because of the detection limit in VSWCB data.
Figure 5-12. (continued).
Figure 5-12. (continued).
VI. SENSITIVITY ANALYSIS OF THE WATER QUALITY MODEL

A primary use of the calibrated and verified model is sensitivity analysis to examine the behavior of the prototype in response to any alteration(s) made. In a series of model runs, for example, the effects on the water quality of increasing or decreasing vertical mixing may be examined. Experiments of this nature would be difficult or impossible to conduct on the prototype. Sensitivity analysis is a powerful tool that can be used to improve understanding of the present water quality conditions and to explore the factors that are primarily responsible.

From the field observations and model application (calibration and verification), three distinct water quality regimes are noted in the tidal Rappahannock River; the lower reach (between km 0-50), the middle reach (between km 80-145) and the upper reach (between km 155-175). The upper reach, immediately downriver of the fall line, receives wastewater discharges from STP’s; DO concentrations lower than 5 mg l⁻¹ can be found depending upon river discharge and water temperature, as well as the quality and quantity of STP discharges. A prior modeling study (Kuo et al. 1991b) has shown that both point and nonpoint source loadings have significant impacts on water quality with their relative importance depending upon the magnitude of the river discharge.

In the lower portion of the river, hypoxia (or even anoxia) persists during summer in the bottom water. In the mid-reach of the river, a characteristic Chl maximum has been frequently observed. For these two parts of the river, sensitivity analysis was performed to study the controlling mechanism(s) of the observed phenomena. The sensitivity analysis was conducted by running the model with all coefficients as in the calibration run except for the one being examined. It should be clearly noted that the subsequent sensitivity analysis is not intended to generate precise predictions of prototype behavior under alternative conditions. The variability of natural systems and the effects
of random events may act to produce results that would differ from the predictions. The model results should be viewed as best estimates if the conditions remain at their calibrated levels except for the sensitivity parameters.

6-1. Lower Part of the Tidal Rappahannock River

In the lower part of the tidal Rappahannock River, hypoxia, or even anoxia, persists during summer in the bottom water. This phenomenon has been studied by many investigators (Kuo & Neilson 1987; Kuo et al. 1991a; Kuo & Park 1992). Kuo & Neilson (1987) made a qualitative investigation of the bottom water DO in the three Virginia estuaries (James, York and Rappahannock rivers). They reported that hypoxia has been observed most frequently in the deep water of the Rappahannock River, but it occurs rarely in the James River even though it receives the heaviest wastewater loadings among the three estuaries. This difference has been attributed in part to the relatively strong gravitational circulation in the James River. Due to the relatively weak circulation in the Rappahannock, the impact of increased urbanization may be more severe there than it has been in the James River.

In their study of the temporal and spatial variability of hypoxia in the lower portion of the Rappahannock River, Kuo et al. (1991a) observed a characteristic longitudinal pattern of bottom water DO in the summer of 1987. The bottom DO concentrations decreased upriver from river mouth, reached a minimum at approximately km 42, upriver of the deepest point of the river, then increased as the water column became shallower. The same pattern was observed in the summer of 1990 and was predicted by the model (Figures 5-3 and 5-6). A similar pattern was observed in the Patuxent River, Maryland (Laubach & Summers 1987), another tributary of Chesapeake Bay. Kuo et al. (1991a) also observed a periodic reoxygenation of bottom water that was closely related to spring tide mixing. The destratification-stratification cycle caused by spring-neap tidal
cycle has been documented in the Rappahannock River as well as other Virginia estuaries (Haas 1977; D'Elia et al. 1981; Ruzecki & Evans 1986).

Using a Lagrangian concept, Kuo et al. (1991a) developed a model for the bottom water DO based on a DO budget of a water parcel travelling upriver along estuarine bottom. In the DO budget, only one source (vertical mixing) and one sink (oxygen demand) were considered. The predictive application of the model was not always satisfactory due to the lack of complete information for input parameters (vertical mixing and oxygen demand); spatially and temporally varying values for input parameters were called for to improve the predictive capability of the model. The diagnostic study using the simple model, however, enabled them to investigate cause-effect relationships, i.e., effect on bottom DO of residual velocity, vertical mixing, oxygen demand and quality of incoming water from the bay.

Sensitivity analysis using the present model was performed to study the controlling mechanism(s). The primary function of this analysis was to test the theory proposed in Kuo & Neilson (1987) and Kuo et al. (1991a) using detailed hydrodynamics and geometry. The sensitivity of the prototype was examined for the following factors that might be responsible for low DO concentration: quality of the incoming bay water, gravitational circulation, vertical mixing, SOD and water column oxygen demand.

6-1-1. Quality of the incoming bay water

It has been suggested that anoxia in the main channel of Chesapeake Bay might contribute to hypoxia in the Rappahannock River. This possibility was examined by adjusting the downstream boundary condition for DO and CBOD. In the calibration and verification runs, the time-varying downstream boundary condition was prepared by linear interpolation of the field data at the mouth from 3 slackwater surveys (June 6, July 5 and August 7).
Two new boundary conditions for DO were constructed by linear interpolation of the data after low DO measurements were brought up to 5.5 (or 7.0) mg l\(^{-1}\). The DO boundary conditions in the bottom layer used in two sensitivity runs are presented in Fig. 6-1. Results from two sensitivity runs in Fig. 6-2 indicate that the DO in the incoming bay water can affect the severity of hypoxia but not the shape of bottom DO distribution, particularly the location of the minimum bottom DO. Furthermore, the bottom water ends up being hypoxic regardless of the DO concentration in the incoming bay water. These results agree with the conclusions of Kuo et al. (1991a), which were based upon a simple DO budget model for bottom water.

The effect of CBOD in the incoming bay water on hypoxia was examined by decreasing the downstream boundary condition for CBOD. Results from a sensitivity run with a zero-CBOD boundary condition in Fig. 6-3, compared to those in Fig. 6-2, show that the hypoxic condition can be relieved more by eliminating CBOD than by increasing DO in the incoming bay water. Results from a second sensitivity run with the lowest DO boundary condition of 7.0 mg l\(^{-1}\) and zero-CBOD boundary condition in Fig. 6-3 indicate that the bottom water ends up being hypoxic regardless of the DO and CBOD concentrations in the incoming bay water.

6-1-2. Gravitational circulation

Differences in the gravitational circulation have been proposed to be responsible for the systematic variability in the bottom water DO in three Virginia estuaries (Kuo & Neilson 1987; Kuo et al. 1991a). The effect on the DO distribution of residual circulation was examined by changing the constant relating salinity to density (k in Eq. 2-6). Results from an initial sensitivity run (not shown) show that an increase in k, thus strengthening the residual current, lowers the DO concentration slightly over the region where gravitational circulation exists; this is because the increased vertical density
difference as well as the enhanced gravitational circulation strengthens the stratification, which in turn reduces the vertical mixing. To alter the strength of the gravitational circulation while minimizing the change in the vertical mixing, only the constant involved in calculating the horizontal pressure (density) gradient (see Eq. 2-39 in Park & Kuo 1993) was modified. Figure 6-4 shows the results from sensitivity runs with 120% and 130% of the calibration value of \( k \) \( (7.5 \times 10^4) \).

In Fig. 6-4, two mechanisms are responsible for the increase in bottom water DO with increasing the constant, \( k \); residual circulation and vertical mixing. The lower half of Fig. 6-5 shows the tidal mean velocity vertically averaged over the bottom layer. (Negative velocity indicates that the water flows in the upriver direction). In the base (calibration) run with \( k = 7.5 \times 10^4 \), the spatial average of tidal mean velocity over the bottom layer is \(-1.7\) cm sec\(^{-1}\). The spatial averages for \( k = 9.0 \times 10^4 \) (120%) and \( 9.75 \times 10^4 \) (130%) are, respectively, \(-2.2\) and \(-3.3\) cm sec\(^{-1}\). Therefore, one mechanism to increase the bottom DO in Fig. 6-4 is that faster water movement allows less time for DO to be consumed as a water parcel travels upriver along the bottom, which confirms the argument in Kuo & Neilson (1987) and Kuo et al. (1991a).

The enhanced gravitational circulation increases the velocity shear \( (\Delta u/\Delta z) \) as well as stratification \( (\Delta \rho/\Delta z) \). The increase in \( \Delta u/\Delta z \) that enhances turbulence is somewhat compensated for by increase in \( \Delta \rho/\Delta z \), making the increase in vertical mixing not as large as it can be with the increase in \( \Delta u/\Delta z \) only. In the present sensitivity runs, increasing the constant, \( k \), only in the horizontal density gradient eliminated its direct effect on \( \Delta \rho/\Delta z \); this made the increase in turbulent mixing due to velocity shear \( (\Delta u/\Delta z) \) more pronounced than the reduction due to increased stratification \( (\Delta \rho/\Delta z) \) by vertical shear straining. The upper half of Fig. 6-5 shows the tidal mean vertical diffusivity \( (K_z) \) vertically averaged over total depth. The spatial averages of tidal mean \( K_z \) over the estuarine portion are \( 1.3, 1.8 \) and \( 2.8\) cm\(^2\) sec\(^{-1}\) for \( k = 7.5 \times 10^4, 9.0 \times \)
and \(9.75 \times 10^{-4}\), respectively. Therefore, another contributing factor for the elevated bottom DO in Fig. 6-4 is the increased vertical mixing. With the present model, which contains all terms in the continuity equation and momentum and mass balance equations (Equations 2-1 through 2-5), it was not possible to strengthen the gravitational circulation without affecting the vertical mixing.

6-1-3. Vertical mixing

The effect of vertical mixing was examined by varying the constant, \(\alpha\), in the vertical mixing coefficients (Equations 2-7 and 2-8). Figure 6-6 shows the results from sensitivity runs with 120% and 150% of the calibrated \(\alpha\) value (\(1.15 \times 10^{-2}\)). It shows that increased vertical mixing does relieve the hypoxic condition in the bottom water, which confirms one of the conclusions in Kuo et al. (1991a). The tidal mean velocity and vertical diffusivity, which are comparable to those in Fig. 6-5, are presented in Fig. 6-7. In the upper half of Fig. 6-7, the spatial averages of tidal mean \(K_z\) over the estuarine portion are 1.3, 1.6 and 2.7 cm² sec⁻¹, respectively, for \(\alpha = 1.15 \times 10^{-2}\) (calibration), \(1.38 \times 10^{-2}\) (120%) and \(1.725 \times 10^{-2}\) (150%). Tidal mean velocity in the lower half of Fig. 6-7 shows that the gravitational circulation increases with increasing \(\alpha\) between km 0-32. The spatial averages of tidal mean velocity over the bottom layer are \(-1.7\), \(-1.9\) and \(-2.8\) cm sec⁻¹, respectively, for \(\alpha = 1.15 \times 10^{-2}\), \(1.38 \times 10^{-2}\) and \(1.725 \times 10^{-2}\).

This increase in gravitational circulation with increasing vertical mixing is contrary to the Hansen and Rattray’s analytical solution (Hansen & Rattray 1965) as well as to the results in Figures 4-17 and 4-18. Hansen and Rattray’s solution dictates that the gravitational circulation decreases as the vertical mixing increases, which is represented by weaker residual velocity during spring tide (Fig. 4-17) compared to neap tide (Fig. 4-18); Hansen and Rattray’s solution, however, was based upon the assumption of constant
longitudinal salinity gradient \( \partial s / \partial x \). It is \( \partial s / \partial x \) integrated over the water column that is the driving force for the gravitational circulation and thus determines its strength. In Fig. 6-8, the lower half repeats the tidal mean velocity of Fig. 6-7 and the upper half shows \( \Sigma(\Delta S_x) = \Sigma(S_i - S_{i+1}) \), the longitudinal gradient of tidal mean salinity integrated over total depth (note constant \( \Delta x \) and \( \Delta z \) were used in the present study). It shows that the driving force for gravitational circulation increases as the vertical mixing increases between km 0-32. To show the effect on the salinity field of increased vertical mixing, two contour plots of tidal mean salinity are presented in Fig. 6-9 for \( \alpha = 1.15 \times 10^{-2} \) and \( 1.725 \times 10^{-2} \). An increase in vertical mixing results in more homogeneous conditions with less salt being transported upriver. In the lower part of the river between km 0-30, increased vertical mixing affects the salinity field such that more salt is mixed upward (increasing the salinity near the surface) and less salt is transported upriver (decreasing the salinity near bottom). This altered salinity field for large \( \alpha \) \( (1.725 \times 10^{-2}) \), along with the same salinity boundary condition at the mouth, increases \( \partial s / \partial x \), which in turn enhances the gravitational circulation.

The conditions used to generate the residual velocities in Figures 4-17 and 4-18 are described in Section 4-4-1. Using the same conditions, the tidal mean characteristics, salinity, \( \Sigma(\Delta S_x) \) and vertically averaged tidal mean velocity over the bottom layer, during spring and neap tides are presented in Fig. 6-10. The salinity distributions in the lower part of the river, like those in Fig. 6-9, show that the enhanced vertical mixing during spring tide increases (decreases) the salinity near surface (bottom). However, the difference between spring and neap tides is so small that it may not cause significant change in \( \partial s / \partial x \), which is evident in the plot of \( \Sigma(\Delta S_x) \) in Fig. 6-10. With virtually the same \( \partial s / \partial x \) during spring and neap tides, the residual velocities in Figures 4-17 and 4-18 follow Hansen and Rattray's analytical solution. That the spring tide provides more mixing energy and thus has weaker residual circulation is shown in the plot of tidal mean

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velocity in Fig. 6-10.

As the vertical mixing increases, it has two opposing effects on the residual circulation. One is to weaken the circulation because more mixing enhances vertical momentum exchange, which process is from now on referred to as ME. The other is to strengthen the circulation by increasing $\partial s/\partial x$ (SG) and thus the driving force for the gravitational circulation as a result of changes in the salinity field. Whether the residual circulation increases or not as the vertical mixing increases depends upon the relative importance of two processes, ME and SG. Since the spring-neap cycle is short compared to the response time of longitudinal salinity distribution, it cannot cause significant change in $\partial s/\partial x$. Then, the residual circulation weakens during spring tide since ME dominates SG. In Figures 6-6 through 6-9, increased (50%) vertical mixing changes the salinity field in such a way that the effect of increased $\partial s/\partial x$ (SG) dominates that of ME resulting in the enhanced circulation.

As in Fig. 6-4, the enhanced DO in Fig. 6-6 is partly due to increased vertical mixing and partly due to faster water movement. Again, the present model, being a complicated model containing all terms in the continuity equation and momentum and mass balance equations (Equations 2-1 through 2-5), cannot separate the effect of the vertical mixing from that due to the gravitational circulation.

6-1-4. Spatial and temporal variations of bottom water DO

Both spatial and temporal variations of the bottom DO distribution in response to spring-neap cycle have been observed in the Rappahannock (Kuo et al. 1991a). The destratification-stratification cycle, closely related to the differential mixing over the spring-neap cycle, has been documented in the Rappahannock River as well as other Virginia tributaries of Chesapeake Bay (Haas 1977; D’Elia et al. 1981; Ruzecki & Evans 1986). The model’s ability to reproduce these spatial and temporal variations was
examined by comparing the DO concentrations during strong spring and neap tides. To eliminate the effect of DO boundary condition, a constant DO downstream boundary condition, that on 7/05/90, was used. Figure 6-11 shows the longitudinal DO distributions during strong spring and neap tides. The more vigorous tidal mixing during strong spring tide than neap tide is well reproduced by the model.

In Fig. 6-11, the location of minimum DO occurs further downriver during strong spring tide compared to neap tide, confirming another conclusion of Kuo et al. (1991a) derived from both field measurements and DO budget model. The conditions near the mouth of the Rappahannock River are such that the DO sink terms are greater than the source terms for the bottom water. The DO concentration, therefore, starts to decrease once a parcel of bottom water enters the river, and keeps decreasing as it travels upriver into the deep basin. As the bottom water travels beyond the deepest point in the basin into shallower waters, the DO replenishment due to vertical mixing increases. Since water depth generally decreases in the upriver direction, the DO source terms eventually become equal to the sink terms, at which point the minimum DO occurs. The location of this point depends on the intensity of vertical mixing. Because the increase in vertical mixing during strong spring tides increases the DO replenishment rate at a given depth, the balance between the source and sink terms will occur earlier in deeper water. The resulting downriver movement of the minimum DO location was observed around the times of strong spring tides (Kuo et al. 1991a), and is well reproduced by the model (Fig. 6-11).

Another view of the effect on bottom DO of the differential mixing over spring-neap cycle is presented as a time series plot of bottom DO (Fig. 6-12b). The tidal range from the surface elevation measured at the mouth (Fig. 6-12a) represents the intensity of tidal mixing. The temporal variation of the bottom DO in response to the differential tidal mixing is evident in Fig 6-12b; note the sudden decrease in bottom DO in response
to that in tidal range around day 31 and the increase in bottom DO during and after strong spring tide around day 49. Figure 6-12b also shows that the temporal variation of bottom DO in response to the differential tidal mixing decreases in the upriver direction.

6-1-5. Sediment and water column oxygen demand

The SOD of 2.0 g m\(^{-2}\) day\(^{-1}\) was obtained from the field measurements and model calibration (Table 5-4). The effect of SOD on hypoxic conditions was assessed in sensitivity runs, in which SOD values of 1.0 and 0.0 g m\(^{-2}\) day\(^{-1}\) were used. Results in Fig. 6-13 show that a decrease in SOD increases the absolute value of the bottom DO, which again confirms one of the conclusions in Kuo et al. (1991a). In Fig. 6-13, however, the shape of DO distribution also changes as SOD is varied, which does not agree with an argument in Kuo et al. (1991a). This difference in sensitivity of DO distribution to SOD change may be attributable to the differences in geometry used. Using spatially uniform SOD values and simple (constant width) geometry, Kuo et al. (1991a) argued that the shape of the longitudinal DO distribution would not be altered by changing the magnitude of SOD. However, Fig. 6-13 shows that when detailed geometry is used, the DO increase is more pronounced around km 40 than around km 20. Oxygen demand in the water column has dimension [M L\(^{-3}\) T\(^{-1}\)] while SOD has [M L\(^{-2}\) T\(^{-1}\)], which suggests that the effect of SOD is inversely proportional to a length scale. For the overall effect in a cross-section, the length scale of importance is volume/(bottom area), which is 9.1 m at km 18.6 and 5.3 m at km 38.6 (see Table 4-1). For each particular layer, the DO consumption due to SOD is proportional to the layer bottom area, \((B_k - B_{k+1}) \cdot \Delta x\) and inversely proportional to the layer volume, \(B_k \cdot \Delta x \cdot \Delta z\). Since constant layer thickness (\(\Delta z = 2\) m) and segment length (\(\Delta x = 2500\) m) are used, the DO consumption due to SOD is proportional to \((B_k - B_{k+1})/B_k\) (see Eq. 2-17b); the vertical mean \((B_k - B_{k+1})/B_k\) is 0.31 at km 18.6 and 0.43 at km 38.6 (see Table 4-1).
is these differences in geometry that make the DO increase due to the SOD reduction more pronounced around km 40 than that around km 20 in Fig. 6-13.

The sensitivity runs for Fig. 6-13 used the same downstream boundary condition and thus the system can have no sensitivity to SOD at the boundary. This suggests that potential sensitivity of DO distribution to any factor may increase with distance from the boundary. However, some factors increase bottom DO more around km 20 than around km 40; see curves (a) and (b) in Fig. 6-15. Therefore, a larger DO increase around km 40 than around km 20 (Fig. 6-13) is not necessarily due to distance from the boundary.

The SOD represents the oxygen demand from the sediment, and three other terms, CBOD decay ($K_c$), nitrification ($K_{AN}$) and algal respiration ($R$), represent the oxygen demand in the water column. The calibrated model has the corresponding rate constants at 20°C of 0.1 day$^{-1}$ (Table 5-4), 0.3 mg l$^{-1}$ day$^{-1}$ (Table 5-2) and 0.17 day$^{-1}$ (Table 5-1). The effect of these water column demand terms was examined in sensitivity runs, in which each of the terms and all three terms were eliminated. Results in Fig. 6-14 show that in the lower part of the river, the CBOD decay consumes the most DO. Field observations, and model calibration and verification (Figures 5-3 and 5-6) show a bimodal distribution of CBOD with one peak in the upper part of the river due to the STP discharges. The other peak in the lower part is due to the downstream boundary condition, and the hypoxic condition can be relieved by eliminating CBOD in the incoming bay water (Fig. 6-3).

To show the relative importance of the four oxygen demanding terms, the increase in the bottom DO that is caused by eliminating each term is presented in Fig. 6-15. It indicates that the DO consumption due to the water column demand (CBOD decay, nitrification and algal respiration) is as important as that due to SOD.
6-1-6. Summary

Hypoxia has been frequently observed during summer in the bottom water of the lower part of the tidal Rappahannock River. The sensitivity analysis shows that the bottom water will become hypoxic regardless of the DO and CBOD concentrations in the incoming bay water. The hypoxic condition can be relieved more by eliminating CBOD than by increasing DO in the incoming bay water. The sensitivity analysis also reveals that hypoxia is caused by a combination of physical and biochemical processes. Among the physical processes, an increase in either residual velocity or vertical mixing also can relieve the hypoxic condition. The present model is complicated, so the effects of vertical mixing and gravitational circulation cannot be separated.

Oxygen demands in both sediment and water column contribute to the formation of hypoxia in the lower part of the river. Water column demand, including CBOD decay, nitrification and algal respiration, is as important as SOD, and the CBOD decay is the most important in the water column.

6-2. Middle Part of the Tidal Rappahannock River

The middle part of the tidal Rappahannock River between km 85-145 is bounded by shallow regions at both boundaries (Fig. 3-2). The upper limit of salt intrusion, which moves up and down the river in response to the freshwater discharge, was located around km 85 in the summer of 1990 (Figures 5-3 and 5-6). In this tidal freshwater portion of the river, a characteristic Chl maximum has been frequently observed (Anderson 1986; Kuo et al. 1991b). As possible controlling mechanisms, Anderson (1986) suggested the hydrodynamic trapping of algal biomass in the region of the turbidity maximum, rapid internal cycling of essential nutrients such as silica, and the demise of freshwater algae in the presence of salt farther downriver.

The high phytoplankton concentration in the tidal freshwater and low salinity...
regions of estuaries has also been frequently observed in many other estuarine environments (Haertel et al. 1969; Lippsone et al. 1979; Cloern et al. 1983; Pennock 1985; Relexans et al. 1988; Schuchardt & Schirmer 1991). Key mechanisms suggested by these investigators are river discharge, water residence time, solar radiation, nutrients, etc. The sensitivity analysis for these suggested mechanisms was performed to study the controlling mechanism(s) for high Chl, and the results from sensitivity runs are shown in Figures 6-16 through 6-20.

6-2-1. Results from sensitivity runs

In Sections 5-2-5 and 5-3-2, the shortcomings of the current model calibration and verification for P2 were noted. Because the quality and quantity of the field data used for the current calibration and verification are limited, more detailed field data to calibrate the present model are needed before a reliable sensitivity analysis of nutrient limitation can be conducted. The current sensitivity analysis pertaining to nutrients, and results from these analysis should be construed with caution.

In model calibration, an external input of nutrients in the form of benthic flux of P2 and N2 was needed to reproduce the observed high Chl concentration in the mid-reach of the river. Results from a sensitivity run without the P2 benthic release are presented in Fig. 6-16, and those without the N2 release in Fig. 6-17. These two sensitivity runs are not intended to assess the limiting nutrient but to assess the degree to which an external input of nutrients (N2 and P2) is needed to maintain the high Chl concentration. Without P2 release from sediment in Fig. 6-16, the model predictions of Chl, P2 and total phosphorus are lower than the field data between km 85-140. In Fig. 6-17, the high Chl between km 85-125 cannot be maintained without the N2 benthic flux and the model predictions of total nitrogen between km 80-165 are low compared to field data. Therefore, both P2 and N2 fluxes from sediment are necessary to maintain the
high Chl in the mid-reach and to reproduce the field measurements of total nitrogen and phosphorus.

The shallow embayments may have high primary production owing to the shallow depths. It, thus was suspected that the side storage areas might be responsible, at least in part, for the high Chl concentration in the main channel. Results from a sensitivity run without the storage area show negative contribution from storage area in the mid-reach of the river (Fig. 6-18), that is, the storage area acts as a sink for Chl. The Chl settling rate of 10 cm day\(^{-1}\) was used in both the main channel and the storage area in model calibration. Results from a sensitivity run (not shown) indicate that the Chl in the main channel increases with zero settling rate of Chl in the storage area. Because of the shallower depth, the loss of Chl due to settling may be higher in the storage area than in the main channel.

The effect of light intensity was examined by increasing and decreasing the light extinction coefficient (\(K_e\)). Results in Fig. 6-19 show that the Chl concentration increases (decreases) significantly as \(K_e\) decreases (increases) upriver of km 145. The light availability used in model calibration is necessary to maintain the high Chl concentration between km 85-145. Finally, the results from model simulations with altered freshwater discharge rates are presented in Fig. 6-20. It shows that the effect of freshwater discharge rate over the range used in the sensitivity runs is important only upriver of km 125.

Results in Figures 6-16 through 6-20 indicate that the availability of light and nutrients, phosphate and ammonia, is essential to maintain the high Chl concentration between km 85-125. As one of the possible controlling mechanisms for the high Chl concentration in the mid-reach of the Rappahannock River, Anderson (1986) suggested the rapid internal cycling of essential nutrients such as silica. The present model, since it does not include the silica cycle, cannot assess the importance of silica. The
sensitivity runs, however, do indicate that the high Chl concentrations observed during
the summer cannot be maintained without an external input of phosphate and ammonia.

6-2-2. Hypothesis

If an external input of nutrients is required to maintain the high Chl concentration,
where do the nutrients come from? Another characteristic of high Chl in the mid-reach
of the river is the downriver boundary that limits the high Chl upriver of km 85 (Figures
5-3 and 5-6). A hypothesis is proposed to account for the source of nutrients and the
downriver limit.

Four STP's discharge wastewater, which is the primary source of inorganic
nutrients, into the upper 10 km reach of the tidal Rappahannock River. It was necessary
in model calibration to have a high settling rate of P2 near the STP discharges and a loss
of phosphate to the sediment has been well established (see Section 5-2-3). These
phosphorus-rich sediment particles are a possible source of P2 for the mid-reach of the
river.

Nichols et al. (1981) investigated the sediment response triggered by the high flow
event in the tidal Rappahannock River. They suggested from the HIFLO observations in
1978 that sediment transport through the freshwater reaches is a stepwise process
involving temporary accumulation followed by resuspension and downriver transport. In
1990, the largest freshwater discharge (368 cms) occurred on May 11; a runoff event of
this size is about eight times the long-term mean discharge rate (46.8 cms). This
"normal" high flow, which has a recurrence interval slightly greater than one year,
although not a major flood, is large enough to transport the phosphate-laden sediments to
the mid-reach of the river (Nichols et al. 1981). The subsequent release of phosphate
from these sediments may be the nutrient source that supports the high Chl
concentration.
If sediments are transported from the vicinity of the STP’s and if subsequent nutrient release from those sediments provides nutrients in the mid-reach, another question is why the Chl maximum stops around km 85? Why is this the downriver limit of high Chl? The mid-reach of the river is shaped like a deep hole with the deepest region occurring around km 100; it is separated from the saline, lower part of the river by a shallow region between km 65-80 (Fig. 3-2). This bottom topography would require a major flood, i.e., freshwater discharge that is much larger than the annual peak discharge, to push the sediment over the shallow region and into the lower part of the river. That is, the geometric trapping of the nutrient-laden sediments in the deep hole in the mid-reach of the river may be responsible for the formation of downriver limit of high Chl around km 85.

The turbidity maximum forms around the null point (Conomos & Peterson 1977; Kuo et al. 1978), which was located around km 85 on 7/5/90. Therefore, another possibility for the downriver limit of high Chl is the hydrodynamic trapping of the nutrient-laden sediments in the region of the turbidity maximum.

Other possibilities for the downriver limit of high Chl suggested by Anderson (1986) are the hydrodynamic trapping of phytoplankton biomass in the region of the turbidity maximum and demise of freshwater phytoplankton as it reaches the saline part of the river. Without trapping of nutrient-laden sediments in the deep hole over the mid-reach, the sediments would be transported downriver into the lower part and release nutrients into the water column. Figure 6-21 shows the model predictions from a sensitivity run in which both N2 and P2 benthic fluxes were extended to the river mouth. The Chl distribution in Fig. 6-21 shows that the hydrodynamic trapping of Chl alone, without trapping of sediments, cannot limit the Chl maximum upriver of km 85 in the Rappahannock River. Results from another sensitivity run without salt, i.e., assuming homogeneous river (note the gravitational circulation and thus the hydrodynamic trapping
of Chl no longer exists), are presented in Fig. 6-22. The Chl distribution in Fig. 6-22 shows that the trapping of sediments alone without the hydrodynamic trapping of Chl can limit the Chl maximum upriver of km 85.

Another interesting point in Fig. 6-22 is the absence of hypoxia in the bottom water without salt in the system. In the calibration run, the gravitational circulation and thus stratification exist in the lower part of the river between km 0-55. Without salt, there is no stratification and thus no reduction in vertical mixing in this lower part of the river. The spatial average of tidal mean $K_z$ over km 0-55, which is 1.3 cm$^2$ sec$^{-1}$ for the calibration, increases to 3.9 cm$^2$ sec$^{-1}$ for the no-salt scenario. Therefore, one mechanism to increase the bottom DO in Fig. 6-22 is the increased vertical mixing. The CBOD in the lower part of the river is due to the transport of CBOD-laden bay water into the river (Fig. 6-5). Without salt, the gravitational circulation no longer exists and water flows downriver at all depths between km 0-55. The CBOD concentration between km 0-55, thus, decreases in the absence of transport of CBOD-laden bay water into the river. Since the CBOD decay is the most important DO consuming process in the water column (Fig. 6-15), another contributing factor for the elevated bottom DO in Fig. 6-22 is the reduced CBOD concentration in the lower part of the river due to the absence of gravitational circulation.

The upper limit of salt intrusion on July 5, 1990 was located around km 85 (Fig. 5-3), which coincides with the downriver boundary of the deep hole over which high Chl was observed. Since the high Chl occurred in the freshwater part and extended downriver to km 85, death of freshwater phytoplankton in the presence of salt might contribute to the formation of downriver limit of high Chl concentration at the limit of salt intrusion.
6-2-3. Summary

High Chl concentrations in the lower portion of tidal freshwater have been observed frequently in the Rappahannock River and many other estuaries. The sensitivity analysis shows that the high Chl cannot be maintained without an external input of nutrients. A hypothesis is proposed to account for the source of nutrients and the formation of downriver limit of high Chl concentration.

It is likely that the sediments are transported from the upper part of the river during times of high freshwater flow and subsequently nutrients are released from the transported sediments. It seems that the geometric and hydrodynamic trapping of nutrient-laden sediments, and possibly the demise of freshwater phytoplankton in the salt water, limit the high Chl concentration to the segment upriver of km 85. To simulate these processes more completely, the water quality model should include a sediment transport model and a sediment diagenesis model. The mechanisms that appear to be of significance include the adsorption of phosphate to sediment particles and subsequent settling, sediment transport in response to high freshwater flow and sediment phosphate release. Differentiation of phytoplankton species is necessary to assess the effect of the demise of freshwater phytoplankton in the salt water on the formation of the downriver limit of high Chl.
Figure 6-1. DO downstream boundary conditions in the bottom layer used in sensitivity runs.
Figure 6-2. Sensitivity to DO downstream boundary condition on 7/05/90.
Figure 6-3. Sensitivity to DO and CBOD downstream boundary conditions on 7/05/90.
Figure 6-4. Sensitivity to gravitational circulation on 7/05/90.
Figure 6-5. Tidal mean vertical diffusivity and velocity on 7/05/90 when varying $k$. 

TIDAL MEAN $K_z$ (cm$^2$ sec$^{-1}$): average over total depth

- CALIBRATION ($k = 0.00075$)
- 120% OF CALIBRATION ($k = 0.0009$)
- 130% OF CALIBRATION ($k = 0.000975$)

NEGATIVE VELOCITY IS IN UPRIVER DIRECTION

TIDAL MEAN VELOCITY (cm sec$^{-1}$): average over bottom layer

DISTANCE FROM MOUTH (km)
CONSTANT, $\alpha$, IN VERTICAL MIXING TERM (Eq. 2-17)

- CALIBRATION (0.0115)
- 120% OF CALIBRATION (0.0138)
- 150% OF CALIBRATION (0.01725)

**Figure 6-6.** Sensitivity to vertical mixing on 7/05/90.
Figure 6-7. Tidal mean vertical diffusivity and velocity on 7/05/90 when varying \( \alpha \).
\[ \Sigma(\Delta S_x) \text{ in ppt} \]

\[ \Delta S_x = \text{longitudinal gradient of tidal mean salinity} \]

**CALIBRATION**
- \[ \alpha = 0.0115 \]
- \[ \alpha = 0.0138 \]
- \[ \alpha = 0.01725 \]

**TIDAL MEAN VELOCITY** (cm sec\(^{-1}\)), average over bottom layer

**DISTANCE FROM MOUTH** (km)

**NEGATIVE VELOCITY IS IN UPRIVER DIRECTION**

Figure 6-8. Tidal mean longitudinal salinity gradient and velocity on 7/05/90 when varying \( \alpha \).
Figure 6-9. Tidal mean salinity distributions on 7/05/90 when varying $\alpha$. 

$\alpha = 0.0115$ (CALIBRATION)

$\alpha = 0.01725$
Figure 6-10. Tidal mean salinity, salinity gradient and velocity during spring and neap tides: the conditions used are described in Section 4-4-1.
Figure 6-11. DO distributions during strong spring and neap tides using constant boundary conditions.
Figure 6-12. Downstream boundary condition for surface elevation (a) and time series of DO at the bottom layer (b).
Figure 6-13. Sensitivity to sediment oxygen demand on 7/05/90.

SOD \( \text{g m}^{-2} \text{ day}^{-1} \)
- 2.0: CALIBRATION
- 1.0
- 0.0

DO CONCENTRATION \( \text{mg l}^{-1} \)

DISTANCE FROM MOUTH \( \text{km} \)

FIELD MODEL
- SURFACE
- BOTTOM
- MID-DEPTH

• MEASURED AT 6 m DEPTH
WHILE TOTAL DEPTH IS 14 m
Figure 6-14. Sensitivity to water column oxygen demand on 7/05/90.
Figure 6-15. Contribution to hypoxia of oxygen demands in water column and sediment on 7/05/90.
Figure 6-16. Sensitivity to benthic flux of phosphate between km 80-147 on 7/05/90.
Figure 6-17. Sensitivity to benthic flux of ammonia between km 80-175 on 7/05/90.
Figure 6-18. Sensitivity to the presence of side storage area on 7/05/90.
Figure 6-19. Sensitivity to light extinction coefficient on 7/05/90.
Figure 6-20. Sensitivity to freshwater discharge rate on 7/05/90.
Figure 6-21. Sensitivity to benthic fluxes of ammonia and phosphate between km 0-80 on 7/05/90.
Figure 6-22. Sensitivity to the presence of salt on 7/05/90.
VII. SUMMARY AND RECOMMENDATIONS

7-1. Summary

A mathematical model has been developed to study the hydrodynamic and water quality characteristics of estuaries. The model, consisting of a hydrodynamic model and a water quality model, is a laterally integrated, two-dimensional, real-time model. The hydrodynamic model is based on the principles of conservation of volume, momentum and mass, and the water quality model on the conservation of mass alone. The model was solved using a two time level, finite difference scheme, and was applied to the tidal Rappahannock River, Virginia.

7-1-1. Hydrodynamic model

The hydrodynamic model, which provides real-time predictions of surface elevation, current velocity and transport of a conservative substance (salt), has been calibrated and verified using field data collected in 1987 and 1990. Results from the mean tide calibration show that the model describes the tidal characteristics along the river very well. The vertical mixing terms were parameterized using Munk and Anderson-type formulations. Calibration of these terms using the salinity data from 1987 slackwater surveys shows that the model provides very good description of prototype salinity distributions. The model capability of reproducing advective transport was verified by simulating the time series measurements of surface elevation and current velocity in 1987. The subtidal variations in surface elevation and current velocity also were examined. Excellent agreement exists between predictions and observations for both the semi-diurnal tidal fluctuations and the subtidal (longer-term) variations. The importance of surface wind stress and bay conditions (velocity and salinity) for the residual velocity was discussed. The model capability of reproducing the diffusive
transport was verified by the agreement between model predictions and 1990 slackwater survey salinity data.

The hydrodynamic model, once calibrated and verified, was used to study the hydrodynamic features of the tidal Rappahannock River. A reverse longitudinal salinity gradient, an increase in salinity in the upriver direction, has been observed frequently in the Rappahannock River. It was thought that the reverse gradient might be explained by the bottom topography of the river and variations in vertical mixing. The saline bay water, that enters the river through the mouth and moves upriver along the bottom, might be deflected upward in the presence of obstacles such as a sloping bottom, thereby creating the reverse gradient. Sensitivity runs indicated that the reverse gradient could be expected to occur frequently in the Rappahannock River, which has upriver-sloping bottom geometry between km 40-50, but that it might be erased by strong mixing during spring tides and/or by strong winds. This argument was further supported by the salinity data from 1981-1990 slackwater surveys by VIMS.

The model predictions of residual velocity showed the two-layer estuarine circulation present in the lower Rappahannock River, and the magnitude was consistent with the field measurements. The response of residual velocity to the spring-neap cycle indicated stronger residual circulation during neap tide than spring tide. The response to increased freshwater discharge of the downriver movement of the limit of salt intrusion and of the null point, where the level of no-net-motion meets the estuary bottom, was faithfully reproduced by the model.

The distinction between the limit of salt intrusion and the limit of gravitational circulation in real estuaries with irregular bottom topography was examined. The null point occurs where the longitudinal density gradient integrated over the total depth (baroclinic) balances the mean surface slope due to the freshwater discharge (barotropic). Then, the location of the null point relative to the limit of salt intrusion is a function of
longitudinal salinity gradient, total depth and surface slope. If the bottom topography in an estuary is such that an increase in freshwater discharge pushes the limit of salt intrusion downriver into a shallow region (e.g., around km 80 in the Rappahannock River), then, despite the augmented longitudinal salinity gradient, the reduced total depth makes the increase in baroclinic forcing not as large as that in barotropic forcing. The balance between baroclinic and barotropic forcing (i.e., null point) occurs further downriver than the limit of salt intrusion. If the freshwater discharge is large enough to push the limit of salt intrusion downriver of the shallow region into the deep part, the null point occurs closer to the limit of salt intrusion. All these features were well reproduced by the model.

7-1-2. Water quality model

The water quality model, supplied with the information of the physical transport processes from the hydrodynamic model, provides real-time predictions of eight water quality parameters: dissolved oxygen, chlorophyll 'a', carbonaceous biochemical oxygen demand, organic nitrogen, ammonia nitrogen, nitrite-nitrate nitrogen, organic phosphorus and inorganic phosphorus.

The water quality model has been calibrated and verified using field data from the summer of 1990. They include the slackwater survey data by VIMS and the data collected by the Virginia Water Control Board as a part of the Chesapeake Bay Fall Line and Tributary Water Quality Monitoring Program. Considering the random variability inherent in natural systems and the goal of consistency in calibrated coefficients, the agreement between model predictions and field observations is more than satisfactory. In general, the agreement between predictions and observations depends upon both the quality and quantity of input data, and the nature and number of observations. The water quality model results are commensurate with the quality and quantity of the data.
available to this study.

The water quality model, calibrated and verified, was used to study the water quality processes in the tidal Rappahannock River. Hypoxia, even anoxia, has been frequently observed during summer in the bottom water of the lower part of the river. The sensitivity analysis indicated that the bottom water will become hypoxic regardless of the DO and CBOD concentrations in the incoming bay water. The hypoxic condition can be relieved more by eliminating CBOD than by increasing DO in the incoming bay water. The sensitivity analysis also revealed that hypoxia is caused by a combination of physical and biochemical processes. Among the physical processes, an increase in either residual circulation or vertical mixing can relieve the hypoxic condition. The present model, being a complicated model, cannot separate the effects of vertical mixing and gravitational circulation though. Oxygen demands in both sediment and water column contribute to the formation of hypoxia. The contribution of water column demands (CBOD decay, nitrification and algal respiration) to hypoxia is as important as that of SOD. In the water column, the CBOD decay is the most important DO consuming process.

High chlorophyll concentrations in the lower portion of tidal freshwater have been observed frequently in the Rappahannock River as well as in many other estuarine environments. Model sensitivity runs showed that the high chlorophyll in the Rappahannock River cannot be maintained without an external input of nutrients. A hypothesis was proposed to account for the source of nutrients and the downriver limit of the high chlorophyll concentrations. It is likely that sediments are transported from the upper part of the river during times of high freshwater flow, and subsequently nutrients are released from the transported sediments. It appears that the geometric and hydrodynamic trapping of nutrient-laden sediments, and possibly the demise of freshwater phytoplankton in the salt water, limit the high chlorophyll concentrations to
the segment upriver of km 85.

7-2. Recommendations

During the present study, the following limitations have been noted. These need to be further investigated and to be included in future models to improve predictive capability.

1) As almost all other investigators have noticed, it is the turbulence closure model that limits the predictive capability of the hydrodynamic model and thus its applicability to other systems. More understanding and better mathematical representation of the turbulent mixing processes are essential to improve the model capability. We should devote more effort studying the behavior of potentially promising methods, which include the K-ε model, Reynolds stress model, Mellor and Yamada Level 2½ model, etc.

2) Coupling of the water quality model with a sediment transport model and a sediment diagenesis model is important to predict the nutrient movement, particularly for phosphate and sediment-nutrient exchanges. The mechanisms that appear to be of significance include the adsorption of phosphate to sediment particles and subsequent settling, sediment transport in response to high freshwater flow and sediment phosphate release.

3) The demise of freshwater phytoplankton in the presence of salt is thought be a possible mechanism that limits the characteristic high chlorophyll concentration to the tidal freshwater portion of the river, as has been frequently observed in many estuarine environments including the Rappahannock River. Therefore, differentiation of phytoplankton species in the water quality model is called for to be able to predict the spatial extent, especially downriver limit, of the high chlorophyll concentration.

4) The current calibration and verification of the water quality model was limited by
the quality and quantity of the field data available. The present model needs to be calibrated with more detailed and extensive data set. Once there is more confidence in model calibration, one can perform the sensitivity analysis pertaining to nutrient limitation.


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