2 Water Quality Model Formulation

Introduction

CE-QUAL-ICM was designed to be a flexible, widely-applicable eutrophication model. Initial application was to Chesapeake Bay (Cerco and Cole 1994). Subsequent additional applications included the Delaware Inland Bays (Cerco et al. 1994), Newark Bay (Cerco and Bunch 1997), San Juan Estuary (Bunch et al. 2000), Virginia Tributary Refinements (Cerco et al. 2002) and the 2002 (Cerco and Noel 2004) and 2010 (Cerco et al. 2010) Chesapeake Bay models. Each application employed a different combination of model features and required addition of system-specific capabilities. This chapter describes general features and site-specific developments of the model as applied to the water column of Chesapeake Bay in the 2015 model verson.

Conservation of Mass Equation

The foundation of CE-QUAL-ICM is the solution to the three-dimensional mass-conservation equation for a control volume. Control volumes correspond to cells on the model grid. CE-QUAL-ICM solves, for each volume and for each state variable, the equation:

$$\frac{\delta V_j \cdot C_j}{\delta t} = \sum_{k=1}^{n} Q_k \cdot C_k + \sum_{k=1}^{n} A_k \cdot D_k \cdot \frac{\delta C}{\delta x_k} + \Sigma S_j \qquad (1)$$

in which:

V_j = volume of j^{th} control volume (m^3)
C_j = concentration in j^{th} control volume (g m^{-3})
t, x = temporal and spatial coordinates
n = number of flow faces attached to j^{th} control volume
Q_k = volumetric flow across flow face k of j^{th} control volume (m^3 s^{-1})
C_k = concentration in flow across face k (g m^{-3})
A_k = area of flow face k (m^2)
D_k = diffusion coefficient at flow face k (m^2 s^{-1})
S_j = external loads and kinetic sources and sinks in j^{th} control volume (g s^{-1})

Solution of Equation 1 on a digital computer requires discretization of the continuous derivatives and specification of parameter values. The equation is solved using the QUICKEST algorithm (Leonard 1979) in the horizontal plane and an implicit central-difference scheme in the vertical direction. Discrete time steps, determined by computational stability requirements, are ≈ 5 minutes.

State Variables

At present, the CE-QUAL-ICM model incorporates 24 state variables in the water column including physical variables, multiple algal groups, and multiple forms of carbon, nitrogen, and phosphorus (Table 2-1).

Algae

Algae are grouped into three model classes: freshwater, spring diatoms, and other green algae. The model formulations for the three groups are virtually identical. The definition of three groups provides flexibility in parameter evaluation to fit various regions of the Bay system. In particular, definition of a freshwater group allows maximum flexibility in parameter specification in freshwater portions of the system which vary greatly in terms of physical characteristics, loading, and surroundings. The spring diatoms are large phytoplankton which produce an annual bloom in the saline portions of the bay and tributaries. Algae which do not fall into the preceding two groups are lumped into the heading of green algae. The green algae represent the mixture that characterizes saline waters during summer and autumn, and freshwater regions in which a specific algal group is not defined. Non-bloom forming diatoms comprise a portion of this mixture.

Organic Carbon

Four organic carbon state variables are considered: dissolved, labile particulate, refractory particulate, and G3 particulate. Labile, refractory, and G3 distinctions are based upon the time scale of decomposition. Labile organic carbon decomposes on a time scale of days to weeks while refractory organic carbon requires more time. G3 particulate carbon is virtually inert in the water column. The three particulate organic carbon groups correspond to the three G groups in the sediment diagenesis model (DiToro and Fitzpatrick 1993) although the decay rates may differ between the water column and sediments.

Nitrogen

Nitrogen is first divided into available and unavailable fractions. Available refers to employment in algal nutrition. Two available forms are considered: reduced and oxidized nitrogen. Ammonium is the single reduced nitrogen form. Nitrate and nitrite comprise the oxidized nitrogen pool. Both reduced and oxidized nitrogen are utilized to fulfill algal nutrient requirements. The primary reason for distinguishing the two is that ammonium is oxidized by nitrifying bacteria into nitrite and, subsequently, nitrate. This oxidation can be a significant sink of oxygen in the water column and sediments.

Unavailable nitrogen state variables are dissolved organic nitrogen, labile particulate organic nitrogen, refractory particulate organic nitrogen, and G3 particulate organic nitrogen.

Phosphorus

As with nitrogen, phosphorus is first divided into available and unavailable fractions. Only a single available form, dissolved phosphate, is considered. Five forms of unavailable phosphorus are considered: dissolved organic phosphorus, labile particulate organic phosphorus, refractory particulate organic phosphorus, G3 particulate organic phosphorus, and particulate inorganic phosphorus.

Chemical Oxygen Demand

Reduced substances that are oxidized by abiotic processes are combined in the chemical oxygen demand pool. The primary component of chemical oxygen demand in saltwater is sulfide released from sediments. Oxidation of sulfide to sulfate may remove substantial quantities of dissolved oxygen from the water column. In freshwater, the primary component is methane which is likewise released from bottom sediments.

Dissolved Oxygen

Dissolved oxygen is required for the existence of higher life forms. Oxygen availability determines the distribution of organisms and the flows of energy and nutrients in an ecosystem. Dissolved oxygen is a central component of the water-quality model.

Salinity

Salinity is a conservative tracer which provides verification of the transport component of the model and facilitates examination of conservation of mass. Salinity also influences the dissolved oxygen saturation concentration and may be used in the determination of kinetics constants which differ in saline and fresh water.

Temperature

Temperature is a primary determinant of biochemical reaction rates. Reaction rates increase as a function of temperature although extreme temperatures may result in the mortality of organisms and a decrease in kinetics rates.

Fixed Solids

Fixed solids are the mineral fraction of total suspended solids. In previous model versions, fixed solids contributed to light attenuation and formed a site for sorption of dissolved inorganic phosphorus. The former role of fixed

solids is now occupied by the four solids classes incorporated in the suspended solids model. The fixed solids variable is retained but has no present function.

The remainder of this chapter is devoted to detailing the kinetics sources and sinks and to reporting parameter values. For notational simplicity, the transport terms are dropped in the reporting of kinetics formulations.

Algae

Equations governing the three algal groups are largely the same. Differences among groups are expressed through the magnitudes of parameters in the equations. Generic equations are presented below.

Algal sources and sinks in the conservation equation include production, metabolism, predation, and settling. These are expressed:

$$\frac{\delta}{\delta t}B = \left(G - BM - Wa \cdot \frac{\delta}{\delta z}\right)B - PR \qquad (2)$$

in which:

B = algal biomass, expressed as carbon (g C m^{-3})
G = growth (d^{-1})
BM = basal metabolism (d^{-1})
Wa = algal settling velocity (m d^{-1})
PR = predation (g C m^{-3} d^{-1})
z = vertical coordinate

Production

Production by phytoplankton is determined by the intensity of light, by the availability of nutrients, and by the ambient temperature.

Light

The influence of light on phytoplankton production is represented by a chlorophyll-specific production equation (Jassby and Platt 1976):

$$P^B = P^Bm \frac{I}{\sqrt{I^2 + Ik^2}} \qquad (3)$$

in which:

P^B = photosynthetic rate (g C g^{-1} Chl d^{-1})
P^Bm = maximum photosynthetic rate (g C g^{-1} Chl d^{-1})
I = irradiance (E m^{-2} d^{-1})

Parameter Ik is defined as the irradiance at which the initial slope of the production vs. irradiance relationship (Figure 2-1) intersects the value of $P^B m$

$$Ik = \frac{P^B m}{\alpha} \qquad (4)$$

in which:

α = initial slope of production vs. irradiance relationship (g C g^{-1} Chl (E m^{-2})$^{-1}$)

Chlorophyll-specific production rate is readily converted to carbon specific growth rate, for use in Equation 2, through division by the carbon-to-chlorophyll ratio:

$$G = \frac{P^B}{CChl} \qquad (5)$$

in which:

CChl = carbon-to-chlorophyll ratio (g C g^{-1} chlorophyll a)

Nutrients

Carbon, nitrogen, and phosphorus are the primary nutrients required for algal growth. Diatoms require silica, as well. Inorganic carbon and silica are usually available in excess and are not considered in the model. The effects of the remaining nutrients on growth are described by the formulation commonly referred to as "Monod kinetics" (Figure 2-2; Monod 1949):

$$f(N) = \frac{D}{KHd + D} \qquad (6)$$

in which:

f(N) = nutrient limitation on algal production ($0 \leq f(N) \leq 1$)
D = concentration of dissolved nutrient (g m^{-3})
KHd = half-saturation constant for nutrient uptake (g m^{-3})

Temperature

Algal production increases as a function of temperature until an optimum temperature or temperature range is reached. Above the optimum, production declines until a temperature lethal to the organisms is attained. Numerous functional representations of temperature effects are available. Inspection of growth versus temperature data indicates a function similar to a Gaussian probability curve (Figure 2-3) provides a good fit to observations:

$$f(T) = e^{-KTg1 \cdot (T - Topt)^2} \quad when \quad T \le Topt$$
$$= e^{-KTg2 \cdot (Topt - T)^2} \quad when \quad T > Topt \qquad (7)$$

in which:

T = temperature (^oC)
Topt = optimal temperature for algal growth (^oC)
KTg1 = effect of temperature below Topt on growth ($^oC^{-2}$)
KTg2 = effect of temperature above Topt on growth ($^oC^{-2}$)

Constructing the Photosynthesis vs. Irradiance Curve

A production versus irradiance relationship is constructed for each model cell at each time step. First, the maximum photosynthetic rate under ambient temperature and nutrient concentrations is determined:

$$P^Bm(N,T) = P^Bm \cdot f(T) \cdot \frac{D}{KHd + D} \qquad (8)$$

in which:

$P^Bm(N,T)$ = maximum photosynthetic rate under ambient temperature and nutrient concentrations (g C g^{-1} Chl d^{-1})

The single most limiting nutrient is employed in determining the nutrient limitation.

Next, parameter Ik is derived from Equation 4. Finally, the production vs. irradiance relationship is constructed using $P^Bm(N,T)$ and Ik. The resulting production versus irradiance curve exhibits three regions (Figure 2-4). For I >> Ik, the value of the term $I / (I^2 + Ik^2)^{½}$ approaches unity and temperature and nutrients are the primary factors that influence production. For I << Ik, production is determined solely by α and irradiance I. In the region where the initial slope of the production versus irradiance curve intercepts the line indicating production at optimal illumination, I ≈ Ik, production is determined by the combined effects of temperature, nutrients, and light.

Irradiance

Irradiance at the water surface is evaluated at each model time step. Instantaneous irradiance is computed by fitting a sin function to daily total irradiance:

$$Io = \frac{\Pi}{2 \cdot FD} \cdot IT \cdot \sin\left(\frac{\Pi \cdot DSSR}{FD}\right) \qquad (9)$$

in which:

Io = irradiance at water surface (E m^{-2} d^{-1})
IT = daily total irradiance (E m^{-2})
FD = fractional daylength ($0 \leq FD \leq 1$)
DSSR = time since sunrise (d)

Io is evaluated only during the interval:

$$\frac{1 - FD}{2} \leq DSM \leq \frac{1 + FD}{2} \qquad (10)$$

in which:

DSM = time since midnight (d)

Outside the specified interval, Io is set to zero.

Irradiance declines exponentially with depth below the surface. The diffuse attenuation coefficient, Ke, is computed as a function of color and concentrations of organic and mineral solids.

Respiration

Two forms of respiration are considered in the model: photo-respiration and basal metabolism. Photo-respiration represents the energy expended by carbon fixation and is a fixed fraction of production. In the event of no production (e.g. at night), photo-respiration is zero. Basal metabolism is continuous energy expenditure to maintain basic life processes. In the model, metabolism is considered to be an exponentially increasing function of temperature (Figure 2-5). Total respiration is represented:

$$R = Presp \cdot G + BM \cdot e^{KTb \cdot (T - Tr)} \qquad (11)$$

in which:

Presp = photo-respiration ($0 \leq Presp \leq 1$)
BM = metabolic rate at reference temperature Tr (d^{-1})
KTb = effect of temperature on metabolism ($^oC^{-1}$)
Tr = reference temperature for metabolism (^oC)

Predation

The predation term includes the activity of zooplankton, other pelagic filter feeders including planktivorous fish, and filter-feeding benthos. Predation in the water column is modeled by assuming predators clear a specific volume of water per unit biomass:

$$PR = F \times B \times M \qquad (12)$$

in which:

F = filtration rate (m^3 g^{-1} predator C d^{-1})
M = planktivore biomass (g C m^{-3})

Detailed specification of the spatial and temporal distribution of the predator population is impossible. One approach is to assume predator biomass is proportional to algal biomass, $M = \gamma B$, in which case Equation 12 can be rewritten:

$$PR = \gamma \cdot F \cdot B^2 \qquad (13)$$

Since neither γ nor F are known precisely, the logical approach is to combine their product into a single unknown determined during the model calibration procedure. Effect of temperature on predation is represented with the same formulation as the effect of temperature on respiration. The final representation of predation is:

$$PR = Phtl \cdot B^2 \qquad (14)$$

in which:

Phtl = rate of water column planktivore predation (m^3 g^{-1} C d^{-1})

Predation by filter-feeding benthos is represented as a loss term only in model cells that intersect the bottom. Details of the benthos computations may be found in Cerco and Noel (2010).

Accounting for Algal Phosphorus

The amount of phosphorus incorporated in algal biomass is quantified through a stoichiometric ratio. Thus, total phosphorus in the model is expressed:

$$TotP = PO_4 + Apc \cdot B + DOP + LPOP + RPOP + G3OP + PIP \qquad (15)$$

in which:

TotP = total phosphorus (g P m^{-3})
PO_4 = dissolved phosphate (g P m^{-3})
Apc = algal phosphorus-to-carbon ratio (g P g^{-1} C)
DOP = dissolved organic phosphorus (g P m^{-3})
LPP = labile particulate organic phosphorus (g P m^{-3})
RPP = refractory particulate organic phosphorus (g P m^{-3})
G3OP = G3 organic phosphorus (g P m^{-3})
PIP = particulate inorganic phosphorus (g P m^{-3})

Algae take up dissolved phosphate during production and release dissolved phosphate and organic phosphorus through respiration. The fate of phosphorus released by respiration is determined by empirical distribution

coefficients. The fate of algal phosphorus recycled by predation is determined by a second set of distribution parameters.

Accounting for Algal Nitrogen

Model nitrogen state variables include ammonium, nitrate+nitrite, dissolved organic nitrogen, labile particulate organic nitrogen, refractory particulate organic nitrogen, and G3 particulate organic nitrogen. The amount of nitrogen incorporated in algal biomass is quantified through a stoichiometric ratio. Thus, total nitrogen in the model is expressed:

$$TotN = NH_4 + NO_{23} + Anc \cdot B + DON + LPON + RPON + G3ON \quad (16)$$

in which:

TotN = total nitrogen (g N m^{-3})
NH_4 = ammonium (g N m^{-3})
NO_{23} = nitrate+nitrite (g N m^{-3})
Anc = algal nitrogen-to-carbon ratio (g N g^{-1} C)
DON = dissolved organic nitrogen (g N m^{-3})
LPON = labile particulate organic nitrogen (g N m^{-3})
RPON = refractory particulate organic nitrogen (g N m^{-3})
G3ON = G3 particulate organic nitrogen (g N m^{-3})

As with phosphorus, the fate of algal nitrogen released by metabolism and predation is represented by distribution coefficients.

Algal Nitrogen Preference

Algae take up ammonium and nitrate+nitrite during production and release ammonium and organic nitrogen through respiration. Nitrate+nitrite is internally reduced to ammonium before synthesis into biomass occurs (Parsons et al. 1984). Trace concentrations of ammonium inhibit nitrate reduction so that, in the presence of multiple nitrogenous nutrients, ammonium is utilized first. The "preference" of algae for ammonium is expressed by a modification of an empirical function presented by Thomann and Fitzpatrick (1982):

$$PN = NH_4 \cdot \frac{NO_{23}}{(KHNH_4 + NH_4) \cdot (KHNH_4 + NO_{23})} + NH_4 \cdot \frac{KHNH_4}{(NH_4 + NO_{23}) \cdot (KHNH_4 + NO_{23})} \quad (17)$$

in which

PN = algal preference for ammonium uptake ($0 \leq PN \leq 1$)
$KHNH_4$ = half saturation concentration for algal ammonium uptake (g N m^{-3})

Our modification substitutes a specific half-saturation concentration for ammonium uptake, $KHNH_4$, for the original use of half-saturation concentration for nitrogen uptake, KHn. We found the modification enforces ammonium use down to lower concentrations that the original formulation.

The preference function has two limiting values (Figure 2-6). When nitrate+nitrite is absent, the preference for ammonium is unity. When ammonium is absent, the preference is zero. In the presence of ammonium and nitrate+nitrite, the preference depends on the abundance of both forms relative to the half-saturation constant for ammonium uptake. When ammonium and nitrate+nitrite are both abundant, the preference for ammonium approaches unity. When ammonium is scarce but nitrate+nitrite is abundant, the preference decreases in magnitude and a significant fraction of algal nitrogen requirement comes from nitrate+nitrite.

Effect of Algae on Dissolved Oxygen

Algae produce oxygen during photosynthesis and consume oxygen through respiration. The quantity produced depends on the form of nitrogen utilized for growth. More oxygen is produced, per unit of carbon fixed, when nitrate is the algal nitrogen source than when ammonium is the source. Equations describing algal uptake of carbon and nitrogen and production of dissolved oxygen (Morel 1983) are:

$$106\ CO_2 + 16\ NH_4^+ + H_2PO_4^- + 106\ H_2O \text{ - - >}$$

$$\text{protoplasm} + 106\ O_2 + 15\ H^+ \qquad (18)$$

$$106\ CO_2 + 16\ NO_3^- + H_2PO_4^- + 122\ H_2O + 17\ H^+ \text{ - - >}$$

$$\text{protoplasm} + 138\ O_2 \qquad (19)$$

When ammonium is the nitrogen source, one mole oxygen is produced per mole carbon dioxide fixed. When nitrate is the nitrogen source, 1.3 moles oxygen are produced per mole carbon dioxide fixed.

The equation that describes the effect of algae on dissolved oxygen in the model is:

$$\frac{\delta}{\delta t} DO = \left[(1.3 - 0.3 \cdot PN) \cdot P - (1 - FCD) \cdot BM\right] \cdot AOCR \cdot B \quad (20)$$

in which:

FCD = fraction of algal metabolism recycled as dissolved organic carbon ($0 \leq FCD \leq 1$)
AOCR = dissolved oxygen-to-carbon ratio in respiration (2.67 g O_2 g^{-1} C)

The magnitude of AOCR is derived from a simple representation of the respiration process:

$$CH_2O + O_2 = CO_2 + H_2O \quad (21)$$

The quantity (1.3 - 0.3 · PN) is the photosynthesis ratio and expresses the molar quantity of oxygen produced per mole carbon fixed. The photosynthesis ratio approaches unity as the algal preference for ammonium approaches unity.

Salinity Toxicity

Some freshwater algae, such as the cyanobacteria *microcystis*, cease production when salinity exceeds 1 to 2 ppt (Sellner et al. 1988). The potential effect of salinity on freshwater algae is represented by a mortality term in the form of a rectangular hyperbola:

$$STOX1 = STF1 \cdot \frac{S}{KHst1 + S} \quad (22)$$

in which

STOX1 = mortality induced by salinity (d^{-1})
STF1 = maximum salinity mortality (d^{-1})
S = salinity (ppt)
KHst1 = salinity at which mortality is half maximum value (ppt)

The spring diatom bloom is limited to saline water. The limiting mechanism is not defined but appears to be related to salinity. The upstream limit of the spring bloom is defined in the model by introducing a mortality term at low salinity:

$$STOX2 = STF2 \times \frac{KHst2}{KHst2 + S} \quad (23)$$

in which

STOX2 = mortality induced by freshwater on spring diatoms (d^{-1})

STF2 = maximum freshwater mortality on spring diatoms (d^{-1})
KHst2 = salinity at which mortality is half maximum value (ppt)

The salinity-related mortality (Figure 2-7) is added to the basal metabolism.

Organic Carbon

Organic carbon undergoes numerous transformations in the water column. The model carbon cycle (Figure 2-8) consists of the following elements:

Phytoplankton production and excretion
Predation on phytoplankton
Dissolution of particulate carbon
Heterotrophic respiration
Settling

Algal production is the primary carbon source to the water column although carbon also enters the system through external loading. Predation on algae by zooplankton and other organisms releases particulate and dissolved organic carbon to the water column. A fraction of the particulate organic carbon undergoes first-order dissolution to dissolved organic carbon. Dissolved organic carbon produced by excretion, by predation, and by dissolution is respired at a first-order rate to inorganic carbon. Particulate organic carbon which does not undergo dissolution settles to the bottom sediments.

Organic carbon dissolution and respiration are represented as first-order processes in which the reaction rate is proportional to concentration of the reactant. An exponential function (Figure 2-5) relates dissolution and respiration to temperature.

Dissolved Organic Carbon

The complete representation of dissolved organic carbon sources and sinks in the model ecosystem is: (24)

$$\frac{\delta}{\delta t} DOC = FCD \cdot R \cdot B + FCDP \cdot PR + Klpoc \cdot LPOC$$

$$+ Krpoc \cdot RPOC + Kg3poc \cdot G3OC - \frac{DO}{KHodoc + DO} \cdot Kdoc \cdot DOC$$

in which:

DOC = dissolved organic carbon (g m^{-3})
LPOC = labile particulate organic carbon (g m^{-3})
RPOC = refractory particulate organic carbon (g m^{-3})
G3OC = G3 particulate organic carbon (g m^{-3})
FCD = fraction of algal respiration released as DOC ($0 < FCD < 1$)

FCDP = fraction of predation on algae released as DOC (0 < FCDP < 1)
Klpoc = dissolution rate of LPOC (d^{-1})
Krpoc = dissolution rate of RPOC (d^{-1})
Kg3poc = dissolution rate of G3OC (d^{-1})
Kdoc = respiration rate of DOC (d^{-1})

Particulate Organic Carbon

The complete representation of labile particulate organic carbon sources and sinks in the model ecosystem is:

$$\frac{\delta}{\delta t} LPOC = FCL \cdot R \cdot B + FCLP \cdot PR - Klpoc \cdot LPOC - Wl \cdot \frac{\delta}{\delta z} LPOC \quad (25)$$

in which:

FCL = fraction of algal respiration released as LPOC (0 < FCL < 1)
FCLP = fraction of predation on algae released as LPOC (0 < FCLP < 1)
Wl = settling velocity of labile particles (m d^{-1})

The equations for refractory and G3 particulate organic carbon are analogous.

Phosphorus

The model phosphorus cycle (Figure 2-9) includes the following processes:

Algal uptake and excretion
Predation
Hydrolysis of particulate organic phosphorus
Mineralization of dissolved organic phosphorus
Dissolution of particulate inorganic phosphorus
Settling and resuspension

External loads provide the ultimate source of phosphorus to the system. Dissolved phosphate is incorporated by algae during growth and released as phosphate and organic phosphorus through respiration and predation. Dissolved organic phosphorus is mineralized to phosphate. A portion of the particulate organic phosphorus hydrolyzes to dissolved organic phosphorus. The balance settles to the sediments. Dissolution of particulate inorganic phosphorus is also possible. Within the sediments, particulate phosphorus is mineralized and recycled to the water column as dissolved phosphate.

Hydrolysis and Mineralization

Within the model, hydrolysis is defined as the process by which

particulate organic substances are converted to dissolved organic form. Mineralization is defined as the process by which dissolved organic substances are converted to dissolved inorganic form. Conversion of particulate organic phosphorus to phosphate proceeds through the sequence of hydrolysis and mineralization. Direct mineralization of particulate organic phosphorus does not occur.

Mineralization of organic phosphorus is mediated by the release of nucleotidase and phosphatase enzymes by bacteria (Ammerman and Azam 1985; Chrost and Overbeck 1987) and algae (Matavulj and Flint 1987; Chrost and Overbeck 1987; Boni et al. 1989). Since the algae themselves release the enzyme and since bacterial abundance is related to algal biomass, the rate of organic phosphorus mineralization is related, in the model, to algal biomass. A most remarkable property of the enzyme process is that alkaline phosphatase activity is inversely proportional to ambient phosphate concentration (Chrost and Overbeck 1987; Boni et al. 1989). Put in different terms, when phosphate is scarce, algae stimulate production of an enzyme that mineralizes organic phosphorus to phosphate. This phenomenon is simulated by relating mineralization to the algal phosphorus nutrient limitation. Mineralization is highest when algae are strongly phosphorus limited and is least when no limitation occurs.

The expression for mineralization rate is:

$$Kdop = Kdp + \frac{KHp}{KHp + PO_4} \cdot Kdpalg \cdot B \qquad (26)$$

in which:

Kdop = mineralization rate of dissolved organic phosphorus (d^{-1})
Kdp = minimum mineralization rate (d^{-1})
KHp = half-saturation concentration for algal phosphorus uptake (g P m^{-3})
PO_4 = dissolved phosphate (g P m^{-3})
Kdpalg = constant that relates mineralization to algal biomass (m^3 g^{-1} C d^{-1})

Potential effects of algal biomass and nutrient limitation on the mineralization rate are shown in Figure 2-10. When nutrient concentration greatly exceeds the half-saturation concentration for algal uptake, the rate roughly equals the minimum. Algal biomass has little influence. As nutrient becomes scarce relative to the half-saturation concentration, the rate increases. The magnitude of the increase depends on algal biomass. Factor of two to three increases are feasible. Exponential functions (Figure 2-5) relate mineralization and hydrolysis rates to temperature.

Dissolved Phosphate

The mass-balance equation for dissolved phosphate is:

$$\frac{\delta}{\delta t} PO_4 = Kdop \cdot DOP + Kpip \cdot PIP - APC \cdot G \cdot B$$
$$+ APC \cdot [FPI \cdot BM \cdot B + FPIP \cdot PR] - Wpo_4 \cdot \frac{\delta}{\delta z} PO_4 \qquad (27)$$

in which:

PIP = particulate inorganic phosphorus (g P m^{-3})
Kpip = dissolution rate of particulate inorganic phosphorus (d^{-1})
FPI = fraction of algal metabolism released as dissolved phosphate ($0 \leq FPI \leq 1$)
FPIP = fraction of predation released as dissolved phosphate ($0 \leq FPIP \leq 1$)
Wpo_4 = settling rate of precipitated phosphate (m d^{-1})

Phosphate settling represents phosphate removal through co-precipitation with iron and manganese during the break-up of seasonal bottom-water anoxia. The settling rate is implemented for a thirty-day period in appropriate portions of the system.

Dissolved Organic Phosphorus

The mass balance equation for dissolved organic phosphorus is:

$$\frac{\delta}{\delta t} DOP = APC \cdot (BM \cdot B \cdot FPD + PR \cdot FPDP) + Klpop \cdot LPOP + Krpop \cdot RPOP + Kg3op \cdot G3OP - Kdop \cdot DOP \qquad (28)$$

in which:

DOP = dissolved organic phosphorus (g P m^{-3})
LPOP = labile particulate organic phosphorus (g P m^{-3})
RPOP = refractory particulate organic phosphorus (g P m^{-3})
G3OP = G3 particulate organic phosphorus (g P m^{-3})
FPD = fraction of algal metabolism released as DOP ($0 < FPD < 1$)
FPDP = fraction of predation on algae released as DOP ($0 < FPDP < 1$)
Klpop = hydrolysis rate of LPOP (d^{-1})
Krpop = hydrolysis rate of RPOP (d^{-1})
Kg3op = hydrolysis rate of G3OP (d^{-1})
Kdop = mineralization rate of DOP (d^{-1})

Particulate Organic Phosphorus

The mass balance equation for labile particulate organic phosphorus is:

$$\frac{\delta}{\delta t} LPOP = APC \cdot (BM \cdot B \cdot FPL + PR \cdot FPLP) - Klpop \cdot LPOP - Wl \cdot \frac{\delta}{\delta z} LPOP \qquad (29)$$

in which:

FPL = fraction of algal metabolism released as LPOP (0 < FPL < 1)
FPLP = fraction of predation on algae released as LPOP (0 < FPLP < 1)

The equations for refractory and G3 particulate organic phosphorus are analogous.

Particulate Inorganic Phosphorus

A large fraction of particulate phosphorus in the Chesapeake Bay system is in inorganic form (Keefe 1994). Examination of dissolved phosphate, fixed solids, and PIP observations indicates the PIP is not loosely sorbed to sediment particles as commonly represented in water quality models. PIP is represented here as a distinct substance which potentially dissolves into phosphate. Otherwise, the ultimate fate of PIP is settling to bottom sediments. The mass balance equation for PIP is:

$$\frac{\partial}{\partial t} PIP = -Kpip \cdot PIP - Wspip \cdot \frac{\delta}{\delta z} PIP \qquad (30)$$

in which:

Wspip = settling rate of particulate inorganic phosphorus (m d^{-1})

Nitrogen

The model nitrogen cycle (Figure 2-11) includes the following processes:

Algal production and metabolism
Predation
Hydrolysis of particulate organic nitrogen
Mineralization of dissolved organic nitrogen
Settling
Nitrification

External loads provide the ultimate source of nitrogen to the system. Available nitrogen is incorporated by algae during growth and released as ammonium and organic nitrogen through respiration and predation. A portion of the particulate organic nitrogen hydrolyzes to dissolved organic nitrogen. The balance settles to the sediments. Dissolved organic nitrogen is mineralized to ammonium. In an oxygenated water column, a fraction of the ammonium is subsequently oxidized to nitrate+nitrite through the nitrification process. Particulate nitrogen which settles to the sediments is mineralized and recycled to the water column, primarily as ammonium. Nitrate+nitrite moves in both directions across the sediment-water interface, depending on relative concentrations in the water column and sediment interstices.

Nitrification

Nitrification is a process mediated by specialized groups of autotrophic bacteria that obtain energy through the oxidation of ammonium to nitrite and oxidation of nitrite to nitrate. A simplified expression for complete nitrification (Tchobanoglous and Schroeder 1987) is:

$$NH_4^+ + 2O_2 \text{ --> } NO_3^- + H_2O + 2H^+ \qquad (31)$$

The simplified stoichiometry indicates that two moles of oxygen are required to nitrify one mole of ammonium into nitrate. The simplified equation is not strictly true, however. Cell synthesis by nitrifying bacteria is accomplished by the fixation of carbon dioxide so that less than two moles of oxygen are consumed per mole ammonium utilized (Wezernak and Gannon 1968).

The kinetics of complete nitrification are modeled as a function of available ammonium, dissolved oxygen, and temperature:

$$NT = \frac{DO}{KHont + DO} \cdot \frac{NH_4}{KHnnt + NH_4} \cdot f(T) \cdot NTm \qquad (32)$$

in which:

NT = nitrification rate (g N m^{-3} d^{-1})
KHont = half-saturation constant of dissolved oxygen required for nitrification (g O_2 m^{-3})
KHnnt = half-saturation constant of NH_4 required for nitrification (g N m^{-3})
NTm = maximum nitrification rate at optimal temperature (g N m^{-3} d^{-1})

The kinetics formulation (Figure 2-12) incorporates the products of two Monod-like functions. The first function diminishes nitrification at low dissolved oxygen concentration. The second function expresses the influence of ammonium concentration on nitrification. When ammonium concentration is low, relative to KHnnt, nitrification is proportional to ammonium concentration. For NH4 << KHnnt, the reaction is approximately first-order. (The first-order decay constant ≈ NTm/KHnnt.) When ammonium concentration is large, relative to KHnnt, nitrification approaches a maximum rate. This formulation is based on a concept proposed by Tuffey et al. (1974). Nitrifying bacteria adhere to benthic or suspended sediments. When ammonium is scarce, vacant surfaces suitable for nitrifying bacteria exist. As ammonium concentration increases, bacterial biomass increases, vacant surfaces are occupied, and the rate of nitrification increases. The bacterial population attains maximum density when all surfaces suitable for bacteria are occupied. At this point, nitrification proceeds at a maximum rate independent of additional increase in ammonium concentration.

The optimal temperature for nitrification may be less than peak temperatures that occur in coastal waters. To allow for a decrease in nitrification at superoptimal temperature, the effect of temperature on nitrification is modeled in the Gaussian form of Equation 7.

Nitrogen Mass Balance Equations

The mass-balance equations for nitrogen state variables are written by summing all previously-described sources and sinks:

Ammonium

$$\frac{\delta}{\delta t} NH_4 = ANC \cdot \left[(BM \cdot FNI - PN \cdot P) \cdot B + PR \cdot FNIP\right] + Kdon \cdot DON - NT \quad (33)$$

in which:

FNI = fraction of algal metabolism released as NH4 ($0 \leq FNI \leq 1$)
PN = algal ammonium preference ($0 \leq PN \leq 1$)
FNIP = fraction of predation released as NH4 ($0 \leq FNIP \leq 1$)

Nitrate+Nitrite

$$\frac{\delta}{\delta t} NO_{23} = - ANC \cdot (1 - PN) \cdot P \cdot B + NT \quad (34)$$

Dissolved Organic Nitrogen

$$\frac{\delta}{\delta t} DON = ANC \cdot (BM \cdot B \cdot FND + PR \cdot FNDP) + Klpon \cdot LPON + Krpon \cdot RPON + Kg3on \cdot G3ON - Kdon \cdot DON \quad (35)$$

in which:

DON = dissolved organic nitrogen (g N m^{-3})
LPON = labile particulate organic nitrogen (g N m^{-3})
RPON = refractory particulate organic nitrogen (g N m^{-3})
G3ON = G3 particulate organic nitrogen (g N m^{-3})
FND = fraction of algal metabolism released as DON ($0 < FND < 1$)
FNDP = fraction of predation on algae released as DON ($0 < FNDP < 1$)
Klpon = hydrolysis rate of LPON (d^{-1})
Krpon = hydrolysis rate of RPON (d^{-1})
Kg3on = hydrolysis rate of G3ON (d^{-1})
Kdon = mineralization rate of DON (d^{-1})

Particulate Organic Nitrogen

The mass balance equation for labile particulate organic nitrogen is:

$$\frac{\delta}{\delta t} LPON = ANC \cdot (BM \cdot B \cdot FNL + PR \cdot FNLP) - Klpon \cdot LPON - Wl \cdot \frac{\delta}{\delta z} LPON \quad (36)$$

in which:

FNL = fraction of algal metabolism released as LPON ($0 < FNL < 1$)
FNLP = fraction of predation on algae released as LPON ($0 < FNLP < 1$)

The equations for refractory and G3 particulate organic nitrogen are analogous.

Chemical Oxygen Demand

Chemical oxygen demand is the concentration of reduced substances that are oxidized through abiotic reactions. The source of chemical oxygen demand in saline water is sulfide released from sediments. A cycle occurs in which sulfate is reduced to sulfide in the sediments and re-oxidized to sulfate in the water column. In freshwater, methane may be released to the water column by bottom sediments. Both sulfide and methane are quantified in units of oxygen demand and are treated with the same kinetics formulation:

$$\frac{\delta}{\delta t} COD = - \frac{DO}{KHocod + DO} \cdot Kcod \cdot COD \quad (37)$$

in which:

COD = chemical oxygen demand concentration (g oxygen-equivalents m^{-3})
KHocod = half-saturation concentration of dissolved oxygen required for exertion of chemical oxygen demand (g O_2 m^{-3})
Kcod = oxidation rate of chemical oxygen demand (d^{-1})

An exponential function (Figure 2-5) describes the effect of temperature on exertion of chemical oxygen demand.

Dissolved Oxygen

Sources and sinks of dissolved oxygen in the water column (Figure 2-13) include:

Algal photosynthesis
Atmospheric reaeration
Algal respiration
Heterotrophic respiration
Nitrification
Chemical oxygen demand

Reaeration

The rate of reaeration is proportional to the dissolved oxygen deficit in model segments that form the air-water interface:

$$\frac{\delta}{\delta t} DO = \frac{Kr}{\Delta z} \cdot (DOs - DO) \qquad (38)$$

in which:

DO = dissolved oxygen concentration (g O_2 m^{-3})
Kr = reaeration coefficient (m d^{-1})
DOs = dissolved oxygen saturation concentration (g O_2 m^{-3})
Δz = model surface layer thickness (m)

In freeflowing streams, the reaeration coefficient depends largely on turbulence generated by bottom shear stress (O'Connor and Dobbins 1958). In lakes and coastal waters, however, wind effects may dominate the reaeration process (O'Connor 1983). The model code provides three options for the reaeration coefficient:

Calculate reaeration as a function of stream velocity and depth.
Calculate reaeration as a function of wind speed.
Specify a reaeration coefficient

The relationship to velocity and depth is based on O'Connor and Dobbins (1958). In SI units, the O'Connor-Dobbins relationship is:

$$Kr = 3.9\sqrt{u/H} \qquad (39)$$

in which:

u = stream velocity (m s^{-1})
H = depth (m)

The relationship to wind is from Hartman and Hammond (1985):

$$Kr = Arear \bullet Rv \bullet Wms^{1.5} \qquad (40)$$

in which:

Arear = empirical constant (≈ 0.1)
Rv = ratio of kinematic viscosity of pure water at 20 ^{o}C to kinematic viscosity of water at specified temperature and salinity
Wms = wind speed measured at 10 m above water surface (m s^{-1})

Hartman and Hammond (1985) indicate Arear takes the value 0.157. In the present model, Arear is treated as a variable to allow for effects of wind sheltering, for differences in height of local wind observations, and for other factors. An empirical function (Figure 2-14) which fits tabulated values of Rv is:

$$Rv = 0.54 + 0.0233 \bullet T - 0.0020 \bullet S \qquad (41)$$

in which:

S = salinity (ppt)
T = temperature (^{o}C)

Dissolved Oxygen Saturation

Saturation dissolved oxygen concentration is influenced by temperature, salinity, and pressure. A general representation of these influences is:

$$DOs = DOf \cdot Fs \cdot Fp \qquad (42)$$

in which:

DOf = dissolved oxygen concentration, as a function of temperature, in freshwater (g O_2 m^{-3})
Fs = salinity correction factor
Fp = pressure correction factor

DOf is from Benson and Krause (1980) as reported by USGS (2011):

$$DOf = exp\left(-139.34 + \frac{1.58x10^{5}}{T} - \frac{6.64x10^{7}}{T^{2}} + \frac{1.24x10^{10}}{T^{3}} - \frac{8.62x10^{11}}{T^{4}}\right) \qquad (43)$$

in which:

T = temperature (^{o}K = ^{o}C+273.15)

Fs is from Benson and Krause (1984) as reported by USGS (2011):

$$Fs = exp\left(-S \cdot \left(0.0177 - \frac{10.75}{T} + \frac{2141}{T^{2}}\right)\right) \qquad (44)$$

in which:

S = salinity (ppt)

Since reaeration occurs at the air-water interface, where atmospheric pressure prevails, Fp is set to unity.

Mass Balance Equation for Dissolved Oxygen

$$\frac{\delta}{\delta t}DO = AOCR \cdot [(1.3 - 0.3 \cdot PN) \cdot P - (1 - FCD) \cdot BM] \cdot B$$
$$- AONT \cdot NT - \frac{DO}{KHodoc + DO} \cdot AOCR \cdot Kdoc \cdot DOC \qquad (45)$$
$$- \frac{DO}{KHocod + DO} \cdot Kcod \cdot COD + \frac{Kr}{H} \cdot (DOs - DO)$$

in which:

AOCR = oxygen-to-carbon mass ratio in production and respiration (= 2.67 g O_2 g^{-1} C)
AONT = oxygen consumed per mass ammonium nitrified (= 4.33 g O_2 g^{-1} N)

Temperature

Computation of temperature employs a conservation of internal energy equation that is analogous to the conservation of mass equation. For practical purposes, the internal energy equation can be written as a conservation of temperature equation. The only source or sink of temperature considered is exchange with the atmosphere. Atmospheric exchange is considered proportional to the temperature difference between the water surface and a theoretical equilibrium temperature (Edinger et al. 1974):

$$\frac{\delta}{\delta t}T = \frac{KT}{\rho \cdot Cp \cdot H} \cdot (Te - T) \qquad (46)$$

in which:

T = water temperature (^oC)
Te = equilibrium temperature (^oC)
KT = Heat exchange coefficient (watt m^{-2} $^oC^{-1}$)
Cp = specific heat of water (4200 watt s kg^{-1} $^oC^{-1}$)
ρ = density of water (1000 kg m^{-3})

Salinity

Salinity is modeled by the conservation of mass equation with no internal sources or sinks

Parameter Values

Model parameter evaluation is a recursive process. Parameters are selected from a range of feasible values, tested in the model, and adjusted until satisfactory agreement between predicted and observed variables is obtained. Ideally, the range of feasible values is determined by observation or experiment.

For some parameters, however, no observations are available. Then, the feasible range is determined by parameter values employed in similar models or by the judgment of the modeler. A review of parameter values was included in documentation of the first application of this model (Cerco and Cole 1994). Parameters from the initial study were refined in successive applications and refined again for the present model. A complete set of parameter values is provided in Table 2-2.

Table 2-1
Water Quality Model State Variables

Temperature	Salinity
Fixed Solids	Freshwater Algae
Spring Diatoms	Other (Green) Algae
Dissolved Organic Carbon	Labile Particulate Organic Carbon
Refractory Particulate Organic Carbon	G3 Particulate Organic Carbon
Ammonium	Nitrate+Nitrite
Dissolved Organic Nitrogen	Labile Particulate Organic Nitrogen
Refractory Particulate Organic Nitrogen	G3 Particulate Organic Nitrogen
Phosphate	Dissolved Organic Phosphorus
Labile Particulate Organic Phosphorus	Refractory Particulate Organic Phosphorus
G3 Particulate Organic Phosphorus	Particulate Inorganic Phosphorus
Chemical Oxygen Demand	Dissolved Oxygen

Table 2-2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
ANC	nitrogen-to-carbon ratio of algae	0.175 (fresh), 0.135 (spring), 0.155 (green)	g N g^{-1} C
AOCR	dissolved oxygen-to-carbon ratio in respiration	2.67	g O_2 g^{-1} C
AONT	mass dissolved oxygen consumed per mass ammonium nitrified	4.33	g O_2 g^{-1} N
APC	algal phosphorus-to-carbon ratio	0.0125 (fresh), 0.0167 (spring) 0.0167 (green)	g P g^{-1} C
BM	basal metabolic rate of algae at reference temperature Tr	0.03 (fresh), 0.01 (spring), 0.02 (green)	d^{-1}
CChl	algal carbon-to-chlorophyll ratio	45 (fresh), 75 (spring), 60 (green)	g C g^{-1} Chl
FCD	fraction of dissolved organic carbon produced by algal metabolism	0.0	$0 \leq FCD \leq 1$
FCDP	fraction of dissolved organic carbon produced by predation	0.5	$0 \leq FCDP \leq 1$
FCL	fraction of labile particulate carbon produced by algal metabolism	0.0	$0 \leq FCL \leq 1$
FCLP	fraction of labile particulate carbon produced by predation	0.3	$0 \leq FCLP \leq 1$
FCR	fraction of refractory particulate carbon produced by algal metabolism	0.0	$0 \leq FCR \leq 1$
FCRP	fraction of refractory particulate carbon produced by predation	0.15	$0 \leq FCRP \leq 1$
FCG3	fraction of G3 particulate carbon produced by algal metabolism	0.0	$0 \leq FCG3 \leq 1$
FCG3P	fraction of G3 particulate carbon produced by predation	0.05	$0 \leq FCG3P \leq 1$
FNI	fraction of inorganic nitrogen produced by algal metabolism	0.45	$0 \leq FNI \leq 1$
FNIP	fraction of inorganic nitrogen produced by predation	0.35	$0 \leq FNIP \leq 1$
FND	fraction of dissolved organic nitrogen produced by algal metabolism	0.2	$0 \leq FND \leq 1$
FNDP	fraction of dissolved organic nitrogen	0.15	$0 \leq FNDP \leq 1$

Table 2-2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
	produced by predation		
FNL	fraction of labile particulate nitrogen produced by algal metabolism	0.23	$0 \leq FNL \leq 1$
FNLP	fraction of labile particulate nitrogen produced by predation	0.28	$0 \leq FNLP \leq 1$
FNR	fraction of refractory particulate nitrogen produced by algal metabolism	0.04	$0 \leq FNR \leq 1$
FNRP	fraction of refractory particulate nitrogen produced by predation	0.1	$0 \leq FNRP \leq 1$
FNG3	fraction of G3 particulate nitrogen produced by algal metabolism	0.08	$0 \leq FNG3 \leq 1$
FNG3P	fraction of G3 particulate nitrogen produced by predation	0.12	$0 \leq FNG3P \leq 1$
FPD	fraction of dissolved organic phosphorus produced by algal metabolism	0.25	$0 \leq FPD \leq 1$
FPDP	fraction of dissolved organic phosphorus produced by predation	0.4	$0 \leq FPDP \leq 1$
FPI	fraction of dissolved inorganic phosphorus produced by algal metabolism	0.75	$0 \leq FPI \leq 1$
FPIP	fraction of dissolved inorganic phosphorus produced by predation	0.5	$0 \leq FPIP \leq 1$
FPL	fraction of labile particulate phosphorus produced by algal metabolism	0.0	$0 \leq FPL \leq 1$
FPLP	fraction of labile particulate phosphorus produced by predation	0.06	$0 \leq FPLP \leq 1$
FPR	fraction of refractory particulate phosphorus produced by algal metabolism	0.0	$0 \leq FPR \leq 1$
FPRP	fraction of refractory particulate phosphorus produced by predation	0.01	$0 \leq FPRP \leq 1$
FPG3	fraction of G3 particulate phosphorus produced by algal metabolism	0.0	$0 \leq FPG3 \leq 1$
FPG3P	fraction of G3 particulate phosphorus produced by predation	0.03	$0 \leq FPG3P \leq 1$
Kcod	oxidation rate of chemical oxygen demand	20 (saltwater), 0.025 (fresh)	d^{-1}
Kdoc	dissolved organic carbon respiration rate	0.025 – 0.05	d^{-1}
Kdon	dissolved organic nitrogen mineralization rate	0.035	d^{-1}
Kdp	minimum mineralization rate of dissolved organic phosphorus	0.025	d^{-1}

Table 2-2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
Kdpalg	constant that relates mineralization rate to algal biomass	0.4	$m^3 g^{-1} C d^{-1}$
KHn	half-saturation concentration for nitrogen uptake by algae	0.01(fresh), 0.025(spring), 0.025 (green)	g N m^{-3}
KHnh4	half-saturation concentration of ammonium in nitrogen preference formula	0.002(fresh), 0.002(spring), 0.002(green)	g N m^{-3}
KHnnt	half-saturation concentration of NH_4 required for nitrification	1.0	g N m^{-3}
KHocod	half-saturation concentration of dissolved oxygen required for exertion of COD	0.1	g O_2 m^{-3}
KHodoc	half-saturation concentration of dissolved oxygen required for oxic respiration	0.1	g O_2 m^{-3}
KHont	half-saturation concentration of dissolved oxygen required for nitrification	1.0	g O_2 m^{-3}
KHp	half-saturation concentration for phosphorus uptake by algae	0.0025	g P m^{-3}
KHst	salinity at which algal mortality is half maximum value	15 (fresh), 2.0 (spring)	ppt
Klpoc	labile particulate organic carbon dissolution rate	0.15	d^{-1}
Klpon	labile particulate organic nitrogen hydrolysis rate	0.12	d^{-1}
Klpop	labile particulate organic phosphorus hydrolysis rate	0.12	d^{-1}
Kpip	particulate inorganic phosphorus dissolution rate	0.0	d^{-1}
Krdo	Reaeration coefficient	1.5	m d^{-1}
Krpoc	refractory particulate organic carbon dissolution rate	0.006	d^{-1}
Krpon	refractory particulate organic nitrogen hydrolysis rate	0.005	d^{-1}
Krpop	refractory particulate organic phosphorus hydrolysis rate	0.005	d^{-1}
Kg3p	g3 particulate organic carbon hydrolysis rate	0.0	d^{-1}
Kg3n	g3 particulate organic nitrogen hydrolysis rate	0.0	d^{-1}
Kg3p	g3 particulate organic phosphorus hydrolysis rate	0.0	d^{-1}

Table 2-2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
KTb	effect of temperature on basal metabolism of algae	0.0322	$^oC^{-1}$
KTcod	effect of temperature on exertion of chemical oxygen demand	0.041	d^{-1}
KTg1	effect of temperature below Tm on growth of algae	0.005 (fresh), 0.0018 (spring), 0.0035 (green)	$^oC^{-2}$
KTg2	effect of temperature above Tm on growth of algae	0.004 (fresh), 0.006 (spring), 0.0 (green)	$^oC^{-2}$
KThdr	effect of temperature on hydrolysis rates	0.069	$^oC^{-1}$
KTmnl	effect of temperature on mineralization rates	0.069	$^oC^{-1}$
KTnt1	effect of temperature below Tmnt on nitrification	0.003	$^oC^{-2}$
KTnt2	effect of temperature above Tmnt on nitrification	0.003	$^oC^{-2}$
KTpr	effect of temperature on predation	0.032	$^oC^{-1}$
NTm	maximum nitrification rate at optimal temperature	0.062 to 0.125	g N m^{-3} d^{-1}
Phtl	predation rate on algae	0.05 (fresh), 0.1 (spring), 0.4 (green)	m^3 g^{-1} C d^{-1}
Pm^B	maximum photosynthetic rate	200 (fresh), 300 (spring), 450 (green)	g C g^{-1} Chl d^{-1}
Presp	photo-respiration fraction	0.25	$0 \leq Presp \leq 1$
STF	salinity toxicity factor	0.3 (fresh), 0.1 (spring)	d^{-1}
Topt	optimal temperature for growth of algae	29 (fresh), 16 (spring), 25 (green)	^oC
Tmnt	optimal temperature for nitrification	30	^oC
Tr	reference temperature for metabolism	20	^oC
Trcod	reference temperature for COD oxidation	23	^oC
Trhdr	reference temperature for hydrolysis	20	^oC
Trmnl	reference temperature for mineralization	20	^oC
Trpr	reference temperature for predation	20	^oC
Wa	algal settling rate	0.0 (fresh), 0.6 (spring), 0.1 to 0.5 (green)	m d^{-1}

Table 2-2
Parameters in Kinetics Equations

Symbol	Definition	Value	Units
Wl	settling velocity of labile particles	1.0	m d^{-1}
Wr	settling velocity of refractory particles	1.0	m d^{-1}
Wg3	Settling velocity of G3 particles	1.0	m d^{-1}
Wpip	Settling velocity of particulate inorganic phosphorus	0.1 to 0.5	m d^{-1}
Wspo4	settling velocity for precipitated phosphate	1.0	m d^{-1}
α	initial slope of production vs. irradiance relationship	3.15 (fresh), 8.0 (spring), 10.0 (green)	g C g^{-1} Chl $(E\ m^{-2})^{-1}$

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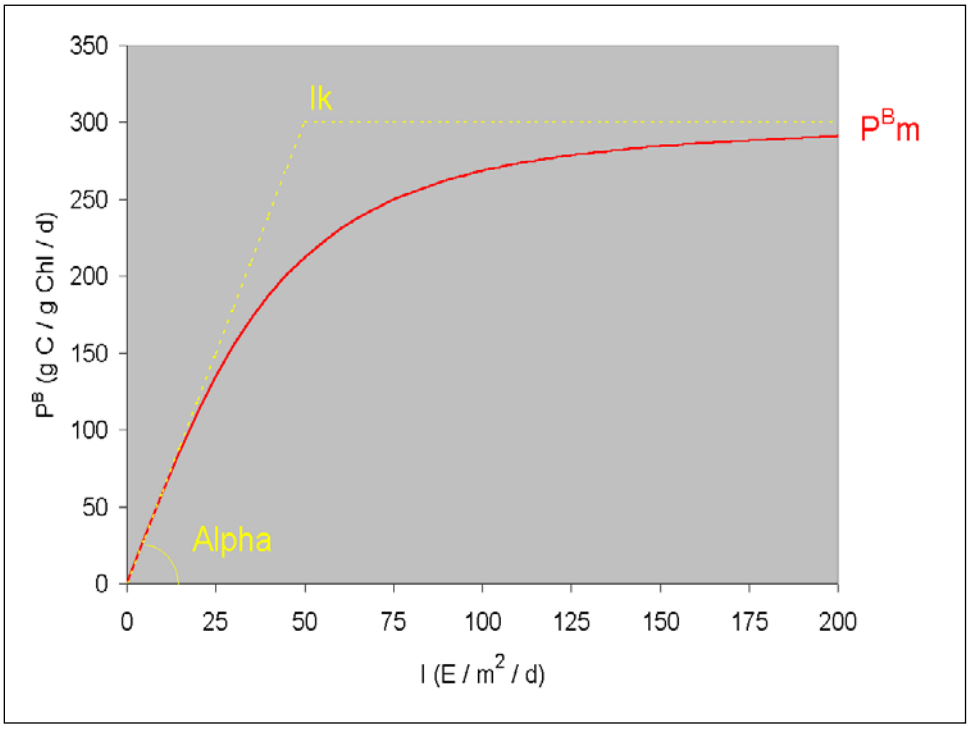

Figure 2-1. Production versus irradiance curve.

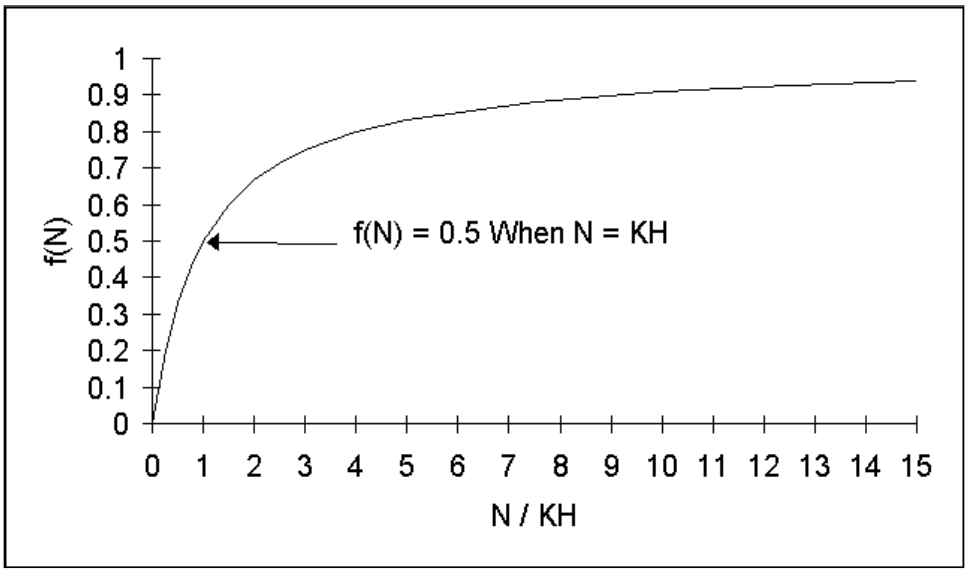

Figure 2-2. Monod formulation for nutrient-limited growth.

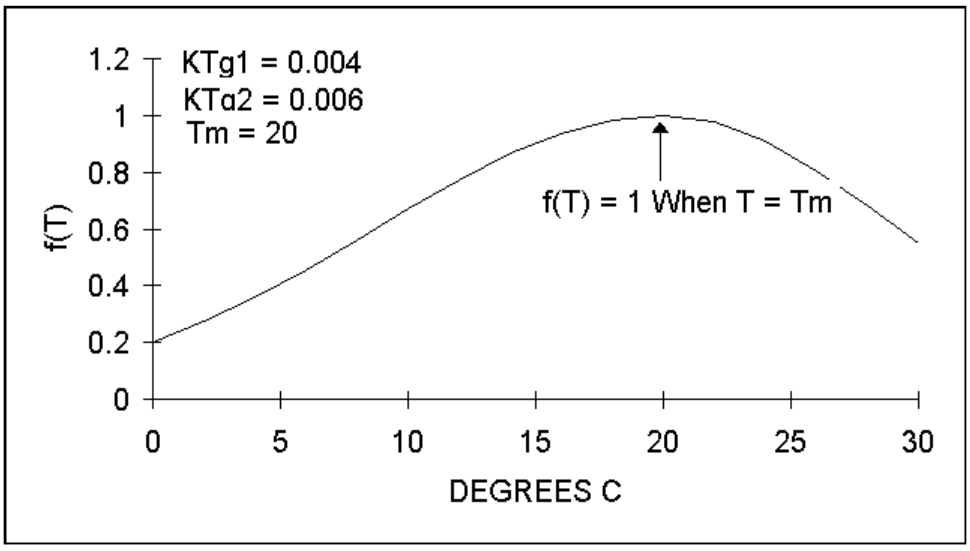

Figure 2-3. Relation of algal production to temperature.

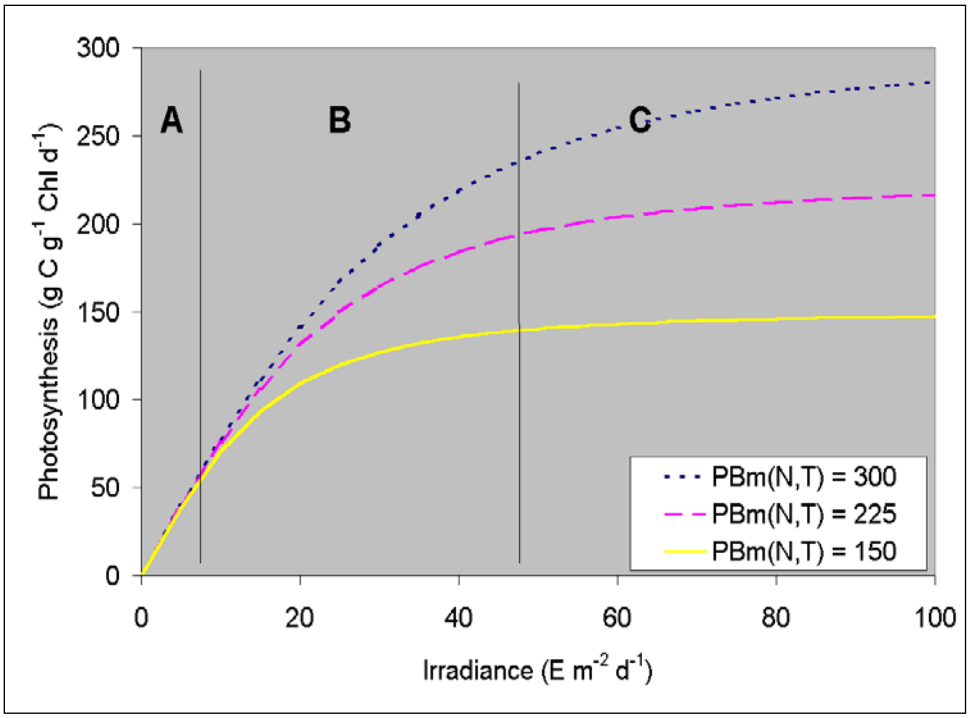

Figure 2-4. Effects of light and nutrients on production versus irradiance curve, determined for α = 8 (g C g^{-1} Chl (E m^{-2})$^{-1}$).

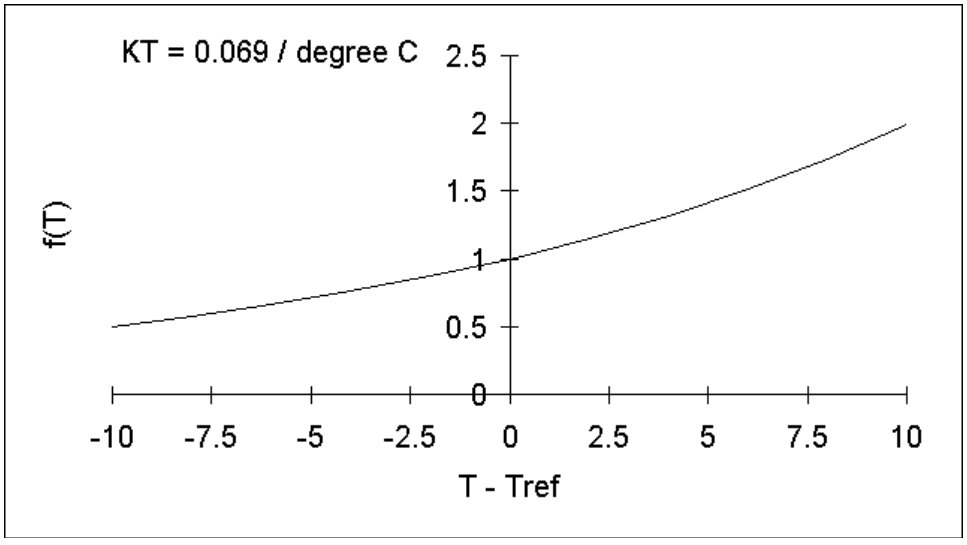

Figure 2-5. Exponential temperature relationship employed for metabolism and other processes

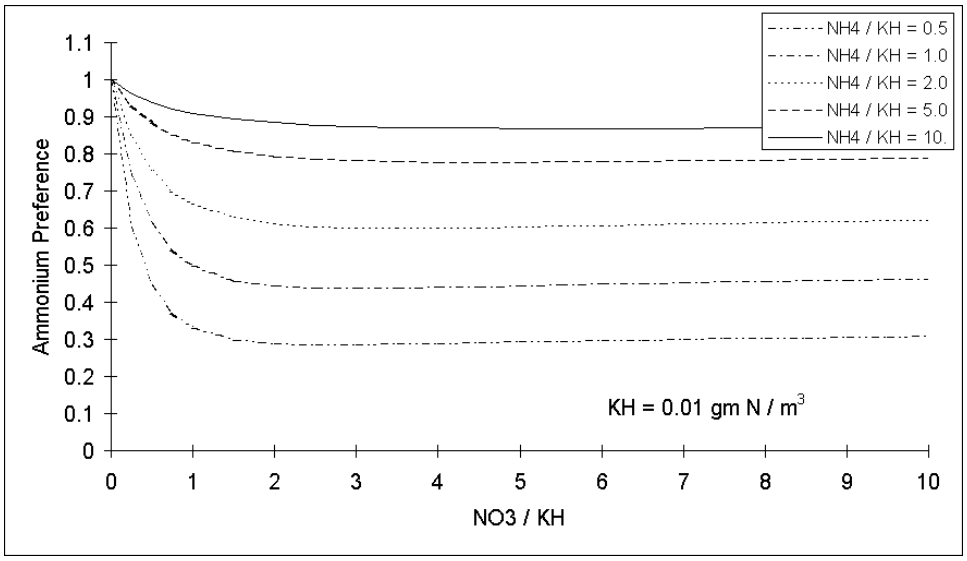

Figure 2-6. Algal ammonium preference

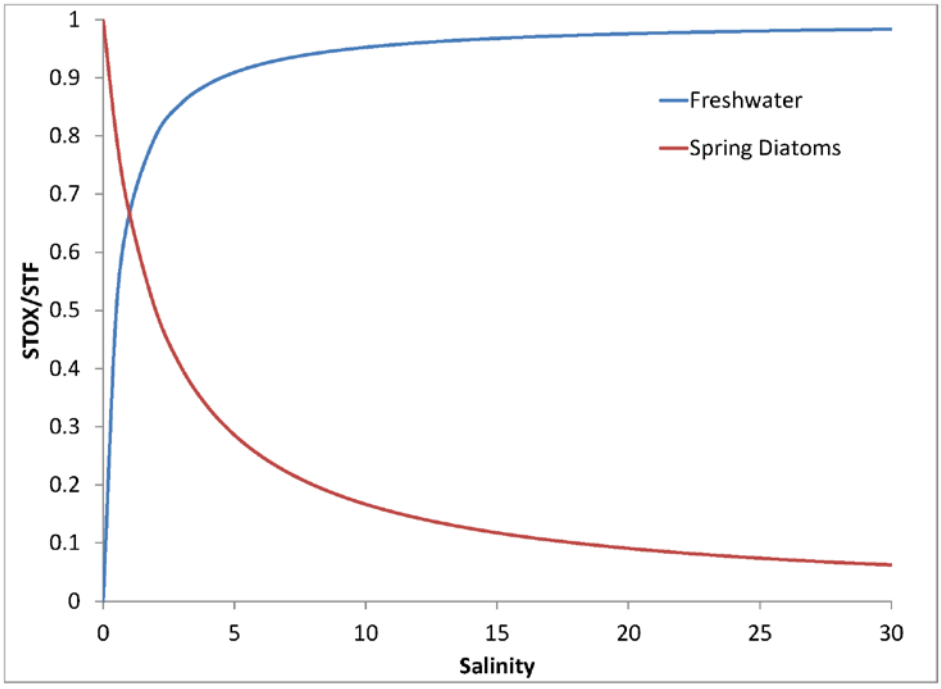

Figure 2-7. Salinity toxicity relationship.

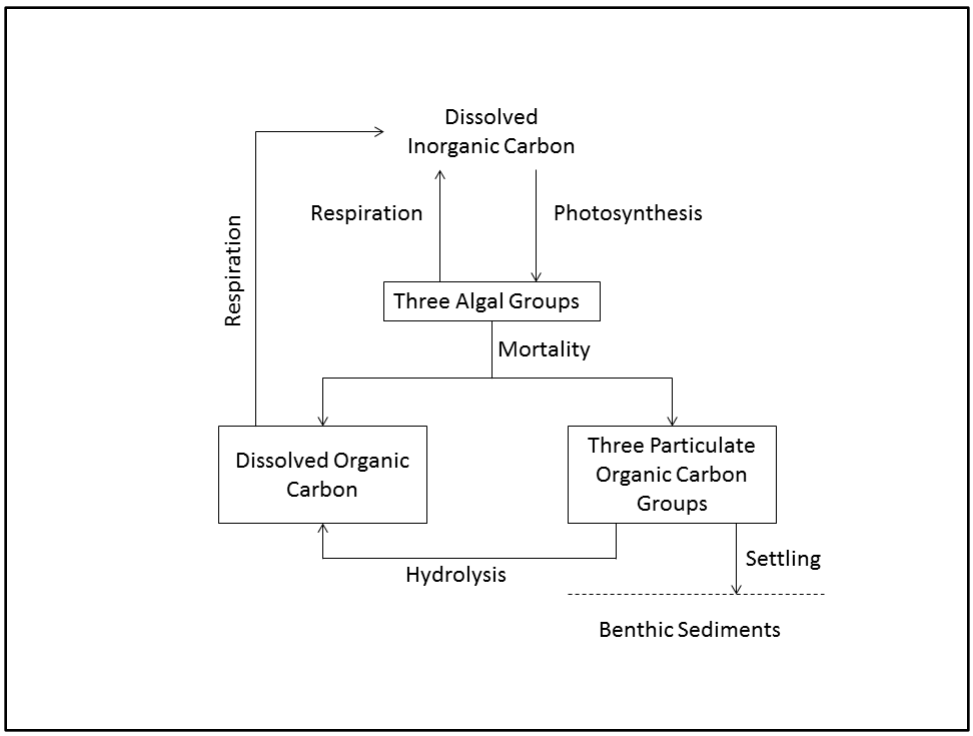

Figure 2-8. Model carbon cycle.

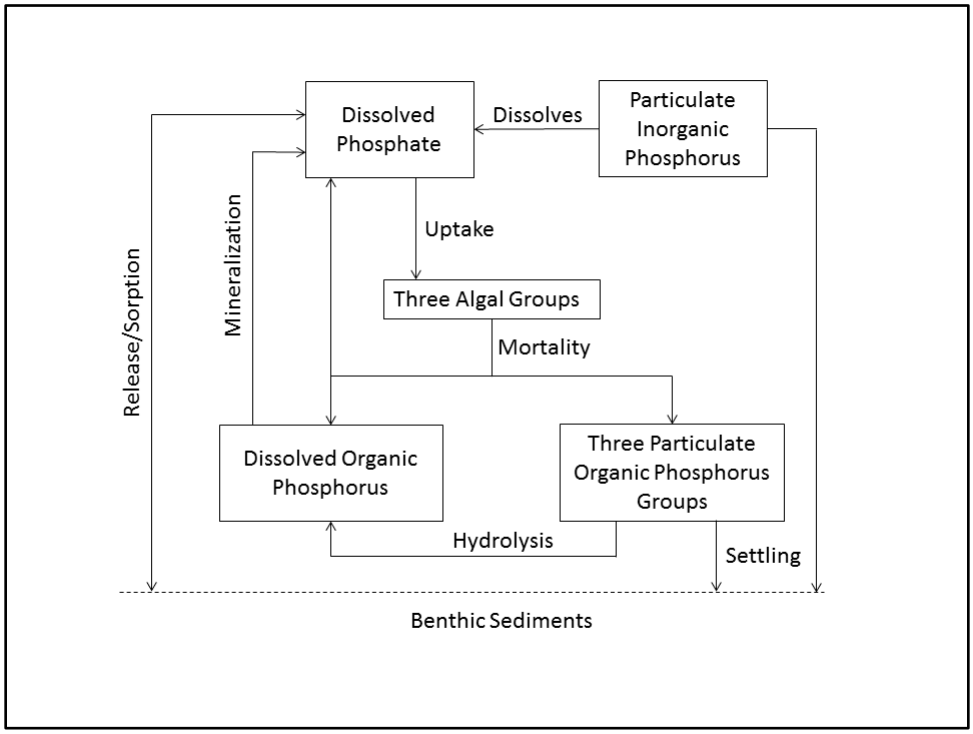

Figure 2-9. Model phosphorus cycle.

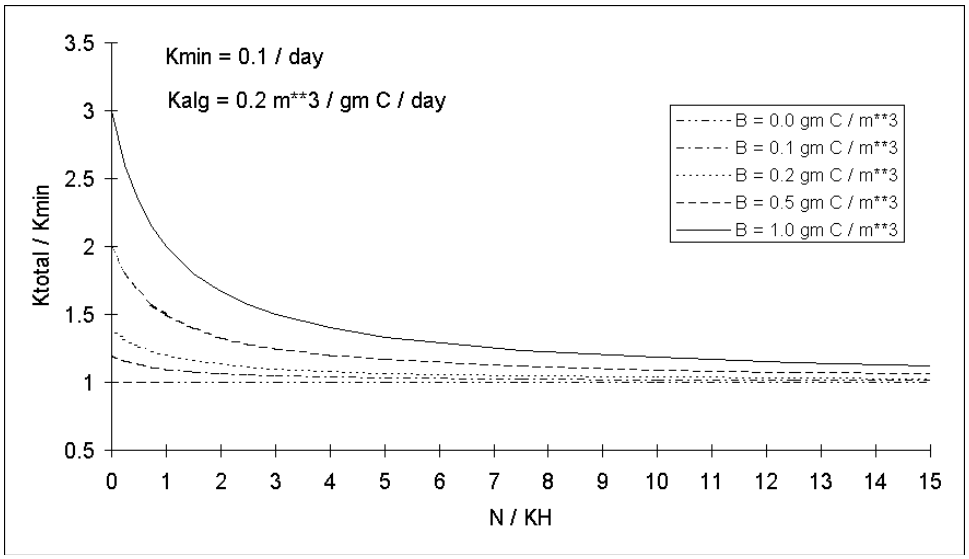

Figure 2-10. Effect of algal biomass and nutrient concentration on phosphorus mineralization.

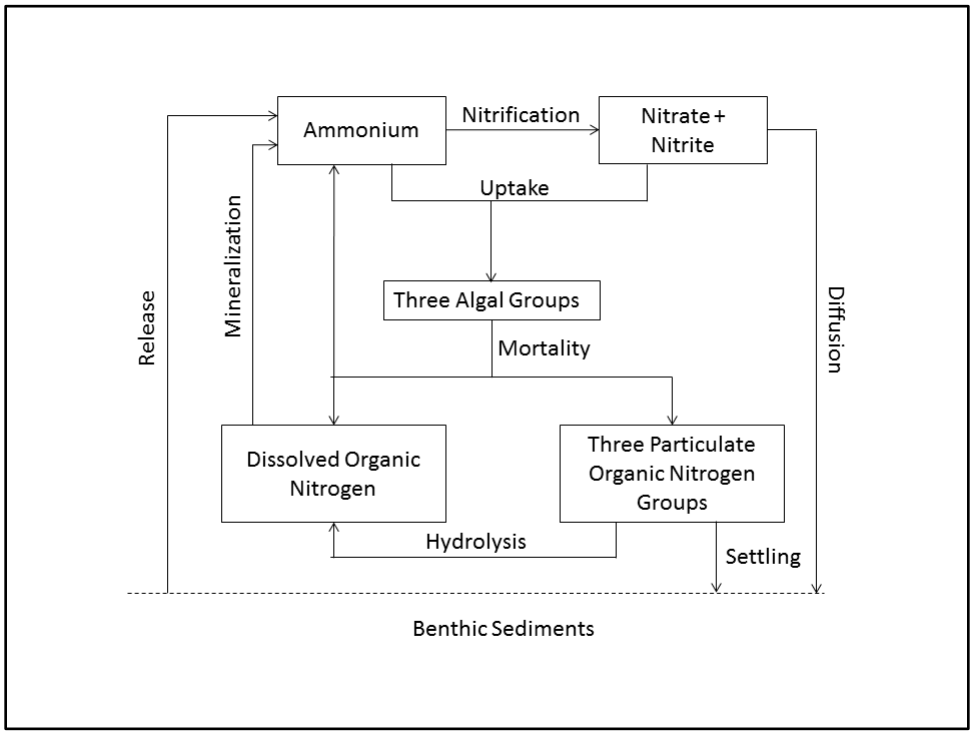

Figure 2-11. Model nitrogen cycle.

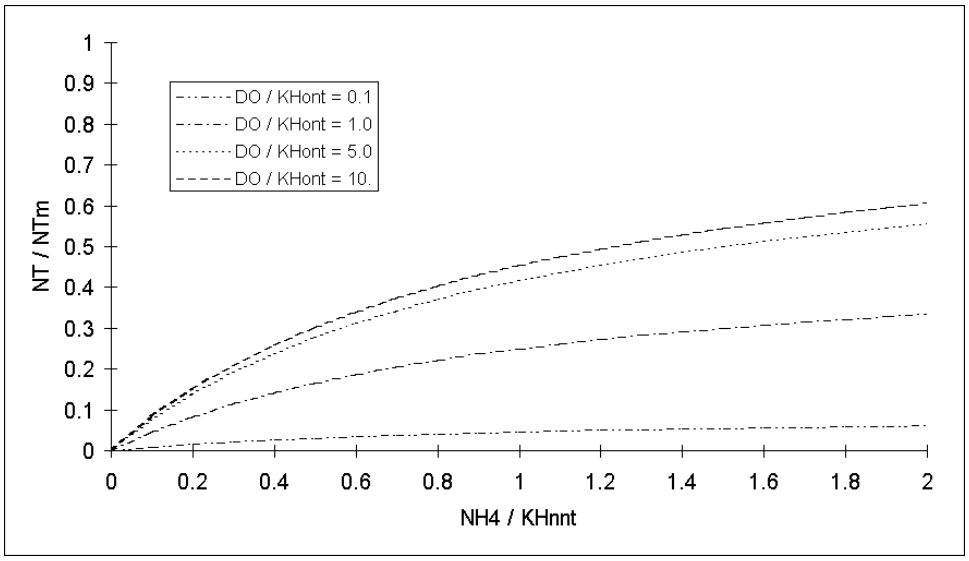

Figure 2-12. Effect of dissolved oxygen and ammonium concentration on nitrification rate.

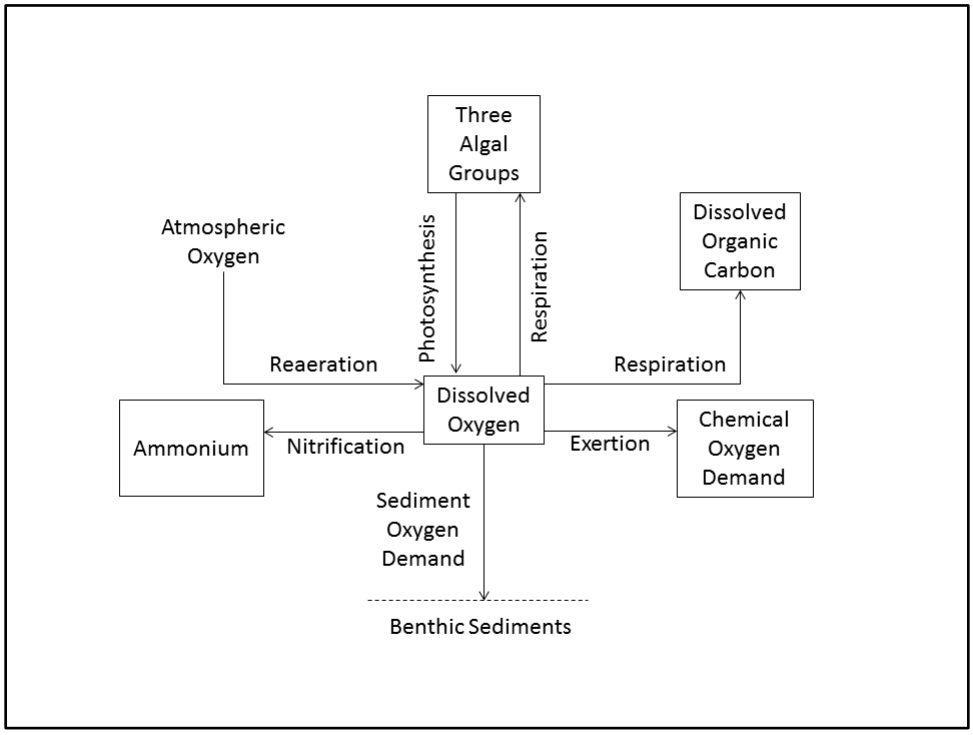

Figure 2-13. Dissolved oxygen sources and sinks.

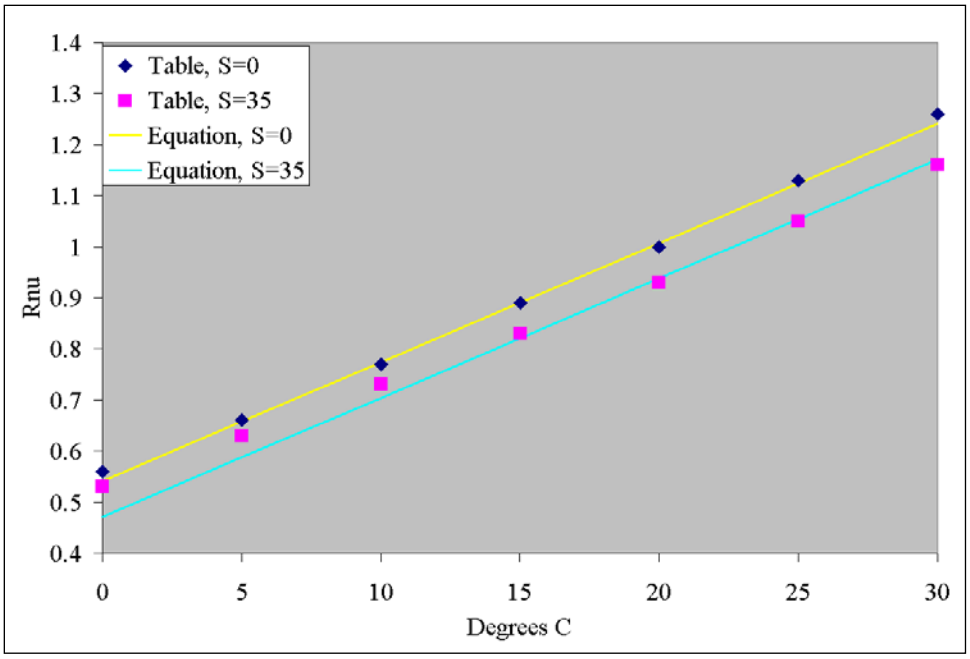

Figure 2-14. Computed and tabulated values of Rv.