September 2023 | www.epa.gov/ord

Water Quality Eutrophication Model (WQEM)

GUIDE TO MODEL THEORY & FORMULATIONS VERSION 1.0

U.S. EPA Office of Research and Development
Center for Environmental Measurement and Modeling

Contents

1.0 Introduction

This document contains a description of the modeling framework implemented in the Water Quality Ecological Model (WQEM). It describes the two types of eutrophication kinetics used by WQEM, Monod and Droop. It also describes the implementation of the instant remineralization algorithm, which is used for the organic matter that settles to the sediment bed.

Eutrophication refers to the process by which an aquatic system becomes enriched with dissolved nutrients, resulting in increased growth of algae and other microscopic plants. This process occurs naturally over many years but can be accelerated by human activities such as fertilizer runoff from farms and sewage input. The nutrients consist mostly of nitrates and phosphates.

Understanding eutrophication is critical in water quality studies. For instance, too many nutrients entering an aquatic system can cause large algal blooms followed by natural die-off and decay which results in low oxygen levels. Low oxygen levels can be detrimental to fish, particularly when levels become hypoxic or even worse, anoxic.

The kinetics equations are based on the Corps of Engineers Water Quality Integrated Compartment Model (CE-QUAL-ICM) (Cerco and Cole, 1995). The mathematical equations are constructed based on the principle of conservation of mass. This is an elementary physical law which is satisfied by macroscopic natural systems.

The water quality constituents of primary interest in WQEM are nutrients, phytoplankton, and dissolved oxygen. Phytoplankton growth is modeled as a function of available nutrients, temperature, and light; other processes such as phytoplankton mortality and herbivorous zooplankton grazing are included. WQEM simulates 18 primary state variables that are common to both Monod and Droop kinetics, 4 Droop-specific state variables, and 1 tracer state variable.

2.0 Development of Eutrophication Equations

A characteristic of eutrophication modeling is the many interactions between nutrients, plankton, and sediments and the transformation reactions describing the conversions between dissolved and particulate phases. In a modeling framework, each interaction is described as a mathematical equation, and the challenge is to define a relatively simple expression to approximate more complex biochemical processes.

2.1 Phytoplankton Growth

WQEM accounts for two phytoplankton classes: diatoms and non-diatoms. We still use the term “greens” for non-diatoms in WQEM’s source code, but the user should keep in mind “greens” is just a label for non-diatoms. The major difference between these classes is silica dependence by the diatoms and differences in settling rates, carbon content, and growth rates at different times of the year. It has been speculated that diatoms grow faster than “non-diatoms” and that they grow better at colder temperatures because one usually observes diatom blooms during the spring in the Great Lakes (Schelske and Stoermer, 1971, 1972; Rousar, 1973; Brooks and Torke, 1977; Bartone and Schelske, 1982; Schelske *et al*., 1986; Fahnenstiel and Scavia, 1987a,b; Scavia and Fahnenstiel, 1987; Rockwell *et al*., 1989; Stoermer, 1993). The kinetic equations used in WQEM are

based on the WASP family of models (Thomann and Di Toro, 1975; Di Toro and Connolly, 1980; Rodgers and Salisbury, 1981a,b) and CE-QUAL-ICM, developed by the United States Army Corps of Engineers (USACE) (Cerco and Cole, 1993). However, note that unlike those found in the WASP family of models, the kinetic equations presented in this chapter do not display a settling rate term. The settling rates are included within the transport algorithm. Thus, settling is accounted for as a transport and not a kinetic process, as it should be. The basic phytoplankton growth equation can be written as:

$$NET\ PRODUCTION\ =\ GROSS\ PRODUCTION - MORTALITY \tag{1}$$

Equation (1) can be represented in mathematical terms as:

$$\frac{dPHYTO}{dt} = \left(k_g - k_d\right)\ PHYTO - k_{gz}\ Z \tag{2}$$

where

PHYTO = phytoplankton concentration (kg · m^{-3})
t = time (s)
k_g = phytoplankton growth rate (s^{-1})
k_d = phytoplankton mortality rate (s^{-1})
k_{gz} = predation rate (s^{-1})
Z = zooplankton concentration (kg · m^{-3})

The growth rate can be written as:

$$k_g = k_{gmax}\, f(N)\, f(T)\, f(I) \tag{3}$$

where

k_{gmax} = optimum growth rate (s^{-1})
f(N) = nutrient growth dependency
f(I) = light growth dependency
f(T) = temperature growth dependency

The optimum growth rate, k_{gmax}, has different values for different types of phytoplankton. Thus, diatoms and non-diatoms have slightly different optimum growth rates. This parameter is represented in the source code with two variable names: PMD, for diatoms, and PMG, for non-diatoms. Table 1 shows default values for the variables.

2.1.1 Nutrient Growth Dependency

For the nutrient growth dependency, f(N), we use the standard Monod equation (Monod, 1949) and variations of it depending whether nitrogen is considered a growth limiting factor or not. Diatoms are treated slightly different from non-diatoms because of the former's silica dependence in addition to nitrogen and phosphorus.

For the non-diatoms, the Liebig's law of minimum (Odum, 1971) applies with no silica dependency and assumes nitrogen is a growth limiting factor.

$$f(N) = Min\left[\left(\frac{NH_4 + NO_3}{k_{sat-N} + NH_4 + NO_3}\right), \left(\frac{P_{av}}{k_{sat-P} + P_{av}}\right)\right] \tag{4}$$

where

Min = minimum of the two expressions (separated by a comma) within the square brackets.
k_{sat-N} = half-saturation coefficient for nitrogen uptake (kg · m^{-3}) (KHNG in Table 1)

k_{sat-P} = half-saturation coefficient for phosphorus uptake (kg · m^{-3}) (KHPG in Table 1)
P_{av} = available phosphorus (kg · m^{-3}), given by Eq. (6) (see below)
NH_4 = ammonia concentration (kg · m^{-3})
NO_3 = nitrate concentration (kg · m^{-3})

If nitrogen is assumed not to be a limiting factor, Eq. (4) simplifies to:

$$f(N) = \frac{P_{av}}{k_{sat-P} + P_{av}} \tag{5}$$

Because we assume that a fraction of the dissolved organic phosphorus (DOP) is readily available for algal uptake, we define the available phosphorus, P_{av}, as follows:

$$P_{av} = SRP + f_{DOP} \bullet DOP \tag{6}$$

where

f_{DOP} = fraction of available DOP (AVFRAC in Table 1)
DOP = dissolved organic phosphorus concentration (kg · m^{-3})
SRP = soluble reactive phosphorus concentration (kg · m^{-3})

The user must specify which of the two nutrient growth dependency equations, Eq. (4), or Eq. (5), to use by setting the general parameter SILIM to specific values. The parameter SILIM is set by the user in the input deck. It is strongly recommended to use Eq. (4) because it applies to all situations, regardless of whether nitrogen is a growth limiting factor or not. Eq. (5) is too restrictive to use because the user must prove, using statistical analysis of field data, that nitrogen is not a growth limiting factor in the aquatic system being studied/simulated.

The diatoms are described using one of three different formulas. The first one uses the product of the silica limitation and the minimum of nitrogen and phosphorus:

$$f(N) = \left(\frac{Si}{k_{sat-Si} + Si}\right) Min\left[\left(\frac{NH_4 + NO_3}{k_{sat-N} + NH_4 + NO_3}\right), \left(\frac{P_{av}}{k_{sat-P} + P_{av}}\right)\right] \tag{7}$$

The second one uses the minimum of silica, nitrogen, and phosphorus:

$$f(N) = Min\left[\left(\frac{Si}{k_{sat-Si} + Si}\right), \left(\frac{NH_4 + NO_3}{k_{sat-N} + NH_4 + NO_3}\right), \left(\frac{P_{av}}{k_{sat-P} + P_{av}}\right)\right] \tag{8}$$

The last one uses the product of silica and phosphorus limitation only:

$$f(N) = \left(\frac{Si}{k_{sat-Si} + Si}\right) \left(\frac{P_{av}}{k_{sat-P} + P_{av}}\right) \tag{9}$$

k_{sat-Si} = half-saturation coefficient for silica (Si) uptake (kg · m^{-3}) (KHSD in Table 1)
Min = minimum of the two expressions (separated by a comma) within the square brackets
k_{sat-N} = half-saturation coefficient for nitrogen uptake (kg · m^{-3}) (KHND in Table 1)
k_{sat-P} = half-saturation coefficient for phosphorus uptake (kg · m^{-3}) (KHPD in Table 1)
Si = dissolved available silica concentration (kg · m^{-3})

Only one equation of the three listed above is used during a particular simulation. The choice of the equation depends on what assumptions are made about the aquatic system. The user specifies which one to use by using the general parameter SILIM in the input deck.

2.1.2 Temperature Growth Dependency

The temperature dependency is expressed using a Gaussian probability function. It is different from most Arrhenius temperature correction factors (Arrhenius, 1889) in that it is two-sided around Tm and has a different shape than the standard $\theta^{(T-20)}$. Thus:

$$f(T) = \begin{cases} exp[-ktg1\ (T - Tm)^2] & where\ T \leq\ Tm \\ exp[-ktg2\ (Tm - T)^2] & where\ T > Tm \end{cases} \quad (10)$$

where

ktg1 = temperature effect below optimum temperature ($°C^{-2}$)
ktg2 = temperature effect above optimum temperature ($°C^{-2}$)
Tm = optimum temperature for phytoplankton growth (°C)
T = water temperature (°C)

The parameters ktg1, ktg2, and Tm are different for diatoms and non-diatoms. The parameter ktg1 is represented in the LM3 source code with the variable name KTGD1 for diatoms and KTGG1 for non-diatoms. The parameter ktg2 is represented with the variable name KTGD2 for diatoms and KTGG2 for non-diatoms. The parameter Tm is represented with the variable name TMD for diatoms and TMG for non-diatoms. Table 1 shows default values for these parameters.

2.1.3 Light Growth Dependency

Several equations have been proposed to describe the effect of light intensity on phytoplankton production. Steele's (1962) equation is one of the most used expressions, while a light saturation equation (like a Monod-type equation) is also frequently used (Di Toro *et al*., 1971). We described light dependency in WQEM according to Steele's equation.

$$f(I) = \frac{I}{I_s} exp\left[-\left(\frac{I}{I_s}\right) + 1\right] \quad (11)$$

where

f(I) = light limitation (fraction between 0 and 1)
I = incident solar light intensity ($W \cdot m^{-2}$)
I_s = saturating light intensity ($W \cdot m^{-2}$) (ISMIN in Table 1)

The Beer-Lambert equation (Parker, 1993) was used to estimate light penetration into the water.

$$I_z = I_o\ exp(-k_{ess}\ z) \quad (12)$$

where

I_z = the light intensity at depth z ($W \cdot m^{-2}$)
I_o = surface light intensity ($W \cdot m^{-2}$)
k_{ess} = light extinction coefficient (m^{-1})
z = depth (m)

Substituting Eq. (12) into Eq. (11):

$$f\big(I(z)\big) = \frac{I_o\ ex\,p(-k_{ess}\ z)}{I_s} exp\left[-\frac{I_o\ exp(-k_{ess}\ z)}{I_s} + 1\right] \quad (13)$$

This equation calculates the light limitation at an instantaneous time and at a specific depth. However, for models like WQEM, we need to estimate the light limitation at a

certain cell (with a given depth range) and over a time (the time step). We thus need to integrate this equation over time and depth. Di Toro *et al*. (1971) formulated an equation assuming a constant light intensity over the photoperiod. They integrated Steele's equation, Eq. (14), over a 24-hour period and the total depth of a segment.

$$f(I_a) = \frac{2.718\, fd}{k_{ess}\, \Delta z}\, [exp(-\alpha_1) - exp(-\alpha_0)] \tag{14}$$

where

$$\alpha_0 = \frac{I_a}{I_s} exp(-k_{ess}\, z_1) \tag{15}$$

$$\alpha_1 = \frac{I_a}{I_s} exp(-k_{ess}\, z_2) \tag{16}$$

fd = the photoperiod, which is the fraction of day with sunlight (unitless)
I_a = average light intensity over the photoperiod ($W \cdot m^{-2}$)
Δz = thickness of water column segment = z_2 - z_1 (m)
z_1 = vertical distance from the water surface to the top face of water segment (m)
z_2 = vertical distance from the water surface to the bottom face of water segment (m)

This approach is commonly used, although it has been criticized for losing the power to represent midday surface inhibition (Di Toro *et al*., 1971; Kremer and Nixon, 1974).

The light formalism allows modelers to use different light intensity update intervals, from one to 12 hours. If the user wants to estimate the light limitation for less than a day and the average light intensity of that period is known, they can solve Steele's equation by averaging it over the depth of a grid cell. Let z_1 and z_2 be the water depth of the top and bottom, respectively, of a grid cell. The averaging is performed as:

$$f(I_a) = \frac{1}{z_2 - z_1} \int_{z_1}^{z_2} \left(\frac{I_0 exp(-k_{ess} z)}{I_s} exp\left[- \frac{I_0 exp(-k_{ess} z)}{I_s} + 1 \right] \right) dz \tag{17}$$

The solution is almost the same as Eq. (14), without the fraction of daylight in the equation.

$$f(I_a) = \frac{2.718}{k_{ess}\, \Delta z}\, [exp(-\alpha_1) - exp(-\alpha_0)] \tag{18}$$

The average light intensity (I_a) here can be calculated as follows:

$$I_a = \frac{\int I_0(t) dt}{\int dt} \tag{19}$$

where

$I_0(t)$ = measured incident solar radiation at time t ($W \cdot m^{-2}$)
t = time (hours)

and can thus be approximated by:

$$I_a = \frac{1}{n} \sum_{i=1}^{n} I_0(t_i) \tag{20}$$

where:

n = number of discrete time intervals at which I_0 is measured.

The light extinction coefficient, k_{ess}, as it appears in Eq. (18) requires some further explanation. This coefficient represents the light attenuation in the water column. It is composed of two fractions: a background value dependent on both the color of the water and concentration of suspended particles, and extinction due to light absorption by ambient chlorophyll.

$$k_{ess} = k_e + k_{echl} \sum_{i=d,g} \frac{PHYTO_i}{(CCHL)_i} \tag{21}$$

where

k_e = background light attenuation (m^{-1})
k_{echl} = light attenuation factor for chlorophyll-*a* ($m^2 \cdot kg^{-1}$)
$PHYTO_i$ = phytoplankton concentration ($kg \cdot m^{-3}$)
$(CCHL)_i$ = carbon-to-chlorophyll ratio in phytoplankton group
d,g = diatoms, non-diatoms

The parameters, k_e and k_{echl} are constant input values specified by the user. Suggested values can be found in Table 1 under the source code names KE and KECHL. The variable $(CCHL)_i$ takes on two parameter values, one for diatoms and one for non-diatoms. The diatoms value is denoted by the source code name of CCHLD and the corresponding one for non-diatoms is denoted by the name CCHLG. These parameters are also constants and specified by the user. Suggested values can be found in Table 1.

Many of the eutrophication parameters default values shown in Table 1 were taken from the Chesapeake Bay eutrophication report (Cerco and Cole, 1994). Others were estimated values that did not have any association with that report or with any calibration exercise. The user must decide whether default values are appropriate or not for a given simulation. Strictly speaking, the default values are initialization values within the source code and are not meant to be a mandatory or even a recommended value.

2.2 Zooplankton Kinetics

Zooplankton predation is important in regulating the phytoplankton densities in aquatic systems, especially during the stratified summer months (Scavia *et al*., 1988). Complex zooplankton equations (e.g., Bowie *et al*., 1985) were avoided in WQEM and chose a relatively simple formulation. The equations describing herbivorous zooplankton growth are based on formulations from the literature (Bowie et al., 1985; Di Toro and Connolly, 1980; Di Toro and Matystik, 1980; Thomann and Mueller, 1987). Thus, for the present discussion, no carnivorous zooplankton is simulated.

The following equation was used:

$$\frac{dZ}{dt} = \left(\varepsilon\, k_{gz} - k_{dz}\right) Z \tag{22}$$

where

Z = zooplankton concentration ($kg \cdot m^{-3}$)
t = time (s)
k_{gz} = zooplankton predation rate (s^{-1})
k_{dz} = mortality rate (s^{-1}) (ZDTH in Table 1)
ε = assimilation efficiency (GREFF in Table 1)

$$k_{gz} = k_{gzmax}\left(\frac{PHYTO_T}{ks + PHYTO_T}\right)\theta^{T-T_{rz}} \quad (23)$$

where

k_{gzmax} = maximum growth rate (s^{-1}) (CGZ in Table 1)
$PHYTO_T$ = total phytoplankton concentration = the sum of diatom and non-diatoms concentrations ($kg \cdot m^3$)
ks = half-saturation coefficient ($kg \cdot m^3$) (KSZ in Table 1)
θ = temperature correction factor (ZTHET in Table 1)
T_{rz} = reference temperature (°C) (TZREF in Table 1)

The maximum growth rate is a term that lumps the filtration and assimilation rates into a single term. The mortality term lumps respiration, excretion, and higher predation into a single term. We can thus write the overall equation:

$$\frac{dZ}{dt} = \left[\varepsilon\, k_{gzmax}\frac{PHTYO_T}{ks + PHYTO_T}\theta^{T-T_{rz}} - k_{dz}\right]Z \quad (24)$$

2.3 Carbon Interactions

Several carbon interactions are described in WQEM, including phytoplankton and zooplankton carbon, carbon loads from tributaries, shoreline erosion, and detrital carbon from plankton. The carbon state variables in WQEM are diatom, non-diatom, and zooplankton carbon; labile particulate organic carbon (LPOC); refractory particulate organic carbon (RPOC); and dissolved organic carbon (DOC). Carbon dioxide (CO_2) is not simulated, although a mineralization reaction is included. Diatom and non-diatom carbon are simulated, as described in the previous section. LPOC refers to the organic detrital carbon from the phytoplankton species which breaks down, as the name implies, relatively rapidly. In contrast, the RPOC is the combination of the fraction of the plankton breaking down, as well as other forms of organic carbon in the system (carbon from tributaries, the sediments, etc). These forms of carbon break down more slowly but are not totally refractory. In the equations, we specify the fractions of labile and refractory carbon. We assume that phytoplankton utilize CO_2 as the carbon source during photosynthesis and release carbon as dissolved (CO_2 and DOC) and particulate (RPOC and LPOC).

2.3.1 Phytoplankton Mortality and Decay

Phytoplankton respiration and non-predatory mortality were grouped together in WQEM as a "mortality" term. The release of carbon from these processes was split into different fractions of dissolved and particulate organic carbon.

$$\frac{dDOC}{dt} = f_{cdd}\, k_{bmd}\, DIA + f_{cdg}\, k_{bmg}\, GRE \quad (25)$$

$$\frac{dRPOC}{dt} = f_{crd}\, k_{bmd}\, DIA + f_{crg}\, k_{bmg}\, GRE \quad (26)$$

$$\frac{dLPOC}{dt} = f_{cld}\, k_{bmd}\, DIA + f_{clg}\, k_{bmg}\, GRE \quad (27)$$

where

DIA = diatoms concentration ($kg \cdot m^{-3}$)
GRE = non-diatoms concentration ($kg \cdot m^{-3}$)

f_{cdd} = fraction of basal metabolism exuded as DOC by diatoms (FCDD in Table 1)
f_{cdg} = fraction of basal metabolism exuded as DOC by non-diatoms (FCDG in Table 1)
f_{crd} = fraction of refractory POC produced by diatoms metabolism (FCRD in Table 1)
f_{crg} = fraction of refractory POC produced by non-diatoms metabolism (FCRG in Table 1)
f_{cld} = fraction of labile POC produced by diatoms metabolism (FCLD in Table 1)
f_{clg} = fraction of labile POC produced by non-diatoms metabolism (FCLG in Table 1)
k_{bmd} = base metabolic rate for diatoms (s^{-1})
k_{bmg} = base metabolic rate for non-diatoms (s^{-1})

The base metabolic rates, k_{bmd} and k_{bmg}, correspond to the term k_d of Eq. (2). They are calculated using the following equations:

$$k_{bmd} = b_{mrd}\, exp[k_{tbd}\,(T - T_{rd})] \tag{28}$$

$$k_{bmg} = b_{mrg}\ exp\left[k_{tbg}\,(T - T_{rg})\right] \tag{29}$$

where

b_{mrd} = diatom base metabolic rate (s^{-1}) (BMRD in Table 1)
b_{mrg} = non-diatom base metabolic rate (s^{-1}) (BMRG in Table 1)
k_{tbd} = metabolism temperature dependence factor for diatoms ($°C^{-1}$) (KTBD in Table 1)
k_{tbg} = metabolism temperature dependence factor for non-diatoms ($°C^{-1}$) (KTBG in Table 1)
T = water temperature (°C)
T_{rd} = metabolism reference temperature for diatoms (°C) (TRD in Table 1)
T_{rg} = metabolism reference temperature for non-diatoms (°C) (TRG in Table 1)

However, phytoplankton carbon is also converted to detrital and DOC through predation (messy feeding) and zooplankton-imposed mortality.

$$\frac{dDOC}{dt} = f_{cdp}\,(1-\varepsilon)\,k_{gz}\,Z \tag{30}$$

$$\frac{dRPOC}{dt} = f_{crp}\,(1-\varepsilon)\,k_{gz}\,Z \tag{31}$$

$$\frac{dLPOC}{dt} = f_{clp}\,(1-\varepsilon)\,k_{gz}\,Z \tag{32}$$

where

f_{cdp} = fraction of DOC from predation (FCDP in Table 1)
f_{crp} = fraction of RPOC from predation (FCRP in Table 1)
f_{clp} = fraction of LPOC from predation (FCLP in Table 1)

2.3.2 Zooplankton Mortality and Decay

The zooplankton mortality term included respiration, non-predatory mortality, and predatory mortality. We assume that the detrital zooplankton carbon consists of dissolved, labile particulate, and refractory particulate fractions.

$$\frac{dDOC}{dt} = f_{cdz}\, k_{dz}\, Z \tag{33}$$

$$\frac{dLPOC}{dt} = f_{clz}\, k_{dz}\, Z \tag{34}$$

$$\frac{dRPOC}{dt} = f_{crz}\, k_{dz}\, Z \tag{35}$$

where

f_{cdz} = fraction of DOC from zooplankton mortality (FCDZ in Table 1)
f_{clz} = fraction of LPOC from zooplankton mortality (FCLZ in Table 1)
f_{crz} = fraction of RPOC from zooplankton mortality (FCRZ in Table 1)

2.3.3 Hydrolysis and Mineralization

Particulate fractions (both labile and refractory) hydrolyze to DOC, while DOC mineralizes to CO_2.

Because we do not explicitly model bacteria in WQEM, their breakdown of carbon is modeled by including a dependency on the phytoplankton, which acts as a surrogate of the heterotrophic bacterial activity in the water. We also calculate a temperature limitation to the hydrolysis and mineralization. The equations can be written as follows:

$$Tf_{mnl} = exp[Tk_{mnl}\ (T - Tr_{mnl})] \tag{36}$$

$$Tf_{hdr} = exp[Tk_{hdr}\ (T - Tr_{hdr})] \tag{37}$$

where

Tf_{mnl} = temperature correction for mineralization (unitless)
Tf_{hdr} = temperature correction for hydrolysis (unitless)
Tk_{mnl} = mineralization temperature coefficient ($°C^{-1}$) (KTMNL in Table 1)
Tk_{hdr} = hydrolysis temperature coefficient ($°C^{-1}$) (KTHDR in Table 1)
Tr_{mnl} = optimum temperature correction for mineralization (°C) (TRMNL in Table 1)
Tr_{hdr} = optimum temperature correction for hydrolysis (°C) (TRHDR in Table 1)

$$\frac{dDOC}{dt} = Tf_{hdr}\left[\left(k_{lc} + k_{lcp}PHYTO_T\right) LPOC + \left(k_{rc} + k_{rcp}PHYTO_T\right) RPOC\right] - Tf_{mnl}\left(k_{dc} + k_{dcp}PHYTO_T\right) DOC \tag{38}$$

$$-\frac{dRPOC}{dt} = Tf_{hdr}\left(k_{rc} + k_{rcp}\, PHYTO_T\right) RPOC \tag{39}$$

$$-\frac{dLPOC}{dt} = Tf_{hdr}\left(k_{lc} + k_{lcp}\, PHYTO_T\right) LPOC \tag{40}$$

where

DOC = dissolved organic carbon concentration ($kg \cdot m^{-3}$)
LPOC = labile particulate organic carbon concentration ($kg \cdot m^{-3}$)
RPOC = refractory particulate organic carbon concentration ($kg \cdot m^{-3}$)
k_{dc} = DOC minimum mineralization rate (s^{-1}) (KDC in Table 1)
k_{dcp} = DOC mineralization relating to phytoplankton ($m^3 \cdot kg\ C^{-1} \cdot s^{-1}$) (KDCALG in Table 1)
k_{rc} = RPOC minimum hydrolysis rate (s^{-1}) (KRC in Table 1)

k_{rcp} = RPOC hydrolysis relating to phytoplankton ($m^3 \cdot kg\ C^{-1} \cdot s^{-1}$) (KRCALG in Table 1)
k_{lc} = LPOC minimum hydrolysis rate (s^{-1}) (KLC in Table 1)
k_{lcp} = LPOC hydrolysis relating to phytoplankton ($m^3 \cdot kg\ C^{-1} \cdot s^{-1}$) (KLCALG in Table 1)

From the last two equations, note that the gain in DOC equals the sum of the loss of RPOC and LPOC.

2.3.4 Low Dissolved Oxygen Contribution to DOC

A low Dissolved Oxygen (O_2) concentration results in no release of CO_2 during phytoplankton's metabolism or phytoplankton's predation by zooplankton, but higher DOC concentration. A low O_2 concentration is considered anything less than 2 mg/L.

If O_2 < 2 mg/L, the following contribution to DOC takes place:

$$\frac{dDOC}{dt} = \left(1 - (f_{cdd} + f_{cld} + f_{crd})\right) k_{bmd}\, DIA + \left(1 - \left(f_{cdg} + f_{clg} + f_{crg}\right)\right)\, k_{bmg}\, GRE \qquad (41)$$

$$\frac{dDOC}{dt} = (1 - \varepsilon)\left(1 - \left(f_{cdp} + f_{clp} + f_{crp}\right)\right) k_{gz}\, Z \qquad (42)$$

where f_{cdd}, f_{cld}, f_{crd}, f_{cdg}, f_{clg}, f_{crg} are defined in Eqs. (25) – (27) (see parameter descriptions below Eq. (27)); k_{bmd}, and k_{bmg} are defined in Eqs. (28) – (29); f_{cdp}, f_{clp}, and f_{crp} are defined in Eqs. (30) – (32) (see parameter descriptions below Eq. (32)); k_{gz} is defined by Eq. (23).

2.3.5 DOC Mineralization

Dissolved organic carbon (DOC) mineralization is the process by which DOC gets transformed to mineral forms such as CO_2. This process removes DOC from the water column. It is modeled as a Monod function with a dependency on the O_2 concentration.

$$\frac{dDOC}{dt} = -\frac{O_2}{O_2 + k_{sat-do}} \left(k_{dc} + k_{dcp} PHYTO_T\right) Tf_{mnl}\, DOC \qquad (43)$$

where

k_{dc} = DOC minimum mineralization rate (s^{-1}). See KDC in Table 1
k_{dcp} = DOC mineralization relating to phytoplankton ($m^3 \cdot kg\ C^{-1} \cdot s^{-1}$). See KDCALG in Table 1
k_{sat-do} = Half-Saturation concentration of dissolved oxygen required for oxic respiration. This parameter is KHODOC in Table 1.
Tf_{mnl} = Mineralization temperature dependence. See Eq. (36).
O2 = Dissolved oxygen concentration ($kg \cdot m^{-3}$)
DOC = Dissolved organic carbon concentration ($kg \cdot m^{-3}$)
$PHYTO_T$ = Total phytoplankton concentration ($kg \cdot m^{-3}$)

2.4 Phosphorus

Phosphorus currently exists as one of four species (in addition to being tied up in the phytoplankton). Note that all four forms are in the same oxidation state; thus, no oxidation reactions occur. The forms are SRP, DOP, and two forms of particulate organic phosphorus (POP), a labile (LPOP), and a refractory (RPOP) form. SRP and a small fraction of the DOP are taken up by the phytoplankton during production

(photosynthesis). They are released due to mortality and predation. Particulate phosphorus is hydrolyzed to DOP, and DOP is hydrolyzed to SRP.

2.4.1 Phosphorus Uptake by Phytoplankton

SRP Uptake:

$$\frac{dSRP}{dt} = -r_{pc}\left(k_{g,dia}\,DIA + k_{g,gre}\,GRE\right)\frac{SRP}{SRP + f_{dop}\,DOP} \tag{44}$$

DOP Uptake:

$$\frac{dDOP}{dt} = -r_{pc}\left(k_{g,dia}\,DIA + k_{g,gre}\,GRE\right)\frac{f_{dop}\,DOP}{SRP + f_{dop}\,DOP} \tag{45}$$

where

r_{pc} = the P:C ratio (unitless) (APCP in Table 1)
$k_{g,dia}$ = diatoms growth rate (s^{-1})
$k_{g,gre}$ = non-diatoms growth rate (s^{-1})
DOP = dissolved organic phosphorus concentration ($kg \cdot m^{-3}$)
SRP = soluble reactive phosphorus concentration ($kg \cdot m^{-3}$)
f_{dop} = available fraction of DOP (AVFRAC in Table 1)

The growth rates for diatoms and non-diatoms are given by Eq. (3).

An interesting concept, common in many phytoplankton models, is the way in which the nutrients, including phosphorus, are accounted for within the phytoplankton. WQEM keeps track of the carbon and uses a constant carbon-to-nutrient ratio to account for the nutrient contents in the phytoplankton.

2.4.2 Phosphorus Release Due to Phytoplankton Metabolism/Mortality

Phytoplankton in the water column are hydrolyzed and mineralized to all four phosphorus forms. During algal metabolic/mortality processes, phytoplankton-P is converted to particulate and dissolved organic forms as well as directly to SRP.

$$\frac{dSRP}{dt} = r_{pc}\left(f_{srp,dia}\,k_{bmd}\,DIA + f_{srp,gre}\,k_{bmg}\,GRE\right) \tag{46}$$

$$\frac{dDOP}{dt} = r_{pc}\left(f_{dop,dia}\,k_{bmd}\,DIA + f_{dop,gre}\,k_{bmg}\,GRE\right) \tag{47}$$

$$\frac{dLPOP}{dt} = r_{pc}\left(f_{lpop,dia}\,k_{bmd}\,DIA + f_{lpop,gre}\,k_{bmg}\,GRE\right) \tag{48}$$

$$\frac{dRPOP}{dt} = r_{pc}\left(f_{rpop,dia}\,k_{bmd}\,DIA + f_{rpop,gre}\,k_{bmg}\,GRE\right) \tag{49}$$

where

$f_{srp,dia}$ = fraction of SRP from diatoms metabolism/mortality (FPID in Table 1)
$f_{srp,gre}$ = fraction of SRP from non-diatoms metabolism/mortality (FPIG in Table 1)
$f_{dop,dia}$ = fraction of DOP from diatoms metabolism/mortality (FPDD in Table 1)
$f_{dop,gre}$ = fraction of DOP from non-diatoms metabolism/mortality (FPDG in Table 1)
$f_{lpop,dia}$ = fraction of LPOP from diatoms metabolism/mortality (FPLD in Table 1)

$f_{lpop,gre}$ = fraction of LPOP from non-diatoms metabolism/mortality (FPLG in Table 1)
$f_{rpop,dia}$ = fraction of RPOP from diatoms metabolism/mortality (FPRD in Table 1)
$f_{rpop,gre}$ = fraction of RPOP from non-diatoms metabolism/mortality (FPRG in Table 1)
DIA = diatoms concentration (kg · m^{-3})
GRE = non-diatoms concentration (kg · m^{-3})
k_{bmd} = base metabolic rate for diatoms, given by Eq. (28)
k_{bmg} = base metabolic rate for non-diatoms, given by Eq. (29)

2.4.3 Phosphorus Release Due to Zooplankton Predation

During phytoplankton predation, zooplankton assimilate only a fraction of the phytoplankton, and the remainder of the detrital phytoplankton is released directly to the water. This process is commonly referred to as "messy feeding." The phosphorus is released in both the dissolved and particulate forms.

$$\frac{dSRP}{dt} = f_{pip}\,(1-\varepsilon)\,r_{pc}\,k_{gz}\,Z \tag{50}$$

$$\frac{dDOP}{dt} = f_{pdp}\,(1-\varepsilon)\,r_{pc}\,k_{gz}\,Z \tag{51}$$

$$\frac{dLPOP}{dt} = f_{plp}\,(1-\varepsilon)\,r_{pc}\,k_{gz}\,Z \tag{52}$$

$$\frac{dRPOP}{dt} = f_{prp}\,(1-\varepsilon)\,r_{pc}\,k_{gz}\,Z \tag{53}$$

where

f_{pip} = fraction of SRP from predation (FPIP in Table 1)
f_{pdp} = fraction of DOP from predation (FPDP in Table 1)
f_{plp} = fraction of LPOP from predation (FPLP in Table 1)
f_{prp} = fraction of RPOP from predation (FPRP in Table 1)
k_{gz} = zooplankton predation rate (s^{-1}), given by Eq. (23)
Z = zooplankton concentration (kg · m^{-3})

2.4.4 Phosphorus Release Due to Zooplankton Mortality

WQEM also includes equations to describe zooplankton mortality. Phosphorus is released to the water column in both the dissolved and particulate forms.

$$\frac{dSRP}{dt} = f_{piz}\,r_{pc}\,k_{dz}\,Z \tag{54}$$

$$\frac{dDOP}{dt} = f_{pdz}\,r_{pc}\,k_{dz}\,Z \tag{55}$$

$$\frac{dLPOP}{dt} = f_{plz}\,r_{pc}\,k_{dz}\,Z \tag{56}$$

$$\frac{dRPOP}{dt} = f_{prz}\,r_{pc}\,k_{dz}\,Z \tag{57}$$

where

f_{piz} = fraction of SRP from zooplankton mortality (FPIZ in Table 1)

f_{pdz} = fraction of DOP from zooplankton mortality (FPDZ in Table 1)
f_{plz} = fraction of LPOP from zooplankton mortality (FPLZ in Table 1)
f_{prz} = fraction of RPOP from zooplankton mortality (FPRZ in Table 1)

2.4.5 Hydrolysis and Mineralization of Phosphorus

Particulate phosphorus is hydrolyzed to DOP and DOP is mineralized back to SRP as follows:

$$\frac{dSRP}{dt} = \left(k_{dp} + k_{dpa}\, PHYTO_T\, \frac{k_{sat-pt}}{SRP + k_{sat-pt}}\right) Tf_{mnl}\, DOP \tag{58}$$

$$\frac{dDOP}{dt} = \left(k_{lp} + k_{lpa}\, PHYTO_T\, \frac{k_{sat-pt}}{SRP + k_{sat-pt}}\right) Tf_{hdr}\, LPOP + \left(k_{rp} + k_{rpa}\, PHYTO_T\, \frac{k_{sat-pt}}{SRP + k_{sat-pt}}\right) Tf_{hdr}\, RPOP - \left(k_{dp} + k_{dpa}\, PHYTO_T\, \frac{k_{sat-pt}}{SRP + k_{sat-pt}}\right) Tf_{mnl}\, DOP \tag{59}$$

$$-\frac{dLPOP}{dt} = \left(k_{lp} + k_{lpa}\, PHYTO_T\, \frac{k_{sat-pt}}{SRP + k_{sat-pt}}\right) Tf_{hdr}\, LPOP \tag{60}$$

$$-\frac{dRPOP}{dt} = \left(k_{rp} + k_{rpa}\, PHYTO_T\, \frac{k_{sat-pt}}{SRP + k_{sat-pt}}\right) Tf_{hdr}\, RPOP \tag{61}$$

where

DOP = dissolved organic phosphorus concentration (kg · m^{-3})
LPOP = labile particulate organic phosphorus concentration (kg · m^{-3})
RPOP = refractory particulate organic phosphorus concentration (kg · m^{-3})
k_{dp} = DOP mineralization coefficient (s^{-1}) (KDP in Table 1)
k_{lp} = LPOP hydrolysis coefficient (s^{-1}) (KLP in Table 1)
k_{rp} = RPOP hydrolysis coefficient (s^{-1}) (KRP in Table 1)
k_{dpa} = DOP mineralization coefficient algal dependence (m^3 · kg^{-1} · s^{-1}) (KDPALG in Table 1)
k_{lpa} = LPOP hydrolysis coefficient algal dependence (m^3 · kg^{-1} · s^{-1}) (KLPALG in Table 1)
k_{rpa} = RPOP hydrolysis coefficient algal dependence (m^3 · kg^{-1} · s^{-1}) (KRPALG in Table 1)
k_{sat-pt} = mean saturation coefficient of algal classes for SRP (kg · m^{-3}) (KHP in Table 1)
Tf_{mnl} = temperature correction for mineralization (unitless); see Eq. (36)
Tf_{hdr} = temperature correction for hydrolysis (unitless); see Eq. (37)

2.5 Nitrogen

The transformation of nitrogen is like phosphorus, although nitrogen exists in more than one oxidation state. Algal nitrogen is released as two forms of particulate organic nitrogen (PON) (labile [LPON], refractory [RPON]), dissolved organic nitrogen (DON),

and ammonia-nitrogen (NH_4). Particulate forms are hydrolyzed to DON. DON is further mineralized to NH_4, and NH_4 is oxidized to NO_3.

2.5.1 Nitrogen Uptake by Phytoplankton

In WQEM we assume that phytoplankton have no preference between NH_4 and NO_3 as a nitrogen source.

$$\frac{dDIN}{dt} = -r_{nc}\left(k_{g,dia}\, DIA + k_{g,gre}\, GRE\right) \tag{62}$$

where

DIN = $NH_4 + NO_3$
NH_4 = ammonia concentration (kg · m^{-3})
NO_3 = nitrate concentration (kg · m^{-3})
r_{nc} = N:C ratio (ANCP in Table 1)
$k_{g,dia}$ = diatoms growth rate (s^{-1}), given by Eq. (3)
$k_{g,gre}$ = non-diatoms growth rate (s^{-1}), given by Eq. (3)

Because we assume no preference, then

$$\frac{dNH_4}{dt} = -\left[\frac{NH_4}{DIN}\right] r_{nc}\left(k_{g,dia}\, DIA + k_{g,gre}\, GRE\right) \tag{63}$$

$$\frac{dNO_3}{dt} = -\left[\frac{NO_3}{DIN}\right] r_{nc}\left(k_{g,dia}\, DIA + k_{g,gre}\, GRE\right) \tag{64}$$

2.5.2 Nitrogen Release Due to Phytoplankton Metabolism/Mortality

Nitrogen bound to phytoplankton can be released as particulate organic, dissolved organic, and NH_4 forms.

$$\frac{dNH_4}{dt} = r_{nc}\left(f_{nh4,dia}\, k_{bmd}\, DIA + f_{nh4,gre}\, k_{bmg}\, GRE\right) \tag{65}$$

$$\frac{dDON}{dt} = r_{nc}\left(f_{don,dia}\, k_{bmd}\, DIA + f_{don,gre}\, k_{bmg}\, GRE\right) \tag{66}$$

$$\frac{dLPON}{dt} = r_{nc}\left(f_{lpon,dia}\, k_{bmd}\, DIA + f_{lpon,gre}\, k_{bmg}\, GRE\right) \tag{67}$$

$$\frac{dRPON}{dt} = r_{nc}\left(f_{rpon,dia}\, k_{bmd}\, DIA + f_{rpon,gre}\, k_{bmg}\, GRE\right) \tag{68}$$

where

$f_{nh4,dia}$ = fraction of NH_4 produced from diatoms metabolic process (FNID in Table 1)
$f_{nh4,gre}$ = fraction of NH_4 produced from non-diatoms metabolic process (FNIG in Table 1)
$f_{don,dia}$ = fraction of DON from diatoms metabolic process (FNDD in Table 1)
$f_{don,gre}$ = fraction of DON from non-diatoms metabolic process (FNDG in Table 1)
$f_{lpon,dia}$ = fraction of LPON from diatoms metabolic process (FNLD in Table 1)
$f_{lpon,gre}$ = fraction of LPON from non-diatoms metabolic process (FNLG in Table 1)
$f_{rpon,dia}$ = fraction of RPON from diatoms metabolic process (FNRD in Table 1)
$f_{rpon,gre}$ = fraction of RPON from non-diatoms metabolic process (FNRG in Table 1)

2.5.3 Nitrogen Release Due to Zooplankton Predation

As described for carbon and phosphorus, the nitrogen balance is affected by the zooplankton through "messy feeding" and zooplankton mortality. For zooplankton grazing:

$$\frac{dDON}{dt} = f_{ndp}\,(1-\varepsilon)\,r_{nc}\,k_{gz}\,Z \tag{69}$$

$$\frac{dNH_4}{dt} = f_{nip}\,(1-\varepsilon)\,r_{nc}\,k_{gz}\,Z \tag{70}$$

$$\frac{dLPON}{dt} = f_{nlp}\,(1-\varepsilon)\,r_{nc}\,k_{gz}\,Z \tag{71}$$

$$\frac{dRPON}{dt} = f_{nrp}\,(1-\varepsilon)\,r_{nc}\,k_{gz}\,Z \tag{72}$$

where

f_{nip} = fraction of NH_4 from predation (FNIP in Table 1)
f_{ndp} = fraction of DON from predation (FNDP in Table 1)
f_{nlp} = fraction of LPON from predation (FNLP in Table 1)
f_{nrp} = fraction of RPON from predation (FNRP in Table 1)

2.5.4 Nitrogen Release Due to Zooplankton Mortality

The release of nitrogen during zooplankton mortality can be expressed similarly to that of phosphorus.

$$\frac{dNH_4}{dt} = f_{niz}\,r_{nc}\,k_{dz}\,Z \tag{73}$$

$$\frac{dDON}{dt} = f_{ndz}\,r_{nc}\,k_{dz}\,Z \tag{74}$$

$$\frac{dLPON}{dt} = f_{nlz}\,r_{nc}\,k_{dz}\,Z \tag{75}$$

$$\frac{dRPON}{dt} = f_{nrz}\,r_{nc}\,k_{dz}\,Z \tag{76}$$

where

f_{niz} = fraction of NH_4 from zooplankton mortality (FNIZ in Table 1)
f_{ndz} = fraction of DON from zooplankton mortality (FNDZ in Table 1)
f_{nlz} = fraction of LPON from zooplankton mortality (FNLZ in Table 1)
f_{nrz} = fraction of RPON from zooplankton mortality (FNRZ in Table 1)

2.5.5 Hydrolysis and Mineralization of Nitrogen

Particulate nitrogen is hydrolyzed to DON and DON is mineralized back to NH_4.

$$\frac{dNH_4}{dt} = \left(k_{dn} + k_{dna}\,PHYTO_T\,\frac{k_{sat-decayN}}{NH_4 + NO_3 + k_{sat-decayN}}\right) Tf_{mnl}\,DON \tag{77}$$

$$\frac{dDON}{dt} = \left(k_{ln} + k_{lna}\, PHYTO_T\, \frac{k_{sat-decayN}}{NH_4 + NO_3 + k_{sat-decayN}}\right) Tf_{hdr}\, LPON + \left(k_{rn} + k_{rna}\, PHYTO_T\, \frac{k_{sat-decayN}}{NH_4 + NO_3 + k_{sat-decayN}}\right) Tf_{hdr}\, RPON - \left(k_{dn} + k_{dna}\, PHYTO_T\, \frac{k_{sat-decayN}}{NH_4 + NO_3 + k_{sat-decayN}}\right) Tf_{mnl}\, DON \quad (78)$$

$$-\frac{dLPON}{dt} = \left(k_{ln} + k_{lna}\, PHYTO_T\, \frac{k_{sat-decayN}}{NH_4 + NO_3 + k_{sat-decayN}}\right) Tf_{hdr}\, LPON \quad (79)$$

$$-\frac{dRPON}{dt} = \left(k_{rn} + k_{rna}\, PHYTO_T\, \frac{k_{sat-decayN}}{NH_4 + NO_3 + k_{sat-decayN}}\right) Tf_{hdr}\, RPON \quad (80)$$

where:

DON	=	dissolved organic nitrogen concentration (kg · m^{-3})
LPON	=	labile particulate organic nitrogen concentration (kg · m^{-3})
RPON	=	refractory particulate organic nitrogen concentration (kg · m^{-3})
k_{dn}	=	minimum DON mineralization rate (s^{-1}) (KDN in Table 1)
k_{dna}	=	DON mineralization rate algal dependence (m^3 · kg^{-1} · s^{-1}) (KDNALG in Table 1)
k_{ln}	=	minimum hydrolysis rate of LPON (s^{-1}) (KLN in Table 1)
k_{lna}	=	LPON hydrolysis rate algal dependence (m^3 · kg^{-1}· s^{-1}) (KLNALG in Table 1)
k_{rn}	=	minimum hydrolysis rate of RPON (s^{-1}) (KRN in Table 1)
k_{rna}	=	RPON hydrolysis rate algal dependence (m^3 · kg^{-1} · s^{-1}) (KRNALG in Table 1)
$k_{sat\text{-}decayN}$	=	organic nitrogen decay half-saturation constant (kg · m^{-3}) (KHN in Table 1)
Tf_{mnl}	=	temperature correction for mineralization (unitless), given by Eq. (36)
Tf_{hdr}	=	temperature correction for hydrolysis (unitless), given by Eq. (37)

2.5.6 Nitrification

Nitrification is the biological oxidation of ammonia into nitrite followed by the oxidation of these nitrites into nitrates. The modeling of the oxidation of NH4 is simplified by assuming that ammonia, NH_4, oxidizes directly into nitrate, NO_3. The mathematical representation of the nitrification process used is:

$$Tf_n = \begin{cases} exp[\text{-}ktnt1\,(T - Tnt)^2] & where\ T < Tnt \\ exp[\text{-}ktnt2\,(Tnt - T)^2] & where\ T \geq Tnt \end{cases} \quad (81)$$

where

Tf_n	=	nitrification temperature dependence function (unitless)
T	=	water temperature (°C)
Tnt	=	optimal temperature for nitrification (°C) (TMNT in Table 1)
ktnt1	=	effect of temperature below optimal temperature for nitrification ($°C^{-2}$) (KTNT1 in Table 1)
ktnt2	=	effect of temperature above optimal temperature for nitrification ($°C^{-2}$) (KTNT2 in Table 1)

$$\frac{dNH_4}{dt} = -k_{ntm}\ Tf_n\ \frac{NH_4}{NH_4 + k_{sat-nitN}}\ \frac{O_2}{O_2 + k_{sat-DO}} \tag{82}$$

$$\frac{dNO_3}{dt} = k_{ntm}\ Tf_n\ \frac{NH_4}{NH_4 + k_{sat-nitN}}\ \frac{O_2}{O_2 + k_{sat-DO}} \tag{83}$$

where

k_{ntm} = nitrification rate coefficient at optimal temperature (kg · m^{-3} · s^{-1}) (NTM in Table 1)
NH_4 = ammonia concentration (kg · m^{-3})
$k_{sat-nitN}$ = half-saturation concentration of NH_4 required for nitrification (kg · m^{-3}). This is KHNNT in Table 1.
k_{sat-DO} = half-saturation concentration of dissolved oxygen required for nitrification (kg · m^{-3}). This is KHDONT in Table 1.

2.5.7 Denitrification

Denitrification is a microbially mediated process that converts nitrate to molecular nitrogen (N_2) under anaerobic conditions using DOC. We assume denitrification happens when O_2 concentration is less than or equal to 2 mg/L. Denitrification reduces the amount of nitrate present in the system.

If $O_2 \leq$ 2m/L, the following process takes place:

$$\frac{dNO_3}{dt} = \frac{NO_3}{NO_3 + k_{sat-denitN}}\ r_{nc}\ k_{denitN}\ DOC \tag{84}$$

where

r_{nc} = nitrification rate coefficient at optimal temperature (kg · m^{-3} · s^{-1}) (ANCP in Table 1)
NO_3 = nitrate concentration (kg · m^{-3})
DOC = dissolved organic carbon concentration (kg · m^{-3})
$k_{sat-denitN}$ = half-saturation concentration of NH_4 required for nitrification (kg · m^{-3}) (KHDENITR in Table 1)
k_{denitN} = half-saturation concentration of dissolved oxygen required for nitrification (kg · m^{-3}). This is KDENITR in Table 1.

2.6 Silica

The behavior of silica is similar to that of phosphorus and nitrogen. Two silica species, particulate biogenic silica or unavailable silica, (SU) and dissolved available silica (SA), are simulated in the lake. Dissolved silica is utilized by phytoplankton, while biogenic silica is released *via* phytoplankton mortality. Dissolved and biogenic silica are released *via* predation upon phytoplankton by zooplankton. Biogenic silica is assumed to mineralize to dissolved silica. The major difference from the other nutrients is that only diatoms have a silica dependency.

The diatom silica consumption can be written as follows:

$$\frac{dSA}{dt} = -r_{sc}\ k_{g,dia}\ DIA \tag{85}$$

where

r_{sc} = Si:C ratio (ASCD in Table 1)

$k_{g,dia}$ = diatoms growth rate (s^{-1}); see Eq. (3)
DIA = diatoms concentration ($kg \cdot m^{-3}$)

Like the other nutrients, silica is released *via* diatom mortality.

$$\frac{dSU}{dt} = r_{sc}\, k_{bmd}\, DIA \tag{86}$$

Both classes of silica can be released *via* zooplankton predation.

$$\frac{dSA}{dt} = f_{sap}\, r_{sc}\, k_{gz}\, Z\, \frac{DIA}{PHYTO_T} \tag{87}$$

$$\frac{dSU}{dt} = f_{sup}\, r_{sc}\, k_{gz}\, Z\, \frac{DIA}{PHYTO_T} \tag{88}$$

where:

f_{sap} = fraction of SA from predation (FSAP in Table 1)
f_{sup} = 1 - f_{sap} = fraction of SU from predation
k_{gz} = zooplankton predation rate (s^{-1}), given by Eq. (23)
Z = zooplankton concentration ($kg \cdot m^{-3}$)

Biogenic silica is mineralized to dissolved silica. This process is described by the following equations:

$$\frac{dSA}{dt} = k_{sua}\, exp[kt_{sua}\, (T - Tr_{sua})]\, SU \tag{89}$$

$$\frac{dSU}{dt} = -k_{sua}\, exp[kt_{sua}\, (T - Tr_{sua})]\, SU \tag{90}$$

where

k_{sua} = particulate silica dissolution rate constant (s^{-1}) (KSUA in Table 1)
kt_{sua} = silica dissolution temperature rate constant ($°C^{-1}$) (KTSUA in Table 1)
Tr_{sua} = silica dissolution reference temperature (°C) (TRSUA in Table 1)
SU = particulate biogenic silica concentration ($kg \cdot m^{-3}$)

We assume that no silica accumulates within the zooplankton. Thus, there are no terms for silica release from zooplankton mortality.

2.7 Dissolved Oxygen

The sources of DO in the water column include algal photosynthesis and reaeration. DO sinks in the water column include algal respiration, organic carbon oxidation (bacterial respiration), and chemical oxygen demand (COD), mainly sulfide oxidation and nitrification.

2.7.1 Dissolved Oxygen Sources from Phytoplankton Production

Phytoplankton generates dissolved oxygen (photosynthesis) when sufficient nutrients, sunlight, and “warmth” (temperature) are available.

$$\frac{dO_2}{dt} = r_{cdo}\, k_{g,dia}\, DIA + r_{cdo}\, k_{g,gre}\, GRE \tag{91}$$

where

$k_{g,dia}$ = diatoms growth rate (s^{-1}). This is defined by Eq. (3) but with diatom-specific parameters.
$k_{g,gre}$ = non-diatom algae growth rate (s^{-1}). This is defined by Eq. (3) but with non-diatom-specific parameters.
r_{cdo} = O_2:C ratio. See RCDO in Table 1.

2.7.2 Dissolved Oxygen Consumption by Phytoplankton Metabolism/Respiration

Phytoplankton consumes oxygen because of respiration.

$$\frac{dO_2}{dt} = -r_{cdo}\left(1-(f_{cdd}+f_{cld}+f_{crd})\right)k_{bmd}\,DIA\; - r_{cdo}\,(1-(f_{cdg}+f_{clg}+f_{crg}))\,k_{bmg}\,GRE \quad (92)$$

where f_{cdd}, f_{cld}, f_{crd}, f_{cdg}, f_{clg}, and f_{crg} are defined in Eqs. (25) – (27) (see parameter descriptions below Eq. (27)); k_{bmd}, and k_{bmg} are defined by Eqs. (28) – (29); DIA and GRE are the diatoms and non-diatoms concentrations; r_{cdo} is the O_2:C ratio.

2.7.3 Dissolved Oxygen Consumption by Zooplankton Predation on Phytoplankton

$$\frac{dO_2}{dt} = -r_{cdo}(1-\varepsilon)\left(1-\left(f_{cdp}+f_{clp}+f_{crp}\right)\right)k_{gz}\,Z \quad (93)$$

Where f_{cdp}, f_{clp}, and f_{crp} are defined in Eqs. (30) – (32); k_{gz} is defined by Eq. (23).

2.7.4 Dissolved Oxygen Sinks from Nitrification

Nitrification is the biological oxidation of ammonia into nitrite followed by the oxidation of these nitrites into nitrates. The modeling of the oxidation of NH_4 is simplified by assuming that ammonia, NH_4, oxidizes directly into nitrate, NO_3. This process consumes O_2, which has the potential to generate anoxic conditions. Nitrification is typically modeled as a double Monod equation with a dependency on both oxygen and ammonia.

$$\frac{dO_2}{dt} = -k_{ntm}\;Tf_n\;\frac{NH_4}{NH_4+k_{sat-nitN}}\;\frac{O_2}{O_2+k_{sat-DO}} \quad (94)$$

where

k_{ntm} = nitrification rate coefficient at optimal temperature (kg · m^{-3} · s^{-1}) (NTM in Table 1)
NH_4 = ammonia concentration (kg · m^{-3})
O_2 = dissolved oxygen concentration (kg · m^{-3})
$k_{sat-nitN}$ = half-saturation concentration of NH_4 required for nitrification (kg · m^{-3}) (KHNNT in Table 1)
k_{sat-DO} = half-saturation concentration of dissolved oxygen required for nitrification (kg · m^{-3}). This is KHDONT in Table 1.
Tf_n = nitrification temperature dependence function (unitless)

The nitrification temperature dependence function, Tf_n, is given by:

$$Tf_n = \begin{cases} exp[-ktnt1\,(T-Tnt)^2] & where\ T < Tnt \\ exp[-ktnt2\,(Tnt-T)^2] & where\ T \geq Tnt \end{cases} \quad (95)$$

where

T	=	water temperature (°C)
Tnt	=	optimal temperature for nitrification (°C) (TMNT in Table 1)
ktnt1	=	effect of temperature below optimal temperature for nitrification ($°C^{-2}$) (KTNT1 in Table 1)
ktnt2	=	effect of temperature above optimal temperature for nitrification ($°C^{-2}$) (KTNT2 in Table 1)

2.7.5 Dissolved Oxygen Sinks from DOC Mineralization

Dissolved oxygen gets removed from the water column by DOC mineralization. This process is modeled as:

$$\frac{dO_2}{dt} = -\frac{O_2}{O_2 + k_{sat-do}} \left(k_{dc} + k_{dcp} PHYTO_T\right) Tf_{mnl}\, DOC\, r_{cdo} \tag{96}$$

where

k_{dc}	=	DOC minimum mineralization rate (s^{-1}). See KDC in Table 1
k_{dcp}	=	DOC mineralization relating to phytoplankton ($m^3 \cdot kg\ C^{-1} \cdot s^{-1}$). See KDCALG in Table 1
k_{sat-do}	=	Half-Saturation concentration of dissolved oxygen required for oxic respiration. This parameter is KHODOC in Table 1.
r_{cdo}	=	Dissolved oxygen-to-carbon ratio (mol of O_2 / mol of C). See RCDO in Table 1.
Tf_{mnl}	=	Mineralization temperature dependence. See Eq. (36).
O_2	=	Dissolved oxygen concentration ($kg \cdot m^{-3}$)
DOC	=	Dissolved organic carbon concentration ($kg \cdot m^{-3}$)
$PHYTO_T$	=	Total phytoplankton concentration ($kg \cdot m^{-3}$)

2.7.6 Dissolved Oxygen Sinks from Chemical Oxygen Demand

Chemical oxygen demand is the concentration (oxygen equivalents) of reduced species in the water that can be rapidly oxidized chemically (absence of microorganisms). Thus, COD will remove O_2 from the water column. It is modeled as a Monod function with a dependency on the O_2 concentration.

$$\frac{dO_2}{dt} = -\frac{O_2}{O_2 + k_{sat-COD}}\, k_{COD}\, COD \tag{97}$$

where

O_2	=	Dissolved oxygen concentration ($kg \cdot m^{-3}$)
k_{COD}	=	COD oxidation rate (s^{-1}). See KCOD in Table 1.
COD	=	Chemical oxygen demand concentration ($kg \cdot m^{-3}$)
$K_{sat-COD}$	=	half-saturation concentration of O_2 required for exertion of COD ($kg \cdot m^{-3}$). See KHOCOD in Table 1.

Note: This process has not been fully tested as of the writing of this document.

2.7.7 Reaeration

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

$$\frac{dO_2}{dt} = \frac{k_{rdo}}{\Delta z}\left(O_{2,sat} - O_2\right) \tag{98}$$

where

$O_{2,sat}$ = dissolved oxygen saturation concentration (kg · m^{-3})
O_2 = dissolved oxygen concentration (kg · m^{-3})
K_{rdo} = reaeration coefficient (m · s^{-1})
Δz = depth/thickness of surface segment (m)

The dissolved oxygen saturation concentration is calculated as:

$$ln\, O_{2,sat} = -139.34411 + \left(\frac{1.575701\ x\ 10^5}{T}\right) - \left(\frac{6.642308\ x\ 10^7}{T^2}\right) + \left(\frac{1.243800\ x\ 10^{10}}{T^3}\right) - \left(\frac{8.621949\ x\ 10^{11}}{T^4}\right) - CHL\left[(3.1929\ x\ 10^{-2}) - \left(\frac{1.9428\ x\ 10^1}{T}\right) + \left(\frac{3.8673\ x\ 10^3}{T^2}\right)\right] \tag{99}$$

where

T = water temperature (°K)
CHL = chlorinity
Chlorinity is calculated as:

$$CHL = \frac{Salinity}{1.80655} \tag{100}$$

The reaeration coefficient is calculated as:

$$k_{rdo} = (0.222\ \times\ ws^2 + 0.333 \times ws)\left(\frac{Sc}{600.0}\right)^{-0.5} \tag{101}$$

where

ws = wind speed (m · s^{-1})
Sc = Schmidt number for O_2 (unitless)

The Schmidt number for dissolved oxygen is:

$$Sc = \begin{cases} 1800.6 - (120.1 \times T) + (3.7818 \times T^2) - (0.047608 \times T^3), & sal < 1 \\ 1953.4 - (128.0 \times T) + (3.9918 \times T^2) - (0.050091 \times T^3), & sal \geq 1 \end{cases} \tag{102}$$

where “sal” stands for salinity.

2.8 Droop Kinetics

The equations of the Droop formulations as implemented in WQEM are detailed below (Droop, 1973; Cerco et al., 2004).

The phosphorus limitation factor of phytoplankton growth is given by:

$$f(P) = \frac{Q(P) - Q_{minP}}{Q(P)} \tag{103}$$

where

Q(P) = P cell quota (kg P kg^{-1} algal C)
Q_{minP} = minimum phosphorus quota (kg P kg^{-1} algal C)

The nitrogen limitation factor is given by:

$$f(N) = \frac{Q(N) - Q_{minN}}{Q(N)} \tag{104}$$

where

Q(P) = N cell quota (kg N kg^{-1} algal C)
Q_{minN} = minimum nitrogen quota (kg N kg^{-1} algal C)

The uptake of P by algae is given by:

$$P_{uptake} = V_{maxP} \frac{PO_4}{K_{hP} + PO_4} \tag{105}$$

where

V_{maxP} = maximum uptake rate (kg P kg^{-1} algal C s^{-1}),
K_{hP} = half-saturation concentration for phosphorus uptake (kg P m^{-3})
PO_4 = dissolved phosphate concentration external to the algae (kg P m^{-3})

PO_4 is calculated as:

$$PO_4 = SRP + frac_{DOP} \cdot DOP \tag{106}$$

where

$frac_{DOP}$ = fraction of DOP available for uptake
SRP = soluble reactive phosphorus and DOP is dissolved organic phosphorus

The uptake of N by the algae is given by:

$$N_{uptake} = V_{maxN} \frac{N_{dis}}{K_{hN} + N_{dis}} \tag{107}$$

where

V_{maxN} = maximum uptake rate (kg N kg^{-1} algal C s^{-1}),
K_{hN} = half-saturation concentration for nitrogen uptake (kg N m^{-3})
N_{dis} = dissolved nitrogen concentration external to the algae (kg N m^{-3})

N_{dis} is calculated as

$$N_{dis} = NH_4 + NO_3 + frac_{DON}\, DON \tag{108}$$

where

NH_4 = ammonium concentration (kg N m^{-3} s^{-1})
NO_3 = nitrate concentration (kg N m^{-3} s^{-1})
DON = dissolved organic nitrogen concentration (kg N m^{-3} s^{-1})
$frac_{DON}$ = fraction of DON available for uptake (unitless)

The mass-balance equations for internal P (P_{int}) and internal N (N_{int}), excluding transport processes, are:

$$\frac{dP_{int}}{dt} = \left(P_{uptake} - BMA * Q(P)\right) * C(algae) - PRA * Q(P) \tag{109}$$

$$\frac{dN_{int}}{dt} = \left(N_{uptake} - BMA * Q(N)\right) * C(algae) - PRA * Q(N) \quad (110)$$

Where BMA is the algal metabolic rate (s^{-1}), C(algae) is the algal concentration (kg C m^{-3}), and PRA is the predation rate (kg C m^{-3} s^{-1}).

See Table 2 for a complete list of input parameters associated with Droop kinetics.

Note: The default values shown in Table 2 are only placeholders in the source code and do not represent realistic values. The user must enter values in the input deck they deem reasonable for a given simulation.

2.9 Instant Remineralization

WQEM has an instant remineralization algorithm (Fennel et al., 2011) for the organic matter deposited to the sediment bed. It serves as a simplified version of sediment processes.

The contribution of the phytoplankton dependence to DOC mineralization is represented in WQEM by Eq. (111)

$$\frac{dDOC}{dt} = -KDCALG \cdot PHYTO_T \cdot DOC \quad (111)$$

where

KDCALG = phytoplankton-related dependence for DOC mineralization (m3 (kg C)$^{-1}$ s^{-1})
$PHYTO_T$ = sum of diatoms and non-diatom algae concentrations (kg C m^{-3})
DOC = dissolved organic carbon concentration (kg C m^{-3}), and t is time (s)

The sediment oxygen demand (SOD), nitrate-nitrite, and ammonium sediment fluxes simulated by WQEM are based on the “instant remineralization” approach, but sediment flux rates are capped to fit within a range observed in Gulf of Mexico’s field studies. The carbon and nitrogen masses reaching the sediment bed are calculated by summing the carbon and nitrogen fractions of the settled masses of phytoplankton and the particulate organic forms of carbon and nitrogen. We assume that the entire carbon and nitrogen sediment pools are available to be oxidized although maximum flux rates derived from field observations were implemented.

Carbon SOD (SOD_{carbon}, kg O_2 m^{-2} s^{-1}) is calculated using settled particulate organic carbon (POC_{sed}, kg C m^{-2} s^{-1}) and a dependency on the oxygen concentration of the overlying water; this is shown in Eq. (112).

$$SOD_{carbon} = POC_{sed} \frac{O_2}{O_2 + KHODOC\_SED} RCDO \quad (112)$$

where

O_2 = dissolved oxygen concentration in the overlying water (kg O_2 m^{-3})
KHODOC_SED = O_2 half-saturation coefficient (kg O_2 m^{-3})
RCDO = O_2:carbon conversion factor (kg O_2 (kg C)$^{-1}$)

The carbon SOD calculation is capped to ensure the modeled total SOD value does not exceed maximum observed SOD measurements in the Gulf of Mexico, which were approximately 1000 mg O_2 m^{-2} d^{-1} (30 mmol O_2 m^{-2} d^{-1}).

Similar to carbon SOD, sediment nitrification was calculated using the settled organic nitrogen in the sediments (PON_{sed}, kg N m^{-2} s^{-1}) and a dependency on the overlying water O_2 concentration; this is shown in Eq. (113).

$$Nitrification = PON_{sed} \frac{O_2}{O_2 + KHDONT\_SED} \quad (113)$$

where

nitrification = sediment nitrification (kg N m-2 s-1)
KHDONT_SED = O2 half-saturation concentration (kg O2 m-3).

The sediment total SOD is calculated as the sum of carbon SOD and sediment nitrification, as in Eq. (114).

$$Total\ SOD = SOD_{carbon} + Nitrification \cdot RNTO \quad (114)$$

where

RNTO = O_2:N conversion factor (kg O_2 (kg N)$^{-1}$)

The remaining settled organic nitrogen that remained after nitrification has occurred was released as ammonium from the sediment bed to the overlying water. The amount of ammonium released is given by Eq. (115).

$$(NH_4)_{sed} = PON_{sed} - Nitrification \quad (115)$$

The remaining carbon, the amount not oxidized by carbon SOD, is available for denitrification using nitrate as an electron acceptor. Sediment denitrification is calculated assuming the process is limited by the carbon remaining in the sediments, as shown in Eq. (116).

$$Denitr = -POC_{sed}\left(1 - \frac{DO}{DO + KHODOC\_SED}\right)(DENIT\_CN\_RATIO)^{-1} \quad (116)$$

where

Denitr = nitrate consumed (kg N m-2 s-1)
DENIT_CN_RATIO = C:N ratio for denitrification

If the amount of nitrate consumed is smaller than the nitrate available in the sediment bed (produced by nitrification in the sediments), the remaining sediment nitrate is released into the bottom layer of the water column as a positive sediment nitrate flux. If the nitrate consumed is larger than the nitrate available in the sediment, nitrate is transported from the bottom water layer into the sediments as a negative flux. Nitrate flux from the water into the sediments is reduced by a relationship based upon the available nitrate concentration in the overlying water and the maximum nitrate flux into the sediment bed is set to 14 mg N m^{-2} d^{-1} (1 mmol N m^{-2} d^{-1}) based on observations in the Gulf of Mexico. If sediment carbon in a model cell is not completely oxidized during the carbon SOD and denitrification calculations, the remaining carbon is available for the calculation during the next time step.

3.0 Table 1: Eutrophication Parameters

Key Name	Description	Default Value	Units
ANCP	N:C ratio for plankton	2.0×10^{-1}	None
APCP	P:C ratio for plankton	1.0×10^{-2}	None
ASCD	Si:C ratio for diatoms	8.0×10^{-1}	None
AVFRAC	Available fraction of DOP	0	None
BMRD	Diatom base metabolic rate	8.6×10^{-7}	s^{-1}
BMRG	Non-Diatom algae base metabolic rate	8.6×10^{-7}	s^{-1}
CCHLD	Carbon:chlorophyll ratio for diatoms	5.0×10^{1}	None
CCHLG	Carbon:chlorophyll ratio for non-diatom algae	5.0×10^{1}	None
CGZ	Zooplankton maximum growth rate	4.6×10^{-6}	s^{-1}
DENIT_CN_RATIO	Denitrification C:N ratio	1.07	None
FCDD	Fraction of basal metabolism exuded as DOC by diatoms	1.0×10^{-1}	None
FCDG	Fraction of basal metabolism exuded as DOC by non-diatoms	1.0×10^{-1}	None
FCDP	Fraction of DOC produced by predation	1.0×10^{-1}	None
FCDZ	Fraction of DOC from zooplankton mortality	1.0×10^{-1}	None
FCLD	Fraction of labile POC produced by diatoms metabolism	1.0×10^{-1}	None
FCLG	Fraction of labile POC produced by non-diatoms metabolism	1.0×10^{-1}	None
FCLP	Fraction of labile PDC from predation	5.5×10^{-1}	None
FCLZ	Fraction of labile PDC from zooplankton mortality	5.5×10^{-1}	None
FCRD	Fraction of refractory POC produced by diatoms metabolism	1.0×10^{-1}	None
FCRG	Fraction of refractory POC produced by non-diatoms metabolism	1.0×10^{-1}	None
FCRP	Fraction of refractory PDC from predation	3.5×10^{-1}	None
FCRZ	Fraction of refractory PDC from zooplankton mortality	3.5×10^{-1}	None
FNDD	Fraction of DON produced by diatom metabolism	8.0×10^{-1}	None
FNDG	Fraction of DON produced by non-diatom algae metabolism	8.0×10^{-1}	None
FNDP	Fraction of DON produced by predation	1.0×10^{-1}	None
FNDZ	Fraction of DON produced by zooplankton mortality	4.0×10^{-1}	None
FNID	Fraction of inorganic nitrogen produced by diatom metabolism	1.0×10^{-1}	None
FNIG	Fraction of Inorganic nitrogen produced by non-diatom algae metabolism	1.0×10^{-1}	None
FNIP	Fraction of inorganic nitrogen produced by predation	0	None
FNIZ	Fraction of inorganic nitrogen produced by zooplankton mortality	1.0×10^{-1}	None
FNLD	Fraction of labile particulate nitrogen produced by diatom metabolism	1.0×10^{-1}	None

Key Name	Description	Default Value	Units
FNLG	Fraction of labile particulate nitrogen produced by non-diatom algae metabolism	1.0×10^{-1}	None
FNLP	Fraction of labile particulate nitrogen produced by predation	5.5×10^{-1}	None
FNLZ	Fraction of LON produced by zooplankton mortality	3.5×10^{-1}	None
FNRD	Fraction of refractory particulate nitrogen produced by diatom metabolism	0	None
FNRG	Fraction of refractory particulate nitrogen produced by non-diatom metabolism	0	None
FNRP	Fraction of RON produced by predation	3.5×10^{-1}	None
FNRZ	Fraction of RON produced by zooplankton mortality	1.5×10^{-1}	None
FPDD	Fraction of DOP produced by diatom metabolism	8.0×10^{-1}	None
FPDG	Fraction of DOP produced by non-diatom algae metabolism	8.0×10^{-1}	None
FPDP	Fraction of DOP produced by predation	1.0×10^{-1}	None
FPDZ	Fraction of DOP produced by zooplankton mortality	4.0×10^{-1}	None
FPID	Fraction of inorganic phosphorus produced by diatom metabolism	1.0×10^{-1}	None
FPIG	Fraction of inorganic phosphorus produced by non-diatom algae metabolism	1.0×10^{-1}	None
FPIP	Fraction of inorganic phosphorus produced by predation	0	None
FPIZ	Fraction of inorganic phosphorus produced by zooplankton mortality	1.0×10^{-1}	None
FPLD	Fraction of LOP produced by diatom metabolism	1.0×10^{-1}	None
FPLG	Fraction of LOP produced by non-diatom algae metabolism	1.0×10^{-1}	None
FPLP	Fraction of LOP produced by predation	5.5×10^{-1}	None
FPLZ	Fraction of LOP produced by zooplankton mortality	3.5×10^{-1}	None
FPRD	Fraction of ROP produced by diatom metabolism	0	None
FPRG	Fraction of ROP produced by non-diatom algae metabolism	0	None
FPRP	Fraction of ROP produced by predation	3.5×10^{-1}	None
FPRZ	Fraction of ROP produced by zooplankton mortality	1.5×10^{-1}	None
FSAP	Fraction of silica made available through predation	0	None
GREFF	Zooplankton grazing efficiency	6.0×10^{-1}	None
ILUM0	Constant value of illumination (this is a user-defined value)	0	$W\ m^{-2}$
ISMIN	Minimum optical illumination factor	6.05×10^{-1}	$W\ m^{-2}$
KCOD	Chemical oxygen demand oxidation rate	1.0	s^{-1}
KDC	Minimum DOC mineralization rate	1.2×10^{-7}	s^{-1}
KDCALG	DOC mineralization rate algal dependence	0	$m^3\ kg^{-1}\ s^{-1}$
KDENITR	Maximum denitrification rate coefficient	1.0	s^{-1}
KDN	Minimum DON mineralization rate	2.3×10^{-7}	s^{-1}
KDNALG	DON mineralization rate algal dependence	0	$m^3\ kg^{-1}\ s^{-1}$

Key Name	Description	Default Value	Units
KDP	Minimum DOP mineralization rate	5.0×10^{-7}	s^{-1}
KDPALG	DOP mineralization rate algal dependence	2.3×10^{-3}	$m^3\ kg^{-1}\ s^{-1}$
KE	Background light attenuation	1.5×10^{-1}	m^{-1}
KECHL	Light attenuation factor for chlorophyll a	1.7×10^{4}	$m^2\ kg^{-1}$
KHDENITR	Half-saturation concentration of NO_3 required for denitrification	1.0	$kg\ m^{-3}$
KHDENITR_SED	Half-saturation concentration of NO_3 required for denitrification in the sediment bed	1.0	$kg\ m^{-3}$
KHDONT	Half-saturation concentration of dissolved oxygen required for nitrification	1.0	$kg\ m^{-3}$
KHDONT_SED	Half-saturation concentration of dissolved oxygen required for nitrification in the sediment bed.	1.0	$kg\ m^{-3}$
KHN	Organic nitrogen decay half-saturation constant	2.5×10^{-5}	$kg\ m^{-3}$
KHND	Mean half-saturation constant for nitrogen uptake by diatoms	2.5×10^{-5}	$kg\ m^{-3}$
KHNG	Mean half-saturation constant for nitrogen uptake by non-diatom algae	2.5×10^{-5}	$kg\ m^{-3}$
KHNNT	Half-saturation concentration of NH_4 required for nitrification	1.0×10^{-4}	$kg\ m^{-3}$
KHOCOD	Half-Saturation concentration of O_2 required for exertion of chemical oxygen demand	1.0	$kg\ m^{-3}$
KHODOC	Half-Saturation concentration of O_2 required for oxic respiration	1.0	$kg\ m^{-3}$
KHODOC_SED	Half-Saturation concentration of O_2 required for oxic respiration in the sediment bed	1.0	$kg\ m^{-3}$
KHP	Organic phosphorus decay half-saturation constant	1.0×10^{-6}	$kg\ m^{-3}$
KHPD	Mean half-saturation constant for diatom phosphorus uptake	1.0×10^{-6}	$kg\ m^{-3}$
KHPG	Mean half-saturation constant for non-diatom algae phosphorus uptake	1.0×10^{-6}	$kg\ m^{-3}$
KHSD	Mean half-saturation constant for diatom silica uptake	3.0×10^{-5}	$kg\ m^{-3}$
KLC	Minimum hydrolysis rate of LOC	8.6×10^{-7}	s^{-1}
KLCALG	LOC hydrolysis rate algal dependence	0	$m^3\ kg^{-1}\ s^{-1}$
KLN	Minimum hydrolysis rate of LON	2.3×10^{-7}	s^{-1}
KLNALG	LON hydrolysis rate algal dependence	0	$m^3\ kg^{-1}\ s^{-1}$
KLP	Minimum hydrolysis rate of LOP	2.3×10^{-7}	s^{-1}
KLPALG	LOP hydrolysis rate algal dependence	2.3×10^{-3}	$m^3\ kg^{-1}\ s^{-1}$
KRC	Minimum hydrolysis rate of ROC	5.0×10^{-8}	s^{-1}
KRCALG	ROC hydrolysis rate algal dependence	0	$m^3\ kg^{-1}\ s^{-1}$
KRN	Minimum hydrolysis rate of RON	5.7×10^{-8}	s^{-1}
KRNALG	RON hydrolysis rate algal dependence	0	$m^3\ kg^{-1}\ s^{-1}$
KRP	Minimum hydrolysis rate of ROP	5.7×10^{-8}	s^{-1}
KRPALG	ROP hydrolysis rate algal dependence	2.3×10^{-3}	$m^3\ kg^{-1}\ s^{-1}$
KSUA	Particulate silica dissolution rate constant	5.0×10^{-8}	s^{-1}

Key Name	Description	Default Value	Units
KSZ	Half-saturation coefficient of zooplankton for phytoplankton	7.5×10^{-4}	kg m^{-3}
KTBD	Metabolism temperature dependence factor for diatoms	6.9×10^{-2}	$°C^{-1}$
KTBG	Metabolism temperature dependence factor for non-diatoms	6.9×10^{-2}	$°C^{-1}$
KTGD1	Effect of temperature below optimal temperature for diatoms	2.5×10^{-3}	$°C^{-2}$
KTGD2	Effect of temperature above optimal temperature for diatoms	6.0×10^{-3}	$°C^{-2}$
KTGG1	Effect of temperature below optimal temperature for non-diatoms	2.5×10^{-3}	$°C^{-2}$
KTGG2	Effect of temperature above optimal temperature for non-diatoms	1.0×10^{-2}	$°C^{-2}$
KTHDR	Hydrolysis temperature dependence	6.9×10^{-2}	$°C^{-1}$
KTMNL	Mineralization temperature dependence	6.9×10^{-2}	$°C^{-1}$
KTNT1	Effect of temperature below optimal temperature nitrification	9.0×10^{-2}	$°C^{-2}$
KTNT2	Effect of temperature above optimal temperature for nitrification	1.1×10^{-6}	$°C^{-2}$
KTSUA	Silica dissolution temperature rate constant	1.1×10^{-6}	$°C^{-1}$
NTM	Nitrification rate coefficient at optimal temperatures	1.2×10^{-12}	kg m^{-3} s^{-1}
PMD	Diatom production under optimal conditions	2.4×10^{-5}	s^{-1}
PMG	Non-diatom algae production under optimal conditions	2.3×10^{-5}	s^{-1}
RCDO	Dissolved Oxygen-to-Carbon ratio	2.67	(mol of O_2) /(mol of C)
TMD	Temperature of optimum growth for diatoms	2.0×10^{-1}	°C
TMG	Temperature of optimum growth for non-diatoms	2.0×10^{-1}	°C
TMNT	Optimal temperature for nitrification	2.0×10^{-1}	°C
TRD	Metabolism reference temperature for diatoms	2.0×10^{1}	°C
TRG	Metabolism reference temperature for non-diatoms	2.0×10^{1}	°C
TRHDR	Reference temperature for hydrolysis	2.0×10^{1}	°C
TRMNL	Reference temperature for mineralization	2.0×10^{1}	°C
TRSUA	Silica dissolution reference temperature	2.0×10^{1}	°C
TZREF	Predation reference temperature	2.0×10^{1}	°C
ZDTH	Zooplankton death/die-off coefficient	3.5×10^{-7}	s^{-1}
ZTHET	Temperature coefficient for predation	1.05	None

4.0 Table 2: Droop Kinetics Parameters

Key Name	Description	Default Value	Units
FIntNID	Fraction of inorganic nitrogen produced by diatoms metabolism	0	None

Key Name	Description	Default Value	Units
FIntNIG	Fraction of inorganic nitrogen produced by non-diatoms metabolism	0	None
FIntNDD	Fraction of dissolved nitrogen produced by diatoms metabolism	0	None
FIntNDG	Fraction of dissolved nitrogen produced by non-diatoms metabolism	0	None
FIntNLD	Fraction of labile nitrogen produced by diatoms metabolism	0	None
FIntNLG	Fraction of labile nitrogen produced by non-diatoms metabolism	0	None
FIntNRD	Fraction of refractory nitrogen produced by diatoms metabolism	0	None
FIntNRG	Fraction of refractory nitrogen produced by non-diatoms metabolism	0	None
FIntPID	Fraction of inorganic phosphorus produced by diatoms metabolism	0	None
FIntPIG	Fraction of inorganic phosphorus produced by non-diatoms metabolism	0	None
FIntPDD	Fraction of dissolved phosphorus produced by diatoms metabolism	0	None
FIntPDG	Fraction of dissolved phosphorus produced by non-diatoms metabolism	0	None
FIntPLD	Fraction of labile phosphorus produced by diatoms metabolism	0	None
FIntPLG	Fraction of labile phosphorus produced by non-diatoms metabolism	0	None
FIntPRD	Fraction of refractory phosphorus produced by diatoms metabolism	0	None
FIntPRG	Fraction of refractory phosphorus produced by non-diatoms metabolism	0	None
FIntLuxNIP	Fraction of luxury inorganic nitrogen produced by predation	0	None
FIntLuxNDP	Fraction of luxury dissolved organic nitrogen produced by predation	0	None
FIntLuxNLP	Fraction of luxury labile nitrogen produced by predation	0	None
FIntLuxNRP	Fraction of luxury refractory nitrogen produced by predation	0	None
FIntStrNIP	Fraction of structural inorganic nitrogen produced by predation	0	None
FIntStrNDP	Fraction of structural dissolved organic nitrogen produced by predation	0	None
FIntStrNLP	Fraction of structural labile nitrogen produced by predation	0	None
FIntStrNRP	Fraction of structural refractory nitrogen produced by predation	0	None
FIntLuxPIP	Fraction of luxury inorganic phosphorus produced by predation	0	None
FIntLuxPDP	Fraction of luxury dissolved organic phosphorus produced by predation	0	None
FIntLuxPLP	Fraction of luxury labile phosphorus produced by predation	0	None
FIntLuxPRP	Fraction of luxury refractory phosphorus produced by predation	0	None

Key Name	Description	Default Value	Units
FIntStrPIP	Fraction of structural inorganic phosphorus produced by predation	0	None
FIntStrPDP	Fraction of structural dissolved organic phosphorus produced by predation	0	None
FIntStrPLP	Fraction of structural labile phosphorus produced by predation	0	None
FIntStrPRP	Fraction of structural refractory phosphorus produced by predation	0	None
KhIntND	Half-saturation concentration for nitrogen uptake in diatoms	2×10^{-5}	kg m^{-3}
KhIntNG	Half-saturation concentration for nitrogen uptake in non-diatoms	2×10^{-5}	kg m^{-3}
KhIntPD	Half-saturation concentration for phosphorus uptake in diatoms	2×10^{-5}	kg m^{-3}
KhIntPG	Half-saturation concentration for phosphorus uptake in non-diatoms	2×10^{-5}	kg m^{-3}
QMINND	Minimum nitrogen quota for diatoms	0.003	kg N kg^{-1} algal C
QMINPD	Minimum phosphorus quota for diatoms	0.003	kg P kg^{-1} algal C
QMINNG	Minimum nitrogen quota for non-diatoms	0.003	kg N kg^{-1} algal C
QMINPG	Minimum phosphorus quota for non-diatoms	0.003	kg P kg^{-1} algal C
QMAXND	Maximum nitrogen quota for diatoms	1.0	kg N kg^{-1} algal C
QMAXNG	Maximum nitrogen quota for non-diatoms	1.0	kg N kg^{-1} algal C
QMAXPD	Maximum phosphorus quota for diatoms	1.0	kg P kg^{-1} algal C
QMAXPG	Maximum phosphorus quota for non-diatoms	1.0	kg P kg^{-1} algal C

5.0 References

Arrhenius, S. 1889. On the Reaction Velocity of the Inversion of Cane Sugar by Acids. Zeitschrift fur Physikalische Chemie, 4:226-232.

Bartone, C.R. and C.L. Schelske. 1982. Lake-wide Seasonal Changes in Limnological Conditions in Lake Michigan in 1976. J. Great Lakes Res., 8(3):413-427.

Bowie, G.L., W.B. Mills, D.B. Porcella, C.L. Campbell, J.R. Pagenkopf, G.L. Rupp, K.M. Johnson, P.W.H. Chan, S.A. Gherini, and C.E. Chamberlin. 1985. Rates, Constants and Kinetic Formulations in Surface Water Quality Modeling. U.S. Environmental Protection Agency, Office of Research and Development, Environmental Research Laboratory, Athens, Georgia. EPA/600/3-85/040, 455 pp.

Brooks, A.S. and B.G. Torke. 1977. Vertical and Seasonal Distribution of Chlorophyll *a* in Lake Michigan. J. Fish. Res. Board Canada, 34(12):2280-2287.

Cerco, C.F. and T. Cole. 1993. Three-Dimensional Eutrophication Model of Chesapeake Bay. J. Environ. Engin., 119(6):1006-1025.

Cerco, C. and T. Cole. 1994. Three-Dimensional Eutrophication Model of Chesapeake Bay, Volume I: Main Report. U.S. Army Corps of Engineers, U.S. Army Engineer Waterways Experiment Station, Baltimore, Maryland. Technical Report EL-94-4, 658 pp.

Cerco, C. and T. Cole. 1995. User's Guide to the CE-QUAL-ICM Three-Dimensional Eutrophication Model. U.S. Army Corps of Engineers, U.S. Army Engineer Waterways Experiment Station, Vicksburg, Mississippi. Technical Report EL-95-15, 2,420 pp.

Cerco, C.F., Noel, M.R., Tillman, D.H., 2004. A practical application of the Droop nutrient kinetics. Water Res. 38, 4446–4454. https://doi.org/10.1016/j.watres.2004.08.027.

Di Toro, D.M., D.J. O'Connor, and R.V. Thomann. 1971. A Dynamic Model of the Phytoplankton Population in the Sacramento-San Joaquin Delta. In: R.F. Gould (Ed.), Non-Equilibrium Systems in Natural Water Chemistry, pp. 131-180. American Chemical Society, Washington, D.C.

Di Toro, D.M. and J.P. Connolly. 1980. Mathematical Models of Water Quality in Large Lakes, Part 2: Lake Erie. U.S. Environmental Protection Agency, Office of Research and Development, Environmental Research Laboratory-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. EPA/600/3-80/065, 97 pp.

Di Toro, D.M. and W.F. Matystik, Jr. 1980. Mathematical Models of Water Quality in Large Lakes, Part 1: Lake Huron and Saginaw Bay. U.S. Environmental Protection Agency, Office of Research and Development, Environmental Research Laboratory-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. EPA/600/3-80/056, 180 pp.

Droop, M., 1973. Some thoughts on nutrient limitation in algae. J. Phycol. 9, 264–272. https://doi.org/10.1111/j.1529-8817.1973.tb04092.x.

Fahnenstiel, G.L. and D. Scavia. 1987a. Dynamics of Lake Michigan Photoplankton: Primary Production and Growth. Canadian J. Fish. Aquat. Sci., 44(3):499-508.

Fahnenstiel, G.L. and D. Scavia. 1987b. Dynamics of Lake Michigan Photoplankton: Recent Changes in Surface and Deep Communities. Canadian J. Fish. Aquat. Sci., 44(3)509-514.

Kremer, J. and S. Nixon. 1974. A Coastal Marine Ecosystem: Simulation and Analysis. Springer Verlag, New York, New York. 217 pp.

Fennel, K., Hetland, R., Feng, Y., DiMarco, S., 2011. A coupled physical-biological model of the Northern Gulf of Mexico shelf: model description, validation and analysis of phytoplankton variability. Biogeosciences 8, 1881–1899. https://doi.org/10.5194/bg-8-1881-2011.

Kremer, J. and S. Nixon. 1974. A Coastal Marine Ecosystem: Simulation and Analysis. Springer Verlag, New York, New York. 217 pp.

Makarewicz, J.C., P. Bertram, and T.W. Lewis. 1998. Changes in Phytoplankton Size-Class Abundance and Species Composition Coinciding With Changes in Water Chemistry and Zooplankton Community Structure of Lake Michigan, 1983 to 1992. J. Great Lakes Res., 24(3):637-657.

Monod, J. 1949. The Growth of Bacterial Cultures. Ann. Rev. Microbiol., 3:371-394.

Odum, E. 1971. Fundamentals of Ecology, 3rd Edition. W.B. Saunders Company, Philadelphia, Pennsylvania. 574 pp.

Parker, S.P. 1993. McGraw-Hill Encyclopedia of Physics, 2nd Edition. McGraw-Hill Companies, New York, New York. 1,624 pp.

Rockwell, D.C., D.K. Salisbury, and B.W. Lesht. 1989. Water Quality in the Middle Great Lakes: Results of the 1985 U.S. EPA Survey of Lakes Erie, Huron and Michigan. U.S.

Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois. EPA/905/6-89/001, 272 pp.

Rodgers, P.W. and D. Salisbury. 1981a. Water Quality Modeling of Lake Michigan and Consideration of the Anomalous Ice Cover of 1976-1977. J. Great Lakes Res., 7(4):467-480.

Rodgers, P.W. and D. Salisbury. 1981b. Modeling of Water Quality in Lake Michigan and the Effects of Anomalous Ice Cover of 1976-1977. Great Lakes Basin Commission, Great Lakes Environmental Planning Study, Great Lakes Basin Commission, Ann Arbor, Michigan. Contribution Number 44, 53 pp.

Rousar, D.C. 1973. Seasonal and Spatial Changes in Primary Production and Nutrients in Lake Michigan. Water Air Soil Pollut., 2(4):497-514.

Scavia, D. and G.L. Fahnenstiel. 1987. Dynamics of Lake Michigan Phytoplankton Mechanisms Controlling Epilimnetic Communities. J. Great Lakes Res., 13(2):103-120.

Scavia, D., G.A. Lang, and J.F. Kitchell. 1988. Dynamics of Lake Michigan Plankton: A Model Evaluation of Nutrient Loading, Competition, and Predation. Canadian J. Fish. Aquat. Sci., 45(1):165-177.

Schelske, C.L. and E.F. Stoermer. 1971. Eutrophication, Silica Depletion, and Predicted Changes in Algal Quality in Lake Michigan. Science, 173(3995):423-424.

Schelske, C.L. and E.F. Stoermer. 1972. Phosphorus, Silica and Eutrophication in Lake Michigan. In: G.E. Likens (Ed.), Nutrients and Eutrophication, pp. 157-171. American Society of Limnology and Oceanography, Lawrence, Kansas.

Schelske, C.F., E.F. Stoermer, G.L. Fahnenstiel, and M. Haibach. 1986. Phosphorus Enrichment, Silica Utilization and Biogeochemical Silica Depletion in the Great Lakes. Canadian J. Fish. Aquat. Sci., 43(2):407-415.

Steele, J.H. 1962. Environmental Control of Photosynthesis in the Sea. Limnol. Oceanogr., 7(2):137-150.

Stoermer, E.F. 1993. Evaluating Diatom Succession: Some Peculiarities of the Great Lakes Case. J. Paleolimnol., 8(1):71-83.

Thomann, R.V. and D.M. Di Toro. 1975. Mathematical Modeling of Phytoplankton in Lake Ontario, Part 1 - Model Development and Verification. U.S. Environmental Protection Agency, Office of Research and Development, Environmental Research Laboratory-Corvallis, Large Lakes Research Station, Grosse Ile, Michigan. EPA/600/3-75/005, 178 pp.

Thomann, R.V. and J.A. Mueller. 1987. Principles of Water Quality Modeling and Control. Harper and Row Publishers, New York, New York. 644 pp.