

DHI Eutrophication Model 2

MIKE ECO Lab Template

Scientific Description



DHI headquarters

Agern Allé 5
DK-2970 Hørsholm
Denmark

+45 4516 9200 Telephone

+45 4516 9333 Support

+45 4516 9292 Telefax

mike@dhigroup.com

www.mikepoweredbydhi.com

CONTENTS

DHI Eutrophication Model 2
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1	Introduction.....	1
2	Applications	3
3	Mathematical Formulations	5
3.1	Phytoplankton	6
3.2	Phytoplankton Carbon (PC)	6
3.3	Phytoplankton Nitrogen (PN)	9
3.4	Phytoplankton Phosphorus (PP).....	10
3.5	Chlorophyll-a (CH)	11
3.6	Zooplankton (ZC)	12
3.7	Detritus	14
3.8	Detritus Carbon (DC)	14
3.9	Detritus Nitrogen (DN).....	15
3.10	Detritus Phosphorus (DP)	16
3.11	Inorganic Nitrogen (IN).....	17
3.12	Ammonia Nitrogen (NH).....	17
3.13	Inorganic Phosphorus (IP)	20
3.14	Oxygen (DO).....	22
3.15	Benthic Vegetation (BC).....	24
4	Data Requirements.....	27
5	List of References	29

1 Introduction

MIKE ECO Lab is a numerical lab for Ecological Modelling. It is a generic and open tool for customising aquatic ecosystem models to describe water quality and eutrophication amongst others. DHI's expertise and knowhow concerning ecological modelling has been collected in predefined ecosystem descriptions (MIKE ECO Lab templates) to be loaded and used in MIKE ECO Lab. So the MIKE ECO Lab templates describe physical, chemical and biological processes related to environmental problems and water pollution. The following is a description of the DHI Eutrophication Model 2.

The template is used in investigations of eutrophication effects and as an instrument in environmental impact assessments. The eutrophication modelling can be applied in environmental impact assessments considering:

- pollution sources such as domestic and industrial sewage and agricultural run-off
- cooling water outlets from power plants resulting in excess temperatures
- physical conditions such as sediment loads and change in bed topography affecting especially the benthic vegetation

The aim of using eutrophication modelling as an instrument in environmental impact assessment studies is to obtain, most efficiently in relation to economy and technology, the optimal solution with regards to ecology and the human environment.

The eutrophication model describes nutrient cycling, phytoplankton and zooplankton growth, growth and distribution of rooted vegetation and macroalgae in addition to simulating oxygen conditions.

The model results describe the concentrations of phytoplankton, chlorophyll-a, zooplankton, organic matter (detritus), organic and inorganic nutrients, oxygen and the area-based biomass of benthic vegetation over time. In addition, a number of derived variables are stored: primary production, total nitrogen and phosphorus concentrations, sediment oxygen demand and secchi disc depth.

The eutrophication module is integrated with the advection-dispersion module which describes the physical transport processes at each grid-point covering the area of interest. Other data required are concentrations at model boundaries, flow and concentrations from pollution sources, water temperature and irradiance etc.

2 Applications

The DHI Eutrophication Model 2 template can be applied in a range of environmental investigations:

- Studies where the effects of alternative nutrient loading scenarios are compared and/or different waste water treatment strategies are evaluated
- Studies of oxygen depletion
- Studies of the effects of the discharge of cooling water
- Comparisons of the environmental consequences of different construction concepts for harbours, bridges etc.
- Evaluation of the environmental consequences of developing new urban and industrial areas.

3 Mathematical Formulations

The Eutrophication 2 template consists of 13 state variables represented by 4 functional groups (phytoplankton, zooplankton, benthic vegetation and detritus), nutrients and oxygen.

13 state variables are used to describe the pelagic system. They are subject to both advection and dispersion and MIKE ECO Lab processes. State variables and functional groups that attach or by other means are fixed to the bottom, such as benthic vegetation, are not subject to transport by water movements or to dispersion.

List of state variables, abbreviations and their unit:

	State variables	Variable abbrev.	Unit
1	Phytoplankton carbon	PC	gC/m ³
2	Phytoplankton nitrogen	PN	gN/m ³
3	Phytoplankton phosphorus	PP	gP/m ³
4	Chlorophyll-a	CH	g/m ³
5	Zooplankton	ZC	gC/m ³
6	Detritus carbon	DC	gC/m ³
7	Detritus nitrogen	DN	gN/m ³
8	Detritus phosphorus	DP	gP/m ³
9	Ammonium	NH	gN/m ³
10	Nitrate	N3	gN/m ³
11	Inorganic phosphorus	IP	gP/m ³
12	Dissolved oxygen	DO	g/m ³
13	Benthic vegetation carbon	BC	gC/m ²

The processes and transfer of carbon, nitrogen, phosphorous and oxygen in the Eutrophication 2 template is illustrated in Figure 3.1.

The processes describing the variations of the state variables in time and space are dependent on external factors such as the salinity, water temperature, the irradiance, and discharges of nutrients and organic matter.

The mathematical formulations of the biological and chemical processes and transformations for each state variable are described one by one below. The differential equations are 1st order, ordinary and coupled.

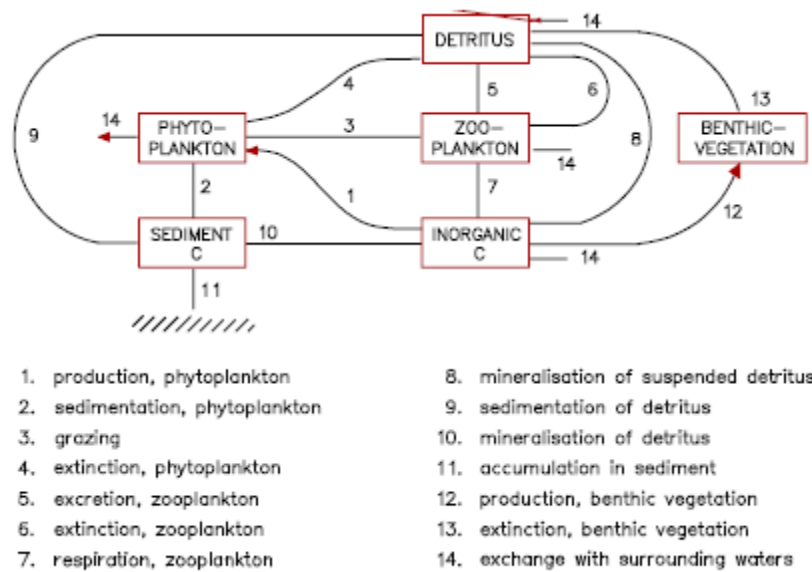


Figure 3.1 Simplified flow diagram of the fluxes of carbon, nitrogen and phosphorus in the eutrophication model

3.1 Phytoplankton

Phytoplankton is represented by one functional group and three state variables: phytoplankton carbon (PC), phytoplankton nitrogen (PN) and phytoplankton phosphorus (PP). The internal pools of phytoplankton nutrients in this model are state variables, because their uptake dynamics are decoupled from the phytoplankton carbon assimilation dynamics, resulting in time-varying PN/PC and PP/PC ratios. However, the nutrient pools being internal to the carbon-based phytoplankton, their source and sink terms are proportional to the corresponding phytoplankton carbon rates.

3.2 Phytoplankton Carbon (PC)

Sources and sinks of phytoplankton carbon include production, respiration, zooplankton grazing, sedimentation and death. These are expressed as:

$$\frac{dPC}{dt} = \text{production} - \text{respiration} - \text{grazing} - \text{sedimentation} - \text{death} \tag{3.1}$$

$$= prpc - repc - grpc - sepc^* - depc$$

* **NOTE:** 'sepc' defined as a special "settling" process taken into account the input from the above layer (n>1) in multilayered systems.

Production (prpc)

The production of phytoplankton depends on the intensity of light, by the availability of nutrients and by the ambient temperature. The gross production is computed with a multiplicative approach considering the maximal rate of production (μ), the influence of light ($F(I)$), temperature ($F_1(T)$) and the internal concentrations of nitrogen and phosphorus $F_1(N,P)$):

$$prpc = \mu \cdot flig(I) \cdot ftem(T) \cdot fnut(N,P) \cdot PC \quad (3.2)$$

Light function

The gross production-irradiance parameterisation is written according to Jassby & Platt (1976) relation between photosynthesis and light without considering light-inhibition:

$$flig(I) = \left[1 - \exp\left(-\frac{\alpha \cdot ipar}{\mu PC}\right) \right] \quad (3.3)$$

Where

α = initial slope in production-irradiance curve [gC/gC/(μ E/m²/s)]

$ipar$ = average available photosynthetic radiation in each vertical layer [μ E/m²/s]

μPC = max gross growth rate of phytoplankton carbon

The production is temporal resolved on a scale of hours to allow for simulating diurnal variation in oxygen concentration. To that end hourly resolved inputs of irradiance at the surface is required. Actual intensity of photosynthetic available radiation within each layer is calculated from surface irradiance and extinction of light due to absorbance by chlorophyll, detritus and water in layers above and within the particular layer using built-in functions in MIKE ECO Lab.

$$ipar = \frac{-io(e^{-eta \cdot dz} - 1)}{eta \cdot dz} \quad (3.4)$$

Where

io = surface irradiance or irradiance at surface of any layer

eta = $pla \cdot CH + dla \cdot DC + bla$

where

pla = chlorophyll a specific absorption constant (mg chla)⁻¹ m⁻¹

dla = detritus specific absorption constant (mg chla)⁻¹ m⁻¹

bla = background extinction (m⁻¹)

Temperature function

The influence of temperature on phytoplankton production is parameterised by an Arrhenius function:

$$ftem(T) = \theta_g^{(T-20)} \quad (3.5)$$

Where
 Θ_g = temperature coefficient for growth

Temperature for phytoplankton plays a major role as a covariate with other factors. Phytoplankton at low temperatures maintain higher concentrations of photosynthetic pigments, enzymes and carbon (Steemann, Nielsen & Jørgensen, 1968), enabling more efficient use of light. There are strong interactions between temperature and μ_{Max} at any light intensity, with day length and production, and with nutrient uptake. In general, all rates increase with increasing temperatures and the irradiance level where maximum photosynthesis is reached is shifted to higher values with increasing temperatures.

Nutrient dependence function

Since phytoplankton growth depends essentially on the size of the internal nutrient pools, the nutrient-dependent growth limitation $F_1(N,P)$ is calculated from the relative saturation of the internal N and P pools. Droop (1973, 1975) provides a theoretical basis for this approach which also has been incorporated in a theoretical model by Nyholm (1977) and in North Sea models by Mommaerts (1978), Tett et al. (1986) and Lancelot & Rousseau (1987).

$$f_{nut} = \frac{2}{\frac{1}{m_{yn}} + \frac{1}{m_{yp}}} \quad (3.6)$$

Where

$$m_{yn} = \frac{PN/PC - pn_{mi}}{pn_{ma} - pn_{mi}} \quad (3.7)$$

$$m_{yp} = \frac{(PP/PC - pp_{mi}) \cdot (kc + pp_{ma} - pp_{mi})}{(pp_{ma} - pp_{mi}) \cdot (kc + PP/PC - pp_{mi})} \quad (3.8)$$

pn_{mi} , pn_{ma} = minimum and maximum internal nitrogen content in algae (gN/gC), respectively

pp_{mi} , pp_{ma} = minimum and maximum phosphorus content in algae (gP/gC), respectively

kc = half saturation constant for phosphorus in phytoplankton (gP/gC)

Respiration of phytoplankton ($repc$)

Loss due to respiration is represented by basal metabolic expenditure to maintain life processes and is considered a constant fraction of biomass that depends on temperature:

$$repc = f_{tem}(T) \cdot r_{phc} \cdot PC \quad (3.9)$$

Where
 f_{tem} = Temperature Arrhenius function
 r_{phc} = constant fraction of biomass (d^{-1})

Grazing of phytoplankton (grpc)

Loss of phytoplankton due to grazing by zooplankton depends on zooplankton carbon and is regulated by zooplankton grazing function modified by a temperature function. The grazing loss is described in detail in the section on zooplankton.

Sedimentation of phytoplankton (sepc)

Nutrient-replete phytoplankton is able to adjust its buoyancy and hence, to minimise sinking rate. Under conditions of nutrient-stress, with the internal nutrient pools at lower levels, sinking rates increase (Smayda, 1970, 1971). At very high concentrations of PC coagulation rate between cells increases (Jackson 1988) resulting in higher sedimentation rates.

The sedimentation rate of PC is described by a 1st order equation depending on internal nutrient status and a 2nd order equation representing coagulation:

$$sepc = \frac{1}{2} k_{sp} \cdot PC \cdot \left(\frac{pnma}{\frac{PN}{PC}} + \frac{ppma}{\frac{PP}{PC}} \right) + k_{sp2} \cdot PC^2 \quad (3.10)$$

Where

k_{sp} = sedimentation rate parameter (d⁻¹)
 k_{sp2} = sedimentation rate constant ((mg/l)⁻¹ d⁻¹)

Death of phytoplankton (depc)

Natural mortality of phytoplankton, or autolysis, has been shown to be a significant phenomenon in the marine ecosystem (Jassby & Goldman, 1974) and this decay of blooms is partly mineralised in the water column (Lancelot et al., 1987). In this model, the mortality of phytoplankton is described by a 1st order equation modified by temperature:

$$depc = deac \cdot F_1(T) \cdot PC \quad (3.11)$$

Where

$deac$ = death rate at 20 °C (d⁻¹)

3.3 Phytoplankton Nitrogen (PN)

The mass balance for phytoplankton nitrogen is analogous to the mass balance of phytoplankton carbon:

$$\begin{aligned} \frac{dPN}{dt} &= uptake - respiration - grazing - sedimentation - death \\ &= upnh + upn3 - repn - grpn - sepn^* - depn \end{aligned} \quad (3.12)$$

* **NOTE:** 'sepn' defined as a special "settling" process taken into account the input from the above layer ($n>1$) in multilayered systems.

Uptake

The nitrogen uptake by phytoplankton is described in detail in section about the inorganic nitrogen.

Grazing (grpn)

Grazing loss of phytoplankton nitrogen is proportional to the grazing loss of phytoplankton multiplied by the ratio of nitrogen to carbon in phytoplankton:

$$grpn = grpc \cdot (PN/PC) \quad (3.13)$$

Sedimentation (sepn)

Loss of phytoplankton nitrogen due to sedimentation is proportional to the sedimentation of phytoplankton carbon multiplied by the ratio of nitrogen to carbon in phytoplankton:

$$sepn = sepc \cdot (PN/PC) \quad (3.14)$$

Death (depn)

Loss of phytoplankton nitrogen due to phytoplankton mortality is proportional to the loss of phytoplankton carbon due to death multiplied by the ratio of nitrogen to carbon in phytoplankton:

$$depn = depc \cdot (PN/PC) \quad (3.15)$$

3.4 Phytoplankton Phosphorus (PP)

The mass balance for phytoplankton phosphorus is analogous to the mass balance of phytoplankton carbon:

$$\begin{aligned} \frac{dPP}{dt} &= uptake - respiration - grazing - sedimentation - death \\ &= uppp - repp - grpp - sepp^* - depp \end{aligned} \quad (3.16)$$

* **NOTE:** 'sepp' defined as a special "settling" process taken into account the input from the above layer ($n>1$) in multilayered systems.

Uptake (uppp)

The phosphorus uptake by phytoplankton is described in detail in section covering the inorganic phosphorus.

Grazing (grpp)

Grazing loss of phytoplankton phosphorus is proportional to the grazing loss of phytoplankton multiplied by the ratio of phosphorus to carbon in phytoplankton:

$$grpp = grpc \cdot (PP/PC) \quad (3.17)$$

Sedimentation (sepp)

Loss of phytoplankton phosphorus due to sedimentation is proportional to the sedimentation of phytoplankton carbon multiplied by the ratio of phosphorus to carbon in phytoplankton:

$$sepp = sepc \cdot (PP/PC) \quad (3.18)$$

Death

Loss of phytoplankton phosphorus due to phytoplankton mortality is proportional to the loss of phytoplankton carbon due to death multiplied by the ratio of phosphorus to carbon in phytoplankton:

$$depp = depc \cdot (PP/PC) \quad (3.19)$$

3.5 Chlorophyll-a (CH)

The mass balance for chlorophyll-a reads:

$$\begin{aligned} \frac{dCH}{dt} &= \text{production} - \text{death} - \text{sedimentation} \\ &= prch - dech - sech^* \end{aligned} \quad (3.20)$$

* **NOTE:** 'sech' defined as a special "settling" process taken into account the input from the above layer ($n > 1$) in multilayered systems.

Production (prch)

$$prch = (CH_{min} / IK) \cdot \exp(F_3(N)) \cdot prpc \quad (3.21)$$

Where

CH_{min} = coefficient determining the minimum chlorophyll-a production ($\mu E/m^2/s$)⁻¹
 $F_3(N)$ = $CH_{max} \cdot \{(PN/PC - PN_{min}) / (PN_{max} - PN_{min})\}$
 CH_{max} = coefficient determining the maximum chlorophyll-a production (dimensionless) in the absence of nutrient limitation.

Sedimentation (sech)

$$sech = sepc \cdot (CH / PC) \quad (3.22)$$

Death (dech)

$$dech = (depc + grpc) \cdot (CH/PC) \quad (3.23)$$

3.6 Zooplankton (ZC)

The zooplankton state variable is a lumped group representing important grazers such as copepods and various microzooplankters. The mass balance for zooplankton reads:

$$\begin{aligned} \frac{dZC}{dt} &= production - respiration - death \\ &= przc - rezc - dezc \end{aligned} \quad (3.24)$$

Grazing (grpc)

The grazing rate of phytoplankton carbon (grpc) by zooplankton is represented by a saturation equation relating food concentration to grazing rate, a threshold food concentration below which no grazing takes place (Kjørboe et al. 1985, Kjørboe & Nielsen 1994), a temperature function and a function of dissolved oxygen suppression grazing at low DO (Roman et al. 1993):

$$grpc = kgrb \cdot F_2(T) \cdot \frac{PC - thpc}{(PC - thpc + mgprc)} \cdot F(DO) \cdot ZC \quad (3.25)$$

Where

$kgrb$	= maximum grazing rate constant at 20°C (d ⁻¹)
hpc	= threshold food concentration (mg C/l)
$mgprc$	= half saturation concentration of PC for carbon uptake in zooplankton (mg C/l)

Temperature function

The influence of temperature on zooplankton grazing is parameterised by an Arrhenius function:

$$F_2(T) = tetz^{(T-20)} \quad (3.26)$$

Where

$Tetz$	= temperature coefficient for grazing rate
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Oxygen dependence function:

$$F(DO) = \frac{DO^{ndo}}{DO^{ndo} + mdo} \quad (3.27)$$

Where

mdo = oxygen concentration indicating depressed grazing rates due to oxygen depletion
ndo = exponent

Production (przc)

The production of zooplankton is overall coupled to the grazing rate on phytoplankton, but growth rate modified by the internal elementary ratios in food PN/PC, PP/PC.

$$przc = vefo \cdot grpc \quad (3.28)$$

Where

vefo = fraction of PC that is assimilated.

At optimal ratios and above of nitrogen to carbon (*znc*) and phosphorus to carbon (*zpc*) in grazed material (i.e. phytoplankton) *vefo* approaches the maximal assimilation fraction (*vefok*). At less than optimal ratios *vefo* is depressed according to:

$$vefo = vefok \frac{2}{\left(\frac{znc}{PN/PC} + \frac{zpc}{PP/PC} \right)} \quad (3.29)$$

In the individual zooplankter grazing rate is unaffected by nutrient status, however the population growth (i.e. numeric response) is depressed by nutrient status.

It follows that a variable fraction of grazed phytoplankton is not assimilated. The unassimilated carbon, nitrogen and phosphorus are entered into the various pools of detritus (see below).

Respiration (rezc)

Respiration of zooplankton carbon is represented by basal metabolism (*bmzc*) that depends on temperature and specific dynamic action (*sda*) that directly scales to assimilation rate (*refo***grpc*):

$$rezc = sda + bmzc = refo \cdot grpc + kgrz \cdot ZC \cdot F_2(T) \quad (3.30)$$

Where

kgrz = proportionality constant for to basal metabolism
refo = proportionality constant for specific dynamic action

Death (dezc)

Zooplankton mortality has a density-independent term representing the longevity of an average zooplankter (Horwood, 1974). The density-dependent quadratic term can be regarded as a surrogate for predation and acts as a closure term, because zooplankton is the highest trophic level explicitly modelled (Steele 1976).

The zooplankton death rate is proportional to the zooplankton concentration, but at high densities the dependence is of second order (predation term) resulting in:

$$dezc = K_{d1} \cdot ZC + K_{d2} \cdot ZC^2 \quad (3.31)$$

Where

K_{d1} = rate constant (d^{-1}) especially important at concentrations below $1 \text{ g} \cdot \text{m}^{-3}$
 K_{d2} = rate constant important at high concentrations $\{d^{-1} \cdot (\text{g}/\text{m}^3)^{-1}\}$

3.7 Detritus

Detritus is defined in the model as particles of dead organic material in the water. The detritus pool receives the dead primary producers, dead zooplankton grazers and unassimilated material left over after grazing. Sedimentation and mineralisation are the only processes draining the detritus pools.

There are three state variables characterising detritus: detritus carbon, nitrogen and phosphorus.

3.8 Detritus Carbon (DC)

The mass balance for detritus carbon reads:

$$\begin{aligned} \frac{dDC}{dt} &= \text{generation} - \text{sedimentation} - \text{mineralization} \\ &= (1 - v_m) \cdot depc + ekzc + debc/h \\ &\quad - sedc^* - redc + dezc \end{aligned} \quad (3.32)$$

* **NOTE:** 'sedc' defined as a special "settling" process taken into account the input from the above layer ($n > 1$) in multilayered systems.

Generation

The detritus generation is the sum of input from dead phytoplankton carbon (depc), dead zooplankton (dezc), non-assimilated material leftover from grazing (ekzc) and death of benthic vegetation (debc).

Here

V_m = fraction of dead phytoplankton, undergoing immediate mineralisation.

Sedimentation (sedc)

The sedimentation of detritus is modelled similarly to the sedimentation of phytoplankton.

$$sedc = U_d / h \cdot DC \quad (3.33)$$

Where

h = DZ

U_d = sedimentation rate parameter (velocity) for detritus (m/d)

Mineralisation (redc)

Bacterioplankton has been included implicitly in the model by giving the detritus a variable mineralisation rate, which is dependent on temperature and oxygen saturation. Thus, detritus causes both oxygen consumption and inorganic nutrient regeneration in the water column and in the benthic system. This implicit approach has the obvious advantage of saving one state variable, but the disadvantage of having to ignore dissolved organic carbon (DOC) as a potential substrate for bacterioplankton.

However, since the largest single source of DOC in aerobic situations is exudates from primary producers with in situ rates of around 10% of net phytoplankton production (Williams, 1975, Smith et al., 1977) this omission is felt to be justifiable.

Nutrient regeneration from the benthic system by mineralisation processes is not dependent on the benthic detritus pool but on the sedimentation rate of pelagic detritus. Proportionality factors define the permanent loss of nutrients (adsorption, complexation, burial, denitrification) from the system.

$$redc = \mu_m \cdot F_3(T) \cdot F_1(DO) \cdot DC \quad (3.34)$$

Where

μ_m = maximum mineralisation rate at 20°C (d⁻¹)

$F_3(T)$ = $\Theta_D^{(T-20)}$

Θ_D = temperature coefficient for mineralisation of detritus

$F_1(DO)$ = $DO^2 / (DO^2 + MDO)$

3.9 Detritus Nitrogen (DN)

The main balance for detritus nitrogen reads:

$$\frac{dDN}{dt} = \text{generation} - \text{sedimentation} - \text{mineralization} \quad (3.35)$$

$$= (1 - vm) \cdot depn + ekzn + dezn + debn - sedn^* - redn$$

* **NOTE:** 'sedn' defined as a special "settling" process taken into account the input from the above layer (n>1) in multilayered systems.

The rates are similar to the ones for detritus carbon.

Generation

Detritus nitrogen is the result of input from dead phytoplankton and death of zooplankton nitrogen and unassimilated nitrogen from grazing. The excretion and death of zooplankton nitrogen are calculated from:

$$ekzn = vzn \cdot ekzc \quad (3.36)$$

$$dezn = vzn \cdot dezc$$

Where

Vzn = nitrogen content of zooplankton assumed to be constant (gN/gC)

The rate for sloughing of benthic nitrogen is calculated from:

$$debn = pnb \cdot (debc/h) \quad (3.37)$$

Where

Pnb = the nitrogen-carbon ratio in benthic vegetation assumed to be constant (gN/gC)

Sedimentation

$$sedn = sedc \cdot DN/DC \quad (3.38)$$

Mineralisation

$$redn = redc \cdot DN/DC \quad (3.39)$$

3.10 Detritus Phosphorus (DP)

The mass balance for detritus phosphorus reads:

$$\frac{dDP}{dt} = \text{generation} - \text{sedimentation} - \text{mineralization} \quad (3.40)$$

$$= (1 - vm) \cdot depp + ekzp + dezp + debp - sedp^* - redp$$

* **NOTE:** 'sedp' defined as a special "settling" process taken into account the input from the above layer ($n > 1$) in multilayered systems.

The rates for phosphorus are similar to the detritus carbon rates.

Generation

This is the sum of phosphorus from dead phytoplankton, death of zooplankton phosphorus, unassimilated phosphorus from grazing and sloughing of benthic vegetation phosphorus.

The excretion and death of zooplankton phosphorus and the sloughing of benthic phosphorus are expressed as:

$$\begin{aligned}
 ekzp &= vzp \cdot ekzc \\
 dezp &= vzp \cdot dezc \\
 debp &= ppb \cdot (debc / h)
 \end{aligned}
 \tag{3.41}$$

Where

vzp = the constant phosphorus content of zooplankton (gP/gC)
 ppb = the constant phosphorus content of benthic vegetation (gP/gC)

3.11 Inorganic Nitrogen (IN)

The inorganic nitrogen is represented by two state variables, namely oxidised forms (sum of nitrate and nitrite) and reduced forms (sum of ammonia and urea).

3.12 Ammonia Nitrogen (NH)

The primary source of ammonia is input from respiration and mineralisation processes and the sinks include uptake by primary producers: phytoplankton ($upnh$) and benthic vegetation ($ubnh$) and nitrification ($rnit$) from nitrate.

$$\begin{aligned}
 \frac{dNH}{dt} &= \text{input from mineralization} - \text{uptake} - \text{nitrification} \\
 &= repn + rebn + redn + rezn + rsnh * \\
 &+ vm \cdot depn - upnh - ubnh - rnit
 \end{aligned}
 \tag{3.42}$$

* **NOTE:** For multilayered model systems only relevant for the bottom layer.

Input from mineralisation

The mineralisation rates of detritus and zooplankton are described above. The mineralisation of sediment nitrogen, which is only relevant for the bottom layer, is described by:

$$resn = k_{SN} \cdot F_5(T) \cdot F_2(DO) \cdot (SEDN + SEPN) \tag{3.43}$$

Where

k_{SN} = proportionality factor at 20°C
 $F_5(T)$ = $\Theta_M^{(T-20)}$
 $F_2(DO)$ = $DO / (DO + MDO)$

Θ_M = temperature coefficient for mineralisation of sediment

The mineralization is expressed as a fraction of the sedimentation of organic matter.

Under anoxic conditions, the release of nutrients is not only a result of recently sedimented material, but also a zero order function where large amounts of nutrient buried in the sediment will be released. This is described by a constant release rate per areal unit:

$$As \ DO < \ MDO \tag{3.44}$$

$$resn = N_{REL} / h$$

Where

N_{REL} = release rate under anoxic conditions (g/m²/d)

Uptake

The "uptake" includes uptake by phytoplankton and by benthic vegetation.

Uptake by phytoplankton

The model for phytoplankton includes modelling of nutrient limited growth determined by intracellular concentrations. If the internal concentration is saturated (pnma) no uptake takes place. At internal N concentrations below pnma the uptake are dependent on ambient concentration of inorganic nitrogen using a Michaelis-Menten equation. Two sources of inorganic nitrogen are considered represented by the oxidised form N₃ (NO₂⁻, NO₃⁻), and the reduced form NH (NH₄⁺, urea). The uptake of either nitrogen form follows standard Michaelis-Menten kinetics with provision for light-dependency of un3 uptake and interaction between N₃ and NH (Flynn & Fasham, 2003). Besides, the ability of phytoplankton to assimilate and reduce N₃ in darkness is regulated by the internal ratio PN:PC.

Uptake of N₃ is described by:

$$upn3 = \begin{cases} 0 & \text{if } \left(pnma - \frac{PN}{PC} \right) \leq epsi \\ un3 & \text{if } \left(pnma - \frac{PN}{PC} \right) > epsi \end{cases} \tag{3.45}$$

$$un3 = PC \cdot \begin{cases} \max up \cdot \frac{N3}{N3 + hupn3} & \text{if } ipar \geq 5 \\ fn3 \cdot \max up \cdot \frac{N3}{N3 + hupn3} & \text{if } ipar < 5 \end{cases} \quad (3.46)$$

Where

- PC* = Concentration of phytoplankton C (mgC l⁻¹)
- PN* = Concentration of phytoplankton N (mgN l⁻¹)
- maxup* = maximal uptake rate of N3 (and NH) (mg l⁻¹)⁻¹ d⁻¹
- hupn3* = half-saturation constant for un3 (mg N3 l⁻¹)
- ipar* = ambient photon flux at depth (μE m⁻² s⁻¹)
- fn3* = function to describe un3 dependence on internal ratio PN:PC during darkness

The dependence of internal PN:PC ratio on the uptake rate of un3 during darkness is described by a sigmoidal function fn3:

$$fn3 = kuptn3 \cdot \frac{\left(1 - \frac{N:C}{pnma}\right)^4}{\left(1 - \frac{N:C}{pnma}\right)^4 + cres2} \quad (3.47)$$

Where

- kuptn3* = is a scalar that regulates the maximum dark:light ratio of un3
- pnma* = ratio of PN:PC in phytoplankton under saturating conditions
- cres2* = constant that affects the shape of sigmoid function

The uptake rate of reduced inorganic nitrogen NH₄ is described by:

$$upnh = \begin{cases} 0 & \text{if } \left(pnma - \frac{PN}{PC}\right) \leq epsi \\ unh & \text{if } \left(pnma - \frac{PN}{PC}\right) > epsi \end{cases} \quad (3.48)$$

Where

$$unh = PC \cdot \max up \cdot \frac{NH}{NH + hupnh} \quad (3.49)$$

- maxup* = maximal uptake rate of NH (mg l⁻¹)⁻¹ d⁻¹
- hupnh* = half-saturation constant for uh (mg NH l⁻¹)

Uptake by benthic vegetation ($unbn$)

The model for the benthic vegetation does not include a nutrient limited growth as a function of intracellular concentration but a slightly more simple approach in which the extracellular nutrient concentration may be growth limiting. The nutrient uptake is then proportional to the net production.

$$unbn = pnb \cdot (prbc/h) \quad (3.50)$$

Where

pnb = nitrogen to carbon ratio (gN/gC)

$prbc$ = production of benthic carbon (see later for the benthic vegetation mass balance)

The growth limitation function is described together with the production of benthic vegetation below.

3.13 Inorganic Phosphorus (IP)

The main balance for inorganic phosphorus (e.g. phosphate) reads:

$$\frac{dIP}{dt} = \text{input from mineralization} - \text{uptake} \quad (3.51)$$

$$= redp + rezp + resp^* + vm \cdot depp - uppp - upbp$$

* **NOTE:** For multilayered system 'resp' is only active in the bottom layer.

Input from mineralisation

The input from mineralisation is the sum of mineralisation of detritus, zooplankton and phytoplankton phosphorus and the release from the sediment.

Release from the sediment, which is only relevant for the bottom layer, is expressed as:

$$resp = K_{SP} \cdot F_5(T) \cdot F_2(DO) \cdot (sedp + sepp) \quad (3.52)$$

Where

K_{SP} = proportionality factor at 20°C

The remainder of the terms in this equation has been explained above.

Under anoxic conditions ($DO < MDO$) a constant release rate is modelled:

$$resp = P_{REL}/h \quad (3.53)$$

Where

P_{REL} = constant release rate (g/m²/d)

Uptake

Uptake by phytoplankton.

Under non-limiting conditions:

$$u_{ppp} = \min \left[\begin{array}{l} V_{kp} \cdot \frac{IP}{IP + KPP} \cdot PC \\ prpc \cdot PP_{\max} \end{array} \right] \quad (3.54)$$

and under limiting conditions:

$$u_{ppp} = \min \left[\begin{array}{l} \max \left[\begin{array}{l} V_{kp} \cdot \frac{IP}{IP + KPP} \cdot PC \\ Mineralization + external\ supply \end{array} \right] \\ prpc \cdot PP_{\max} \end{array} \right] \quad (3.55)$$

Where

V_{kp} = uptake rate for phosphorus ($d^{-1} \cdot (mg\ P/l)^{-1}$)
 KPP = halfsaturation concentration for P uptake ($mg\ P/l$)

The uptake by benthic vegetation:

$$u_{pbp} = ppb \cdot (prbc/h) \quad (3.56)$$

Where

Ppb = the phosphorus to carbon content (gP/gC)
 $prbc$ = production of benthic vegetation explained later

3.14 Oxygen (DO)

The oxygen balance includes the production of oxygen by the primary producers, the consumption oxygen due to mineralisation and respiration and exchange of oxygen between water and air, i.e. reaeration. The mass balance then reads:

$$\begin{aligned} \frac{dDO}{dt} &= \text{production} - \text{consumption} + \text{reaeration} \\ &= odpc + odbc - orpc - odzc - oddc - odsc \\ &\quad - orbc - opcd + rear - orni \end{aligned} \tag{3.57}$$

Production

Oxygen is produced during the phototrophic production by phytoplankton and benthic vegetation. Depending on the oxidation state of inorganic nitrogen that are assimilated (i.e. N_3 = oxidised; NH = reduced) the stoichiometric ratio $C:O_2$ varies between 106:138 (N_3) to 106:106 (NH). In mass terms the ratio thus can vary between 3.47 and 2.67 g O_2 produced per g C produced. The contribution of oxidised nitrogen forms in supporting primary production varies across different types of surface waters and seasons, but overall it depends on the availability of the two nitrogen forms. As a default the model assumes an equal contribution from N_3 and NH , and a stoichiometric ratio between $O_2:C$ (g/g) of 3.07.

$$odpc = Vo \cdot prpc \tag{3.58}$$

$$odbc = Vo \cdot (prbc/h)$$

Where

Vo = oxygen to carbon ratio at production (g O_2 /gC)

Consumption

The oxygen consumption is due to mineralisation of organic matter in water and sediment, to oxidise ammonia (nitrification), to respiration of zooplankton and phytoplankton, and to mineralisation of the part of the phytoplankton, which is mineralised immediately without entering the detritus pool.

$$oddc = Vo \cdot redc \tag{3.59}$$

$$odzc = Vo \cdot rezc$$

Respiration of phytoplankton:

$$orpc = Vo \cdot repc \tag{3.60}$$

Respiration of macroalgae:

$$orbc = Vo \cdot rebc \quad (3.61)$$

Mineralisation of dead phytoplankton:

$$opcd = Vo \cdot vm \cdot depc \quad (3.62)$$

The oxygen demand by the nitrification process uses a stoichiometric ratio between O₂/N (g/g) of 4.3.

$$orni = vhn \cdot rnit \quad (3.63)$$

Where

Vhn = g O₂ used to oxidise 1 g NH₄ to 1 g NO₃ (stoichiometry)

The sediment oxygen demand is related to the carbon mineralisation in the sediment which again is related to the sedimentation of organic matter (detritus and phytoplankton).

$$resc = K_{MSC} \cdot F_5(T) \cdot F_2(DO) \cdot (sepc + sedc) \quad (3.64)$$

Where

K_{MSC} = proportionality factor at 20°C and oxidised condition

$F_5(T)$ = $\Theta_M^{(T-20)}$
 Θ_M = temperature coefficient for mineralisation
 $F_2(DO)$ = $DO/(DO+MDO)$

The oxygen consumption is then found from:

$$odsc = Vo \cdot resc \quad (3.65)$$

Reaeration

The reaeration is calculated from the oxygen saturation concentration and the reaeration rate:

$$rear = K2 / dz \cdot (csair - DO) \quad (3.66)$$

Where

$K2$ = reaeration rate (d⁻¹)

$csair$ = oxygen saturation concentration (g/m³)

$$= 14.652 - 0.0841 \cdot S + T \cdot \{0.00256 \cdot S - 0.41022 + T \cdot (0.007991 - 0.0000374 \cdot S - 0.000077774 \cdot T)\}$$

T = water temperature (°C)

S = Salinity (o/oo)

The reaeration rate is calculated from horizontal current velocity and wind speed (at 10 m) using a combination of empirical models developed by ():

$$K2 = 3.93 \cdot \frac{\sqrt{vsp}}{dz^{1.5}} + (2.07 + 0.215 \cdot w_{sp}^{1.7}) \cdot \frac{24}{100} \quad (3.67)$$

Where
 V_{sp} = horizontal current velocity
 dz = depth of layer
 w_{sp} = wind speed at 10 m above water surface

3.15 Benthic Vegetation (BC)

The benthic vegetation is assumed to be rooted and/or attached to stones, etc. Fixed nitrogen to carbon and phosphorus to carbon ratios are assumed. The mass balance for the benthic vegetation is:

$$\frac{dBC}{dt} = \text{production} - \text{loss} = prbc - debc \quad (3.68)$$

Production (PRBC)

$$prbc = \mu_B \cdot F_6(T) \cdot F_3(I) \cdot F_4(N,P) \cdot RD \cdot BC \quad (3.69)$$

Where
 μ_B = net specific growth rate at 20°C
 RD = relative day length
 $F_6(T)$ = $\Theta_B^{(T-20)}$
 Θ_B = temperature coefficient for benthic vegetation growth
 $F_2(I)$ = $\begin{cases} I_B / I_{KB}, I_B < I_{KB} \\ 1, I_B \geq I_{KB} \end{cases}$
 I_B = light intensity at bottom (E/m²/d)
 I_{KB} = light saturation intensity for the benthic vegetation (E/m²/d)
 $F_4(N,P)$ = $\frac{2}{\left(\frac{1}{F_2(N)} + \frac{1}{F_2(P)}\right)}$
 $F_2(N)$ = $\frac{IN}{IN + KBN}$
 KBN = Half saturation constant for the nitrogen limitation function (g/m³)
 $F_2(P)$ = $\frac{IP}{IP + KBP}$
 KBP = half saturation constant for the phosphorus limitation function (g/m³)

Loss/sloughing (SLBC)

$$debc = \mu_s \cdot F_7(T) \cdot (BC - babc) \quad (3.70)$$

Where

μ_s

= sloughing or loss rate at 20°C (d⁻¹)

$F_7(T)$

= $\Theta_s^{(T-20)}$

Θ_s

= temperature coefficient for loss

$Babc$

= minimum area based biomass of benthic vegetation (g/m²)

4 Data Requirements

- Basic Model Parameters
 - Model grid size and extent
 - Time step and length of simulation
 - Type of output required and its frequency
- Bathymetry and Hydrodynamic Input
- Combined Advection-Dispersion Model
 - Dispersion coefficients
- Initial Conditions
 - Concentration of parameters
- Boundary Conditions
 - Concentration of parameters
 - Pollution Sources
 - Discharge magnitudes and concentration of parameters
- Process Rates
 - Size of coefficients governing the process rates. Some of these coefficients can be determined by calibration. Others will be based on literature values or found from actual measurements and laboratory tests.

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