MOHID Course
Water Modelling System

Water Quality Manual

Lisbon, September de 2006

Version 1.0

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1 Integration Philosophy

MOHID Water Modelling System (http://www.mohid.com), a modelling platform developed at Instituto Superior Técnico (IST), Lisbon, was designed to simulate surface water bodies (MOHID Water), porous media flow and infiltration (MOHID Soil) and watersheds (MOHID Land). It is a modular finite volumes water modelling system written in ANSI FORTRAN 95, using an object oriented programming philosophy (Braunschweig, 2004). This integrated modelling tool is able to simulate physical and biogeochemical processes in the water column and in the sediments, and the coupling between these two domains and atmospheric processes. Figure 1 represents schematically the different modules included in MOHID Water distributed along the different environmental compartments.

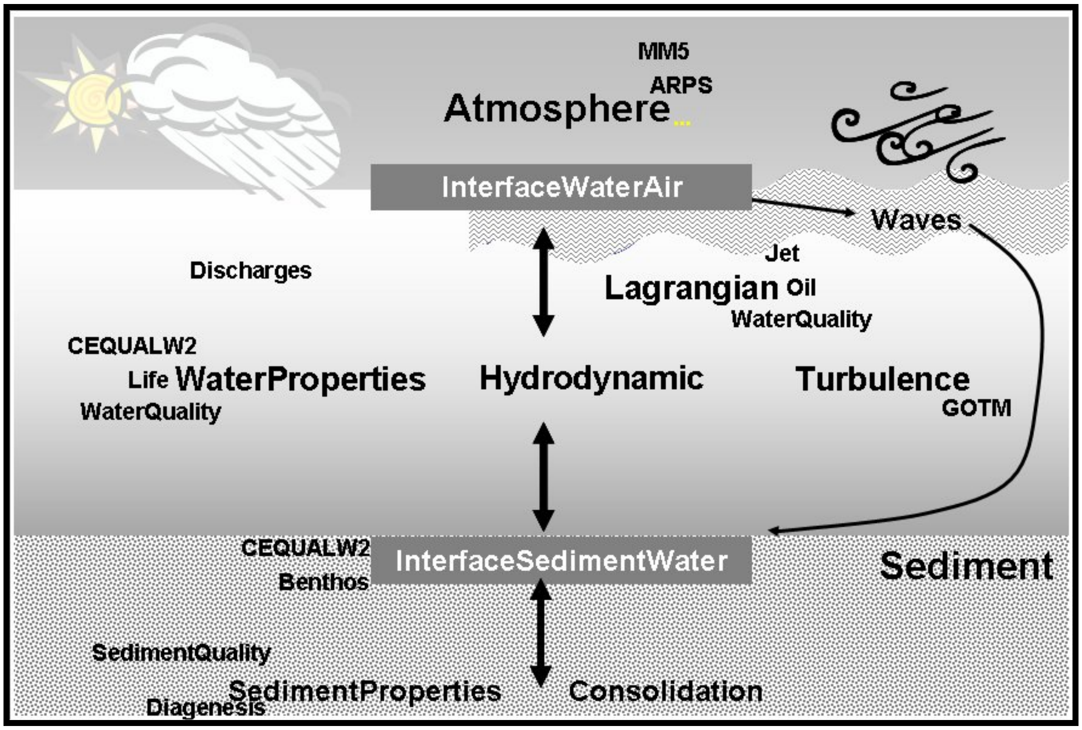

Figure 1. MOHID modular structure.

Pelagic Biogeochemical Processes Simulation

The water column entity is embodied by *Module WaterProperties* which uses *Module Hydrodynamic* to compute water fluxes, then used to compute water properties transport. Transport phenomena in the water column for a given property (P), can be described by the 3D advection-diffusion differential equation:

$$\frac{dP}{dt} = \frac{\partial P}{\partial t} + u_j \frac{\partial P}{\partial x_j} = \frac{\partial}{\partial x_j}\left(k_\Theta \frac{\partial P}{xj} \right) + (Sources - Sinks)$$

P is the concentration (ML^{-3}), j is the index for the correspondent Cartesian axis (x_1, x_2, x_3) or (x,y,z), K_Θ is the turbulent mass diffusion coefficient (horizontal/vertical). MOHID Water is prepared to simulate properties such temperature, salinity, cohesive sediments, phytoplankton, nutrients, contaminants, etc. These properties can either be (i) dissolved in the water, therefore following the currents; (ii) particulate phase or adsorbed on to particulate matter, thus being subjected to one more transport variable: the settling velocity. This enables particulate properties to deposit in the bottom and thus become a part of the sediment compartment.

Sources and sinks relate to reaction processes taken place inside the assumed control volume, which undertakes local production and destruction terms. The sink and source terms can be computed by MOHID using three different modules, differing mainly in terms of processes description complexity level:

- *Module CE-QUAL-W2,* using CE-QUAL-W2 ecological formulations, developed at the Corps of Engineers. The model is able to simulate 22 properties, including temperature, nutrients (nitrogen, phosphorus and silica biogeochemical cycles), oxygen and several species of algae (microalgae). The model does not simulate macroalgae, neither the influence of zooplankton in the primary production;

- *Module WaterQuality*, type of WASP (U.S. Environmental Protection Agency). The model considers 18 properties, including nutrients and organic matter (nitrogen, phosphorus and silica biogeochemical cycles), oxygen and organisms. The model enables the user to choose between the simulation of one group of phytoplankton (for simple applications) or two groups (for more complex applications) – flagellates and diatoms. The same type of option is made for secondary producers: one generic group of zooplankton or two groups – microzooplankton and mesozooplankton. The model is also able to simulate heterotrophic bacteria in the water column.
- *Module Life, type of ERSEM* . This is a more complex model, able to simulate not only nutrients (nitrogen, phosphorus and silica biogeochemical cycles) but also several species of primary producers, secondary producers and decompositors in the water column. The model computes the variability of N:P:C content in the organism's tissue. More complex and detailed studies can be performed using this model.

2 Technical Description

The paradigm behind the MOHID system was inspired by Prof. DiToro's (member of HydroQual) words: "Phytoplankton does not have GPS", meaning that biochemical processes are 0D and do not depend on the referential and dimensions considered to quantify transport. In the MOHID case, the methodology consists in building a biogeochemical module, where the external forcing conditions are given (ex: light, temperature, salinity) and mass fluxes between state variables (ex: nitrate, phytoplankton and zooplankton) are computed for each control volume. This is an efficient way to guarantee a high level of robustness in the code and to maintain it. This approach is also followed by DHI's MIKE system, which like MOHID, has several transport models.

2.1 Coupling hydrodynamic and biogeochemical models

One way to accomplish the coupling of a biogeochemical pelagic module with different eulerian transport models is to build a biochemical module that computes the reactions for one control volume. Consequently, the biochemical subroutines have to be called inside the loops, a method proved to be computational time consuming. The alternative is to build a module that solves the biochemical processes for a 1D array of control volumes. The MOHID system has an interface called *ModuleInterface*, responsible for transferring information (forcing conditions and state variables) from 1D, 2D or 3D structured grids to a 1D array and for calling the 0D biochemical module subroutines. MOHID system was developed following an object-oriented programming philosophy. This interface is a class (or module) currently used to transfer information from the module responsible for the transport processes in the water column to the module responsible for the biochemical process in the sediment. The same happens between the sediment transport module and sediment biochemical processes modules. In this way, *ModuleWaterQuality* is a zero-dimensional ecological model, which can be used by the eulerian or lagrangian transport modules. Figure 1 represents the information flux between the water quality module and other modules.

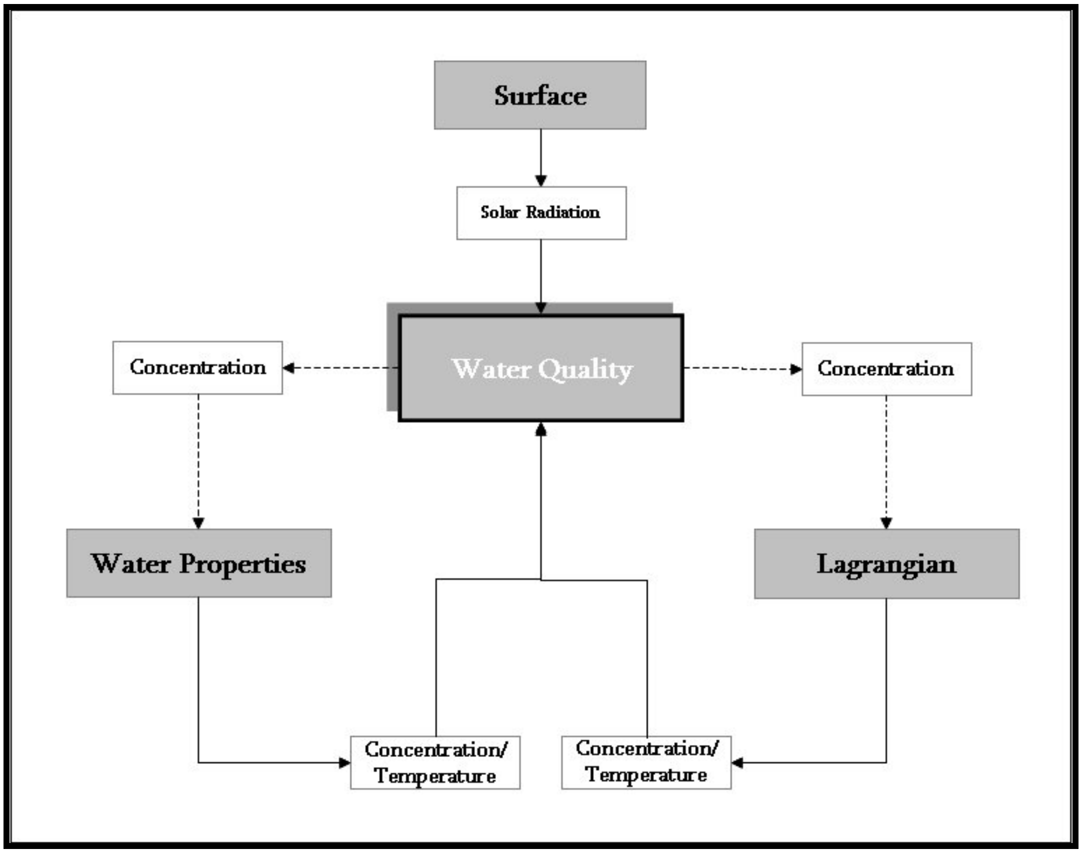

Figure 2. Information flux between Water Quality Module and the other modules.

2.2 Constructing the Interface

The interface construction phase consists on the memory allocation and options consistency to couple the transport model to the biochemical model. Thus, the variables needed to initialize the interface are:

- Name of the biochemical model to be executed;

- An array with the names of the state variables (properties) being modeled by the transport model, which have been defined to have sinks and sources terms using the defined biochemical equations; this is important, so that properties are defined coherently in both models and the properties indexing task can be performed straightforwardly;
- A mapping matrix (WaterPointsxD, being x the number of dimensions) that takes the value of 0 for land points and 1 for water points; this is used to define the size of the 1D arrays where most information will be stored and then given to the biochemical module.
- A size variable (SizexD, being x the number of dimensions), used to translate (loop through) 2D and 3D matrixes to 1D arrays.

2.3 Interfacing during the run

ModuleInterface first task is to gather information on state variables needed by the biochemical models. So, the transport model must loop through all properties, sending its concentration as an argument. Optionally, other variables can also be sent, like radiation at the top of the control volume, control volume thickness and the light extinction coefficient field. Mapping arrays (WaterPointsxD and OpenPointsxD) must be given so that biochemical processes can be computed, if desired, for example, only in covered cells. OpenPointsxD is a variable, which takes the value of 0 if the cell is uncovered and 1 if it is covered with water.

State variables information (i.e. concentration of properties which have sinks and sources defined by the biochemical module) is stored in a bi-dimensional array with size equal to the number of properties versus the number of control volumes, with each property properly indexed in this array. The indexing is done in the constructing phase in agreement with the two models. On the other hand, properties like temperature and salinity as well as light and mapping variables, are stored in specific 1D arrays.

The loop through all the properties continues until all information is gathered. This is achieved by creating a logical array with the indexed properties, defining the ones that have already been added to the state variables array. When everything is ready, the biochemical model is then called, looping through the number of control volumes, changing the state variables values.

The biochemical model time step can be, and often is, different from the transport model time step. The latter needs, due to numerical reasons, smaller time steps than the biochemical models. Thus, in each biochemical time step the state variables values are previously stored in another array, allowing to compute the concentration variation during this time step. This flux is then available to the transport model to actualize the properties concentration in its own time step.

3 Pelagic Processes Description

The ecological model described in *Module Water Quality* is adapted from EPA (1985) and pertain to the category of ecosystem simulations models i.e. sets of conservation equations describing as adequately as possible the working and the interrelationships of real ecosystem components. The nitrogen, oxygen, phosphorus and silica biogeochemical cycles are included. A brief description of these cycles is presented in the next sections.

Many of the equations are written as dependent on a regulating factor, which contains the functional response of the organism to some environmental parameters such as light, nutrients or temperature. When growth is a function of many resources, there is a large range of functional forms that might express the joint dependence. To control the various possibilities, it is common to think of separate resources as limiting factors reducing some theoretical maximum growth rate - factors that can be determined separately and the combined by a small number of ways.

Each growth limitation factor can range from a value of 0 to 1. A value of 1 means the factor does not limit growth (i.e. is at optimum intensity, nutrients are available in excess, etc) and a value of 0 means the factor is so severely limiting that growth is inhibit entirely.

The model uses:

- A minimum formulation only for nutrients limitation, in which the most severely limiting factor alone is assumed to limit growth. This formulation is based on “Liebig’s law of the minimum” which states that the factor in shortest supply will control the growth of algae;
- A multiplicative formulation for the three main limiting factors (light, nutrients and temperature) in which all factors are multiplied together. This approach assumes that several factors in short supply will more severely limit growth than a single factor in short supply. The major criticism of this approach is that the computed growth rates may be excessively low when several factors are limiting. Also, the severity of the reduction increases with the number of limiting nutrients considered in the model, making comparison between models difficult.

3.1 State Variables

Table 1. Water Quality Module available State Variables.

Variable	Description		Unit
Φ^{phy}	Flagellates Concentration	Organism	[mg C/l]
Φ^{dia}	Diatoms Concentration		[mg C/l]
Φ^{zoo}	Mesozooplankton Concentration		[mg C/l]
Φ^{cil}	Microzooplankton Concentration		[mg C/l]
Φ^{bact}	Bacteria Concentration		[mg C/l]
Φ^{NH_4}	Ammonia Concentration	Nitrogen	[mg N/l]
Φ^{NO_2}	Nitrite Concentration		[mg N/l]
Φ^{NO_3}	Nitrate Concentration		[mg N/l]
Φ^{PON}	Particulate Organic Nitrogen Concentration		[mg N/l]
Φ^{DONnr}	Dissolved Organic Nitrogen Non Refractory Concentration		[mg N/l]
Φ^{DONre}	Dissolved Organic Nitrogen Refractory Concentration		[mg N/l]
Φ^{IP}	Inorganic Phosphorus Concentration	Phosphorus	[mg P/l]
Φ^{POP}	Particulate Organic Phosphorus Concentration		[mg P/l]
Φ^{DOPnr}	Dissolved Organic Phosphorus Non Refractory Concentration		[mg P/l]
Φ^{DOPre}	Dissolved Organic Phosphorus Refractory Concentration		[mg P/l]
Φ^{DissSi}	Dissolved Silica Concentration	Silica	[mg Si/l]
Φ^{BioSi}	Biogenic Silica Concentration		[mg Si/l]
Φ^{oxy}	Dissolved Oxygen Concentration	Oxygen	[mg O_2/l]

3.2 Organisms

3.2.1 Flagellates and Diatoms

Flagellates and Diatoms are described in terms of carbon concentration (mgC / l). The model assumes three limitations affecting the organisms maximum growth rate, μ_{max}^{X}: Temperature $\Psi(T)^{X}$, light effect $\Psi(E)^{X}$ and nutrient limitation, which is computed as the minimum of $\Psi(N)^{X}$, $\Psi(P)^{X}$ (and $\Psi(Si)^{X}$ for Diatoms simulation). These two groups of primary producers share the same formulations for the most part of the processes differing just in terms of parameters used by the model. The model is able to consider either one or the two groups of primary producers.

The simulation of the primary producers (Flagellates and/or Diatoms) is developed with the following considerations (Figure 3):

- Organisms consume inorganic nutrients (ammonia and nitrate from the nitrogen cycle and inorganic phosphorus from the phosphorus cycle, and silicate in the case of diatoms) depending on their availability;
- Organisms' growth is also influenced by the temperature and availability of light as a source of energy for photosynthesis;
- Dissolved oxygen is produced during respiration process consumes oxygen and produces ammonia;
- By excretion phytoplankton produces dissolved organic material (DONr, DONnr, DOPr and DOPnr);
- By mortality phytoplankton increases the dissolved organic material and the particulate organic material (PON and POP) in the system;
- By zooplankton grazing, the concentration of flagellates and diatoms decreases.
- By ciliates grazing, the concentration of flagellates decreases;
- Settling process is modeled in the *ModuleWaterProperties* as for any other particulate property in the model.

The rate equation used by the model to compute flagellates and diatoms evolution and the processes formulations are synthetically described in the next tables. Table 9 and Table 10 list the default values considered by the model to compute flagellates and diatoms evolution, respectively.

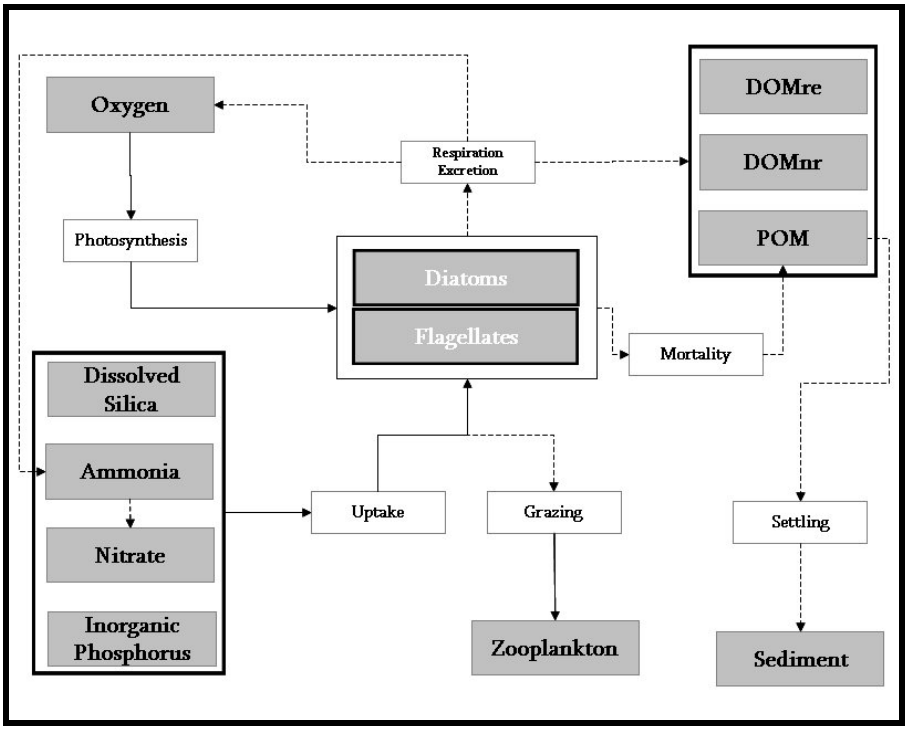

Figure 3. Flagellates and Diatoms Processes.

$$\frac{\partial \Phi^X}{\partial t} = \left(\mu^X - r^X - ex^X - m^X\right)\Phi^X - G^X \qquad X \equiv phy, dia$$

μ^X	Gross Growth Rate	[d-1]
r^X	Total Respiration Rate	[d-1]
ex^X	Excretion Rate	[d-1]
m^X	Natural Mortality Rate (non-predatory)	[d-1]
G^X	Grazing Rate1	[mg C/l.d-1]

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[1] Described in section 3.2.4

Table 2. Flagellates/Diatoms Gross Growth Rate

Symbol	*Description*	*Unit*	*Formulation*
μ^X	Gross Growth Rate	d^{-1}	$\mu^{phy} = \mu_{max}^{phy}.\Psi(T)^{phy}.\Psi(I)^{phy}.Min\left[\Psi(N)^{phy}, \Psi(P)^{phy}\right]$
			$\mu^{dia} = \mu_{max}^{dia}.\Psi(T)^{dia}.\Psi(I)^{dia}.Min\left[\Psi(N)^{dia}, \Psi(P)^{dia}, \Psi(Si)^{dia}\right]$

$\mu_{max}^X(T_{ref})$	Maximum Gross growth Rate at the reference temperature	$[d^{-1}]$
$\Psi(T)^X$	Temperature Limitation Factor	adim
$\Psi(I)^X$	Light Limitation Factor	adim
$\Psi(N)^X$	Nitrogen Limitation Factor	adim
$\Psi(P)^X$	Phosphorus Limitation Factor	adim
$\Psi(Si)^{dia}$	Silica Limitation Factor	adim

Table 3. Temperature Limitation Factor.

Symbol	*Description*	*Unit*	*Formulation*
$\Psi(T)^X$	Temperature Limitation Factor	adim	$\Psi(T)^X = K_A(T)^X K_B(T)^X$
$K_A(T)^X$	-	adim	$K_A(T)^X = \dfrac{K_1{}^X.e^{\gamma_1{}^X.\left(T-T_{\min}^X\right)}}{1+K_1{}^X.\left(e^{\gamma_1{}^X.\left(T-T_{\min}^X\right)}-1\right)}$
$K_B(T)^X$	-	adim	$K_B(T)^X = \dfrac{K_4{}^X.e^{\gamma_2{}^X.\left(T_{\max}^X-T\right)}}{1+K_4{}^X.\left(e^{\gamma_2{}^X.\left(T_{\max}^X-T\right)}-1\right)}$
$\gamma_1{}^X$	-	adim	$\gamma_1{}^X = \dfrac{Ln\dfrac{K_2{}^X\left(1-K_1{}^X\right)}{K_1{}^X\left(1-K_2{}^X\right)}}{T_{opt\min}^X - T_{\min}^X}$
$\gamma_2{}^X$	-	adim	$\gamma_2{}^X = \dfrac{Ln\dfrac{K_3{}^X\left(1-K_4{}^X\right)}{K_4{}^p\left(1-K_3{}^X\right)}}{T_{opt_{\max}}^X - T_{\max}^X}$

$K_1{}^X$	Constant to control temperature response curve shape	adim
$K_2{}^X$	Constant to control temperature response curve shape	adim
$K_3{}^X$	Constant to control temperature response curve shape	adim
$K_4{}^X$	Constant to control temperature response curve shape	adim
$T_{\min}^X$	Minimum tolerable temperature	[ºC]
$T_{\max}^X$	Maximum tolerable temperature	[ºC]
$T_{opt_{\min}}^X$	Minimum temperature of the optimal interval for organism activity	[ºC]
$T_{opt_{\max}}^X$	Maximum temperature of the optimal interval for organism activity	[ºC]

Table 4. Light Limitation Factor.

Symbol	*Description*	*Unit*	*Formulation*	
$\Psi(I)^X$	Light Limitation Factor	adim	$\Psi(I)^X = \frac{e^1}{k^X.z} \times \left(e^{-\frac{I_0}{I_{opt}^X} \times e^{(-k^X.z)}} - e^{-\frac{I_0}{I_{opt}^X}} \right)$	
k	Light extinction coefficient in the water column	[m^{-1}]	*Constant*	$k = \text{Constant}$
			Parsons et al. 1984	$k = 0.04+0.0088\text{Chla}+0.54\text{Chla}^{2/3}$
			Portela, 1996 *(Tagus Estuary)*	$k = 1.24 + 0.036SPM$
			Combined Parsons and Portela	$k = [0.04 + 0.0088Chla + 0.54Chla^{2/3}] \times 0.7 + [0.036 \times 0.5 \times SPM]$
			Multiparameters	$k = \sum k^X \Phi^X$
Chla	Chlorophyll a concentration	µgChla/l	$Chla = \Phi^X \times \alpha_{Chla:C} \times 1000$	
SPM	Solid Suspended Matter Concentration	adim	$SPM = \sum \Phi^X \quad X \equiv coesivese\,\text{dim}\,ents, PON, POP, phy, dia, zoo$	
z	Depth	[m]		
I_{o}[2]	Incident Radiation	[W/m^2]		
I_{opt}^X	Optimum light intensity for photosynthesis	[W/m^2]		
$\alpha_{Chloa:C}$	Chlorophyll_a/C Ratio	[µgChla/ µgC]		

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[2] Computed in Light Extinction Module

Table 5. Nutrients Linitation Factor.

Symbol	*Description*	*Unit*	*Formulation*
$\Psi(N)^X$	Nitrogen Limitation Factor	adim	$\Psi(N)^X = \dfrac{\Phi^{\mathrm{NH_4}} + \Phi^{\mathrm{NO_3}}}{K_N^X + \Phi^{\mathrm{NH_4}} + \Phi^{\mathrm{NO_3}}}$
$\Psi(P)^X$	Phosphorus Limitation Factor	adim	$\Psi(P)^X = \dfrac{\Phi^{IP}}{K_P^X + \Phi^{IP}}$
$\Psi(Si)^{dia}$	Silica Limitation Factor in diatoms growth	adim	$\Psi(Si)^{dia} = \dfrac{\Phi^{DissSi}}{K_{Si}^{dia} + \Phi^{DissSi}}$
K_N^X	Nitrogen half-saturation constant	[mgN/l]	
K_P^X	Phosphorus half-saturation constant	[mgP/l]	
K_{Si}^{dia}	Silica half-saturation constant	[mgSi/l]	

Table 6. Total Respiration Rate.

Symbol	Description	Unit	Formulation
r^X	Total Respiration Rate	d^{-1}	$r^X = k_{re}^X \, e^{(0.069T)} + k_{rp}^X \mu^X$ [EPA, 1985]
T	Temperature	[ºC]	
k_{re}^X	Endogenous respiration constant	$[d^{-1}]$	
k_{rp}^X	Photorespiration fraction	adim	
μ^X	Growth Rate	$[d^{-1}]$	

Table 7. Excretion Rate.

Symbol	Description	Unit	Formulation
ex^X	Excretion Rate	d^{-1}	$ex^X = \varepsilon^X \mu^X (1 - \psi(I)^X)$ [EPA, 1985]
ε^X	Excretion constant	adim	
μ^X	Growth Rate	$[d^{-1}]$	
$\psi(I)^X$	Light Limitation Factor	adim	

Table 8. Natural Mortality (Non Grazing) Rate.

Symbol	*Description*	*Unit*	*Formulation*
m^X	Natural Mortality Rate	d^{-1}	$m^X = m_{\max}^X \dfrac{\dfrac{\Phi^X}{\mu^X}}{K_m^X + \dfrac{\Phi^X}{\mu^X}}$
$m_{\max}^X$	Maximum mortality rate	$[d^{-1}]$	
K_m^X	Mortality half-saturation rate	$[mgC/l.d^{-1}]$	
μ^X	Growth Rate	$[d^{-1}]$	

Table 9. Flagellates Parameters.

Symbol	*Description*	*Unit*	*Default Value*	*Keyword*
$\mu^{phy}_{\max}$	Flagellates Maximum gross growth rate	d^{-1}	2	GROWMAXF
k^{phy}_{re}	Endogenous respiration constant for flagellates	d^{-1}	0.0175	FENDREPC
k^{phy}_{rp}	Fraction of actual photosynthesis which is oxidized by photorespiration for flagellates	adim	0.125	PHOTORES
ε^{phy}	Excretion Constant for flagellates	adim	0.07	EXCRCONS
$m^{phy}_{\max}$	Maximum Mortality Rate for flagellates	d^{-1}	0.02	FMORTMAX
K^{phy}_{m}	Mortality half-saturation rate for flagellates	mg C $l^{-1}d^{-1}$	0.3	FMORTCON
E^{phy}	Assimilation efficiency of the flagellates by zooplankton	adim	0.8	ASS_EFIC
K^{phy}_{N}	Nitrogen half-saturation constant for flagellates	mg N l^{-1}	0.014	NSATCONS
K^{phy}_{P}	Phosphorus half-saturation constant for flagellates	mg P l^{-1}	0.001	PSATCONS
I^{phy}_{opt}	Optimum light intensity for flagellates photosynthesis	Wm^{-2}	121	PHOTOIN
$T^{phy}_{opt_{\min}}$	Minimum temperature of the optimal interval for flagellates photosynthesis	ºC	25	TOPTFMIN
$T^{phy}_{opt_{\max}}$	Maximum temperature of the optimal interval for flagellates photosynthesis	ºC	26.5	TOPTFMAX
$T^{phy}_{\min}$	Minimum tolerable temperature for flagellates photosynthesis	ºC	4	TFMIN
$T^{phy}_{\max}$	Maximum tolerable temperature for flagellates photosynthesis	ºC	37	TFMAX
K^{phy}_{1}	Constant to control temperature response curve shape on flagellates	adim	0.05	TFCONST1
K^{phy}_{2}	Constant to control temperature response curve shape on flagellates	adim	0.98	TFCONST2
K^{phy}_{3}	Constant to control temperature response curve shape on flagellates	adim	0.98	TFCONST3
K^{phy}_{4}	Constant to control temperature response curve shape on flagellates	adim	0.02	TFCONST4
$\alpha^{phy}_{N:C}$	Flagellates Nitrogen/Carbon Ratio	mgN/mgC	0.18	FRATIONC
$\alpha^{phy}_{P:C}$	Flagellates Phosphorus/Carbon Ratio	mgP/mgC	0.024	FRATIOPC
f^{phy}_{inorg}	Fraction of soluble inorganic material excreted by flagellates	adim	0.4	FSOLEXCR
f^{phy}_{orgD}	Fraction of dissolved organic material excreted by flagellates	adim	0.5	FDISSDON

Table 10. Diatoms Parameters.

Symbol	*Description*	*Unit*	*Default Value*	*Keyword*
$\mu_{\max}^{dia}$	Diatoms Maximum gross growth rate	d-1	3	DIGROWMAX
k_{re}^{dia}	Diatoms Endogenous respiration constant	d-1	0.0175	DIFENDREPC
k_{rp}^{dia}	Fraction of actual photosynthesis which is oxidized by photorespiration for Diatoms	adim	0.125	DIPHOTORES
ε^{dia}	Diatoms Excretion Constant	adim	0.07	DIEXCRCONS
$m_{\max}^{dia}$	Maximum Mortality Rate for Diatoms	d-1	0.02	DIMORTMAX
K_{m}^{dia}	Half-saturation for mortality for Diatoms	mg C l-1d-1	0.3	DIMORTCON
E^{dia}	Assimilation efficiency of Diatoms by zooplankton	adim	0.8	DIASS_EFIC
K_{N}^{dia}	Nitrogen half-saturation constant for Diatoms	mg N l-1	0.015	DINSATCONS
K_{P}^{dia}	Phosphorus half-saturation constant for Diatoms	mg P l-1	0.002	DIPSATCONS
K_{Si}^{dia}	Silicate half-saturation constant for Diatoms	mg Si l-1	0.08	DISISATCONS
I_{opt}^{dia}	Optimum light intensity for Diatoms photosynthesis	Wm-2	121	DIPHOTOIN
$T_{opt_{\min}}^{dia}$	Minimum temperature of the optimal interval for Diatoms photosynthesis	ºC	25	DITOPTMIN
$T_{opt_{\max}}^{dia}$	Maximum temperature of the optimal interval for Diatoms photosynthesis	ºC	26.5	DITOPTMAX
$T_{\min}^{dia}$	Minimum tolerable temperature for Diatoms growth	ºC	4	DITMIN
$T_{\max}^{dia}$	Maximum tolerable temperature for Diatoms growth	ºC	37	DITMAX
K_{1}^{dia}	Constant to control temperature response curve shape on Diatoms	adim	0.1	DITCONST1
K_{2}^{dia}	Constant to control temperature response curve shape on Diatoms	adim	0.98	DITCONST2
K_{3}^{dia}	Constant to control temperature response curve shape on Diatoms	adim	0.98	DITCONST3
K_{4}^{dia}	Constant to control temperature response curve shape on Diatoms	adim	0.02	DITCONST4
$\alpha_{N:C}^{dia}$	Diatoms Nitrogen/Carbon Ratio	mgN/mgC	0.18	DIRATIONC
$\alpha_{P:C}^{dia}$	Diatoms Phosphorus/Carbon Ratio	mgP/mgC	0.024	DIRATIOPC
$\alpha_{Si:C}^{dia}$	Diatoms Silica/Carbon Ratio	mgSi/mgC	0.6	DIRATIOSIC
f_{inorg}^{dia}	Fraction of soluble inorganic material excreted by Diatoms	adim	0.4	DISOLEXCR
f_{orgD}^{dia}	Fraction of dissolved organic material excreted by Diatoms	adim	0.5	DIDISSDON

3.2.2 Micro and Mesozooplankton

Figure 4 represents the main processes considered by the model for microzooplankton and mesozooplankton simulation and the tables below describe the formulations used to compute the properties concentration evolution in time, described in carbon concentration (mg C/l). Like in primary producers, the two zooplankton groups have similar formulation differing in terms of specific parameters and grazing possibilities. Globally, zooplankton (micro and mesozooplankton) considers:

- Organisms' growth is influenced by the temperature and prey concentration;
- Respiration process consumes oxygen and produces ammonia;
- Excretion represents a source of dissolved and particulate organic material (DONr, DONnr, DOPr and DOPnr) in the system;
- By mortality, zooplankton increases the particulate organic material (PON and POP);
- Microzooplankton grazing on bacteria and flagellates;
- Mesozooplankton grazing on diatoms and flagellates.

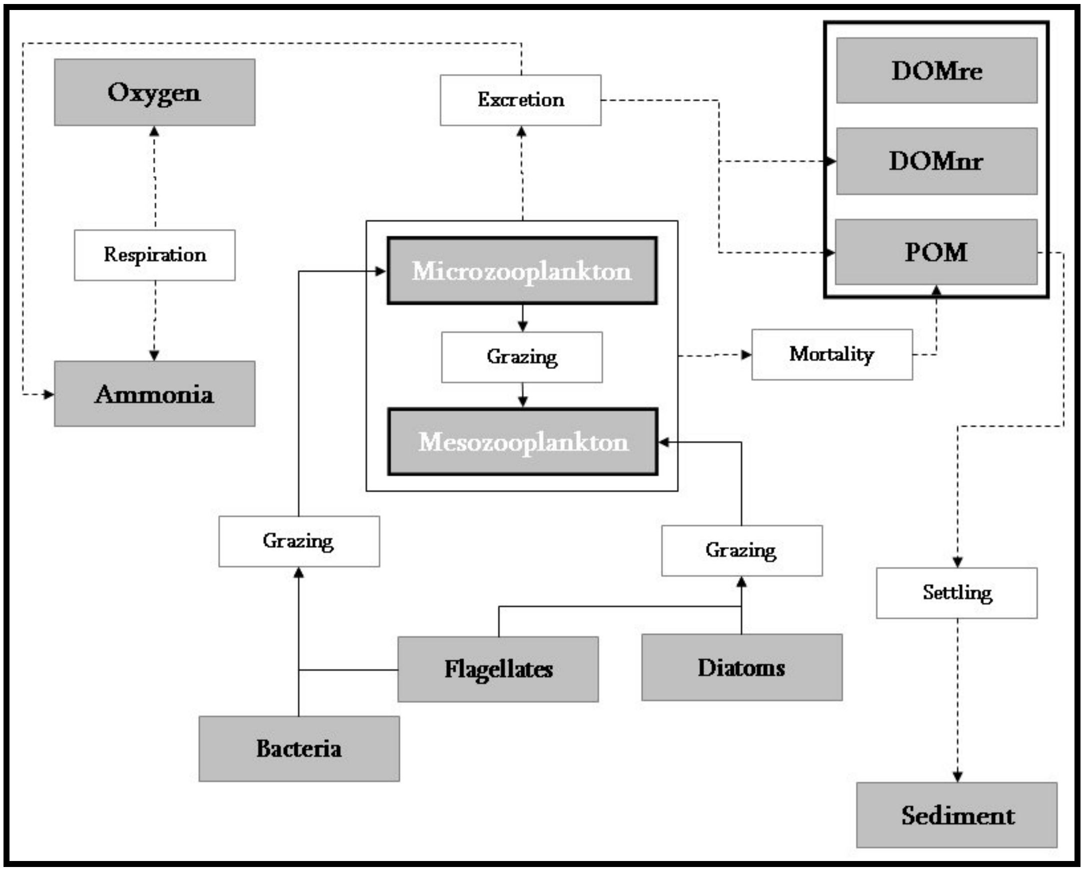

Figure 4. Micro and Mesozooplankton Processes.

$$\frac{\partial \Phi^X}{\partial t} = \left(\mu^X - r^X - ex^X - m^X\right)\Phi^X - G^X \qquad X \equiv zoo, cil$$

μ^X	*Gross Growth Rate*	*[d^{-1}]*
r^X	*Total Respiration Rate*	*[d^{-1}]*
ex^X	*Excretion Rate*	*[d^{-1}]*
m^X	*Natural Mortality Rate (non-predatory)*	*[d^{-1}]*
G^X	*Grazing Rate*[3]	*[mg C/l.d^{-1}]*

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[3] Described in section 3.2.4

Table 11. Micro and Mesozooplankton Formulations.

Symbol	*Description*	*Unit*	*Formulation*	
μ^X	Gross Growth Rate	d^{-1}	1 Flagellates Group 1 Zooplankton Group	$\mu^{zoo} = \mu_{\max}^{zoo}.\Psi\left(T\right)^{zoo}.\Psi\left(F\right)^{zoo}$
			>1 Flagellates Group >1 Zooplankton Group	$\mu^{zoo} = \sum g_{zoo}^X G_{zoo}^X \qquad X \equiv phy, dia, cil$
				$\mu^{cil} = \sum g_{cil}^X G_{cil}^X \qquad X \equiv phy, bact$
$\Psi(T)^X$	Temperature Limitation Factor	adim	*See Table 3*	
$\Psi(F)^{zoo}$	Food Limitation Factor	adim	$\Psi\left(F\right)^{zoo} = \begin{cases} 1 - e^{-\Lambda(\Phi^X - \Phi_{\min X}^{zoo})} \\ 0 \;\; if \;\; \Phi_{phy} < \Phi_{\min X}^{zoo} \end{cases}$	
r^X	Respiration Rate	d^{-1}	$r^X = \rho_{carbon}^X \Psi(T)^{zoo}$	
ex^X	Excretion Rate	d^{-1}	$ex^X = \left(k_{ex}^X b_{ex}^X\right)^T$	
m^X	Natural Mortality Rate (Non-grazing mortality	d^{-1}	$m^X = \begin{cases} \dfrac{a_m^X}{\Phi^{prey}} + m_{\min}^X & if\, \Phi^{prey} > \Phi_{\min_{prey}}^X \\ m_{\max}^X & if\, \Phi^{prey} \leq \Phi_{\min_{prey}}^X \end{cases}$	$\Phi^{prey} = \sum \Phi^Y$ $Y \equiv \begin{cases} phy, dia, cil & if\ X = zoo \\ phy, bact & if\ X = cil \end{cases}$
G^{zoo}	Grazing Rate	d^{-1}	$G^{zoo} = p^{zoo} \Phi^{zoo}$	

$\mu_{\max}^X$	Maximum Gross growth Rate	[d^{-1}]
g_Y^X	Assimilation Coefficient of Y by X	adim
Λ	Ivlev grazing constant	[l/mgC]
ρ_{carbon}^X	Carbon consumption Rate in respiration	[d^{-1}]
k_{ex}^X	Excretion Rate at 0º	[d^{-1}]
b_{ex}^X	Constant for excretion curve	adim
a_m^X	Constant for mortality curve	adim
$m_{\min}^X$	Minimum Natural Mortality Rate	[d^{-1}]
$m_{\max}^X$	Maximum Natural Mortality Rate	[d^{-1}]
$\Phi_{\min_{prey}}^X$	Minimum prey concentration for grazing	[mgC/l]
p^{zoo}	Zooplankton predatory mortality rate: predation by higher trophic levels	[d^{-1}]
G_Y^X	Y Grazing on X	[mg C/l.d^{-1}]

Table 12. Mesozooplankton Parameters.

Symbol	*Description*	*Unit*	*Value*	*Keyword*
$\mu_{\max}^{zoo}$	Zooplankton Maximum gross growth rate	d-1	0.15	GROWMAXZ
$\alpha_{N:C}^{zoo}$	Zooplankton Nitrogen/Carbon Ratio	mg N/mgC	0.15	ZRATIONC
$\alpha_{P:C}^{zoo}$	Zooplankton Phosphorus/Carbon Ratio	mg P/mgC	0.024	ZRATIOPC
f_{inorg}^{zoo}	Soluble inorganic fraction on the mesozooplankton excretions	adim	0.4	ZSOLEXCR
f_{orgD}^{zoo}	Fraction of dissolved organic material excreted by mesozooplankton	adim	0.5	ZDISSDON
$T_{opt_{\min}}^{zoo}$	Minimum temperature of the optimal interval for mesozooplankton growth	ºC	24.8	TOPTZMIN
$T_{opt_{\max}}^{zoo}$	Maximum temperature of the optimal interval for mesozooplankton growth	ºC	25.1	TOPTZMAX
$T_{\min}^{zoo}$	Minimum temperature mesozooplankton growth	ºC	5	TZMIN
$T_{\max}^{zoo}$	Minimum temperature of the optimal interval for mesozooplankton growth	ºC	35	TZMAX
K_1^{zoo}	Constant to control temperature response curve shape on mesozooplankton	adim	0,05	TZCONST1
K_2^{zoo}	Constant to control temperature response curve shape on mesozooplankton	adim	0,98	TZCONST2
K_3^{zoo}	Constant to control temperature response curve shape on mesozooplankton	adim	0,98	TZCONST3
K_4^{zoo}	Constant to control temperature response curve shape on mesozooplankton	adim	0,02	TZCONST4
ρ_{carbon}^{zoo}	Rate of mesozooplankton consumption of Carbon by respiration and non-predatory mortality	d-1	0.036	ZREFRESP
Λ	Ivlev grazing constant	l/mgC	1.6	IVLEVCON
p^{zoo}	Zooplankton predatory mortality rate: predation by higher trophic levels	d-1	0.02	ZPREDMOR
$\Phi_{\min_{prey}}^{zoo}$	Minimum prey concentration for mesozooplankton grazing	mgC/l	0.0045	ZOOPREYMIN
$\Phi_{\min_{cil}}^{zoo}$	Minimum Microzooplankton concentration for mesozooplankton grazing	mgC/l	0.0045	GRAZCILMIN
$\Phi_{\min_{phy}}^{zoo}$	Minimum Flagellates concentration for mesozooplankton grazing	mgC/l	0.0045	GRAZFITOMIN
$\Phi_{\min_{dia}}^{zoo}$	Minimum Diatoms concentration for mesozooplankton grazing	mg C/l	0.0045	DIGRAZMIN
k_{ex}^{zoo}	Zooplankton Excretion Rate	d-1	0.02	ZEXCFAC
b_{ex}^{zoo}	Constant for mesozooplankton excretion curve	adim	1.0305	ZEXCCONS
a_m^{zoo}	Constant for mesozooplankton mortality curve	adim	0.0	MORTZCOEF
$m_{\min}^{zoo}$	Minimum Rate for mesozooplankton Natural Mortality	d-1	0.001	MINMORTZ
$m_{\max}^{zoo}$	Maximum Rate for mesozooplankton Natural Mortality	d-1	0.04	MAXMORTZ
K_{graz}^{zoo}	Half-Saturation Constant for Grazing	mgC/l	0.85	INGCONSZ
c_{phy}^{zoo}	Capture Efficiency of flagellates by mesozooplankton	adim	0.8	ZOOEFFCAPHY
c_{cil}^{zoo}	Capture Efficiency of Microzooplankton by mesozooplankton	adim	0.2	ZOOEFFCAPCIL
c_{dia}^{zoo}	Capture efficiency of Diatoms by mesozooplankton	adim	0.8	DIZOOEFFCAP
$I_{\max}^{zoo}$	Zooplankton maximum ingestion rate	d-1	1.0	ZINGMAX
g_{phy}^{zoo}	Assimilation Coefficient of Flagellates by mesozooplankton	adim	0.8	ZOPHYASS
g_{cil}^{zoo}	Assimilation Coefficient of Microzooplankton by mesozooplankton	adim	0.8	ZOCILASS
g_{dia}^{zoo}	Assimilation Coefficient of Diatoms by mesozooplankton	adim	0.8	DIZOASS
ρ_{phy}^{zoo}	Proportion of flagellates in mesozooplankton ingestion	adim	0.3	PHYRATING
ρ_{cil}^{zoo}	Proportion of Microzooplankton in mesozooplankton ingestion	adim	0.3	CILRATINGZOO
ρ_{dia}^{zoo}	Proportion of Diatoms in mesozooplankton ingestion	adim	0.3	DIRATINGZOO

Table 13. Microzooplankton Parameters.

Símbolo	*Description*	*Unit*	*Value*	*Keyword*
$\alpha_{N:C}^{cil}$	Microzooplankton Nitrogen/Carbon Ratio	mg N/mgC	0.16	CRATIONC
$\alpha_{P:C}^{cil}$	Microzooplankton Phosphorus/Carbon Ratio	mg P/mgC	0.024	CRATIOPC
$\Phi_{\min_{bact}}^{cil}$	Minimum concentration of bacteria for Microzooplankton grazing	mgC/l	0.0045	GRAZBACMIN
$\Phi_{\min_{phy}}^{cil}$	Minimum concentration of flagellates for Microzooplankton grazing	mgC/l	0.0045	CILGRAZPHYMIN
$\Phi_{\min_{prey}}^{cil}$	Minimum concentration of prey for Microzooplankton grazing	mgC/l	0.0045	CILPREYMIN
$r^{cil}(T^{ref})$	Microzooplankton respiration rate at the reference temperature	d^{-1}	0.02	CREFRESP
κ_{ex}^{cil}	Microzooplankton Excretion Rate	d^{-1}	0.02	CEXCFAC
b_{ex}^{cil}	Constant for Microzooplankton excretion curve	adim	1.03505	CEXCCONS
a_{m}^{cil}	Constant for Microzooplankton mortality curve	adim	0.0	MORTCICOEF
$m_{\min}^{cil}$	Minimum Rate for Microzooplankton Natural Mortality	d^{-1}	0.0	MINMORTCI
$m_{\max}^{cil}$	Maximum Rate for Microzooplankton Natural Mortality	d^{-1}	0.044	MAXMORTCI
K_{graz}^{cil}	Half-Saturation Constant for Microzooplankton Grazing	mgC/l	0.85	INGCONSC
c_{bact}^{cil}	Capture efficiency of bacteria by Microzooplankton	adim	0.5	CILEFFCAPBA
c_{phy}^{cil}	Capture efficiency of flagellates by Microzooplankton	adim	0.5	CILEFFCAPPHY
$I_{\max}^{cil}$	Microzooplankton maximum ingestion rate	d^{-1}	1.0	CINGMAX
g_{bact}^{cil}	Assimilation Coefficient of bacteria by Microzooplankton	adim	0.5	CILBACASS
g_{phy}^{cil}	Assimilation Coefficient of flagellates by Microzooplankton	adim	0.5	CILPHYASS
ρ_{bact}^{cil}	Proportion of bacteria in Microzooplankton ingestion	adim	0.5	BACINGCIL
ρ_{phy}^{cil}	Proportion of flagellates in Microzooplankton ingestion	adim	0.5	PHYINGCIL

3.2.3 Bacteria

Figure 5 represents the main processes involving heterotrophic bacteria, described in the model in terms of carbon concentration (mg C/l). Formulations used to compute bacteria concentration evolution in time are shown in the tables below. Globally the model considers:

- The specific uptake rate of bacteria is dependent on resource availability (organic substrate), accordingly to a Michaelis-Menten function, and on temperature;
- For ammonium uptake to take place, DOM or POM concentrations must be higher than the bacteria minimum substrate concentration needed for growth, representing the Carbon limitation for bacteria growth;
- For DOM or/and POM uptake to take place, ammonium concentrations must be higher than the bacteria minimum substrate concentration needed for growth, representing the Nitrogen limitation for bacteria growth;
- Total uptake rate of bacteria is the sum of the specific uptake rate for each one of the nutrient sources (DOMnr, ammonium, and POM);
- Nitrogen uptake is converted in carbon units using the N:C ratio of bacteria;
- Excretion represents a source of dissolved organic material (Non-Refractory Dissolved Organic Nitrogen) in the system;
- By mortality, bacteria increases the particulate organic material (Particulate Organic Nitrogen) and ammonia.
- Microzooplankton grazing on bacteria.

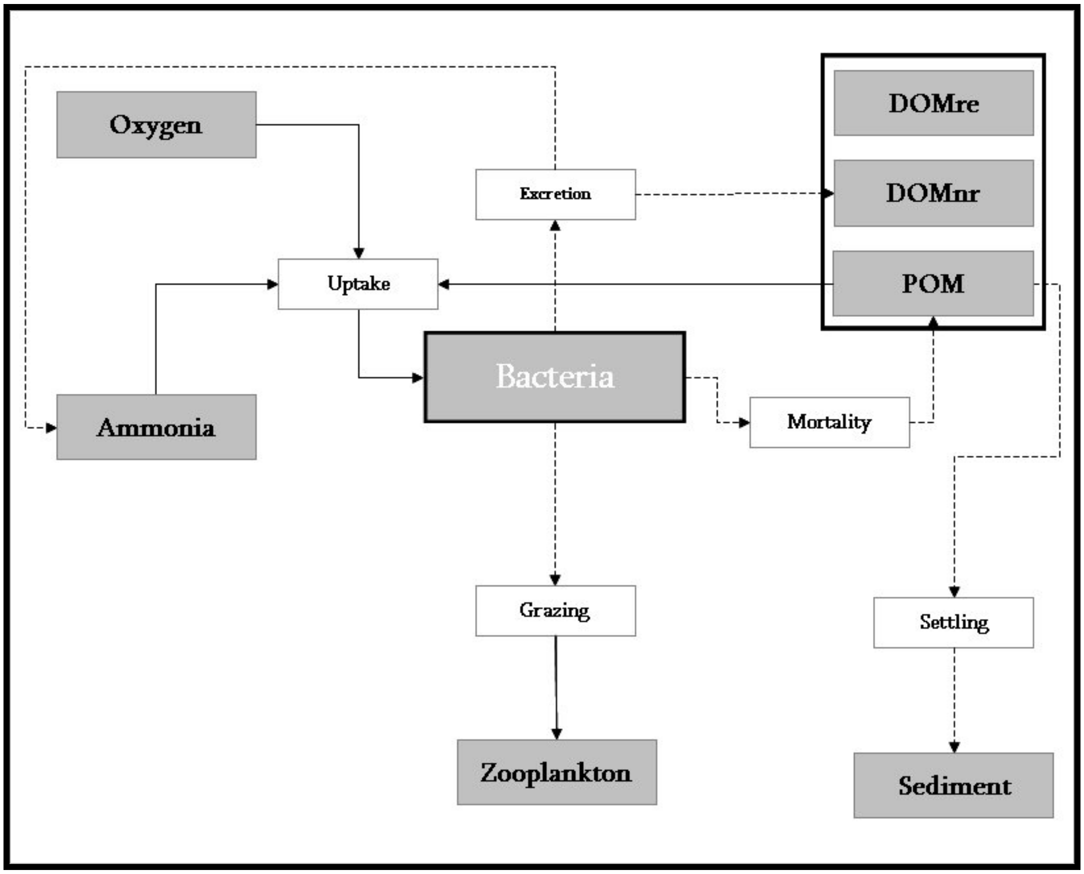

Figure 5. Bacteria processes..

$$\frac{\partial \Phi^{bact}}{\partial t} = \left(\mu^{bact} - e^{bact} - m^{bact} \right) \Phi^{bact} - G^{bact}$$

μ^{bact}	Total bacterial uptake	$[d^{-1}]$
e^{bact}	Excretion Rate	$[d^{-1}]$
m^{bact}	Natural Mortality Rate (non-predatory)	$[d^{-1}]$
G^{X}	*Grazing Rate*[4]	*[mg C/l.d*$^{-1}$*]*

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[4] Described in section 3.2.4

Table 14. Bacteria formulations.

Symbol	*Description*	*Unit*	*Formulation*
μ^{bact}	Total Bacterial Uptake	d^{-1}	$\mu^{bact} = \sum_{Y=1}^{n} \mu_Y^{bact} \quad Y \equiv NH_4, DONnr, PON$
μ_Y^{bact}	Specific uptake rate for each nutrient source	d^{-1}	$\mu_{NH_4}^{bact} = \frac{\mu_{\max}^{bact} . \Psi(T)^{bact} . \Psi(F)_{NH_4}^{bact}}{\alpha_{N:C}^{bact}}$
			$\mu_Y^{bact} = \frac{\mu_{\max}^{bact} . \Psi(T)^{bact} . \Psi(F)_Y^{bact}}{\alpha_{N:C}^{OM}} \quad Y \equiv DONnr, PON$
$\Psi(F)_Y^{bact}$	Food Limitation Factor	adim	$\Psi(F)_Y^{bact} = \begin{cases} \frac{\Phi^Y}{K_N^{bact} + \Phi^Y} \\ 0 \quad if\ \Phi^Y < \Phi_{\min}^{subs} \end{cases} \quad Y \equiv NH_4, DONnr, PON$
$\Psi(T)$	Temperature Limitation Factor	adim	See Table 3
$\mu_{\max}^{bact}(T_{ref})$	Bacteria Maximum Nutrient Uptake at the reference temperature		[mgN/mgC.d^{-1}]
$\alpha_{N:C}^{bact}$	Bacteria Nitrogen/Carbon Ratio		[mg N/mgC]
$\alpha_{N:C}^{OM}$	Organic Matter Nitrogen/Carbon Ratio		[mg N/mgC]
$\Phi_{\min}^{subs}$	Bacteria Minimum Substract Concentration for uptake		mgN/l
K_N^{bact}	Half-Saturation constant for nutrient uptake		[mgN/l]
m^{bact}	Natural Mortality Rate (non-predatory)		[d^{-1}]

Table 15. Bacteria Parameters.

Symbol	*Description*	*Unit*	*Value*	*Keyword*
$\alpha_{N:C}^{bact}$	Bacteria Nitrogen/Carbon Ratio	mg N/mgC	0.2	BRATIONC
m^{bact}	Bacteria Natural Mortality Rate	d-1	0.1	NATMORB
ex^{bact}	Bacteria Excretion Rate	d-1	0.01	BARESPCO
$\mu_{\max}^{bact}$	Bacteria Maximum Nutrient Uptake at the reference temperature	mgN/mgC.d^{-1}	0.251	BMAXUPTA
$\Phi_{\min}^{subs}$	Bacteria Minimum Substract Concentration for uptake	mgN/l	0.010	BACMINSUB
K_N^{bact}	Half-Saturation constant for nutrient uptake	mgN/l	0.0008	BACNCONS
$T_{opt_{\min}}^{bact}$	Minimum temperature of the optimal interval for bacteria growth	ºC	24.8	TOPTBMIN
$T_{opt_{\max}}^{bact}$	Maximum temperature of the optimal interval for bacteria growth	ºC	25.1	TOPTBMAX
$T_{\min}^{bact}$	Minimum temperature for bacteria growth	ºC	5	TBMIN
T_{max}^{bact}	Maximum temperature for bacteria growth	ºC	35	TBMAX
K_1^{bact}	Constant to control temperature response curve shape on bacteria	adim	0,05	TBCONST1
K_2^{bact}	Constant to control temperature response curve shape on bacteria	adim	0,98	TBCONST2
K_3^{bact}	Constant to control temperature response curve shape on bacteria	adim	0,98	TBCONST3
K_4^{bact}	Constant to control temperature response curve shape on bacteria	adim	0,02	TBCONST4

3.2.4 Grazing Formulations

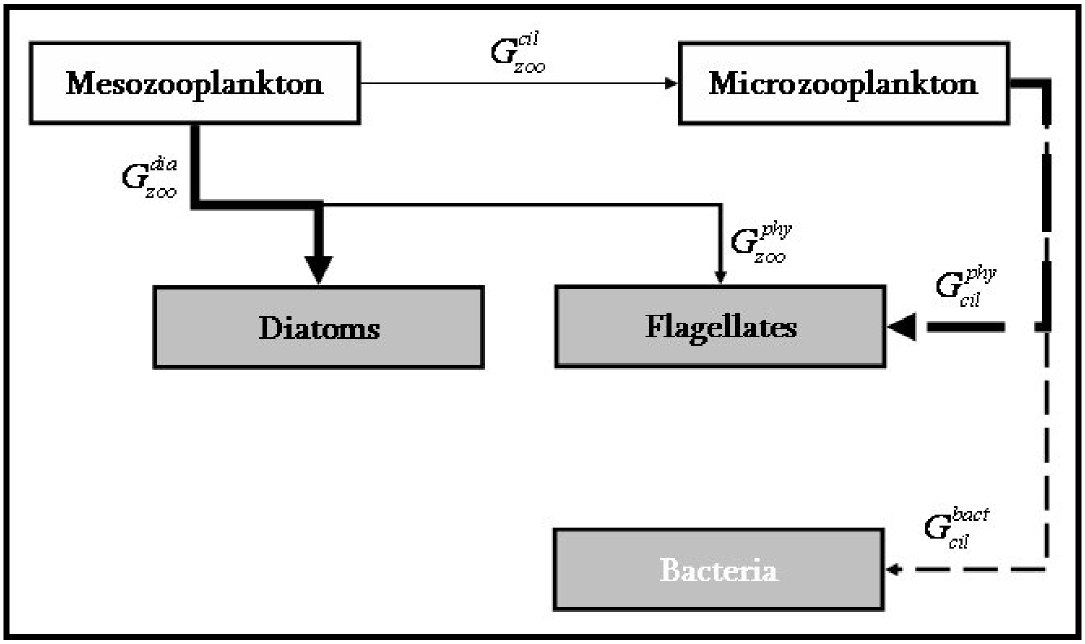

Figure 6. Grazing Options.

G^X	Total Grazing Rate on X	mgC(X)/l.d-1
G_Y^X	Y Grazing on X	d^{-1}

$$G^{phy} = G_{cil}^{phy}\Phi^{cil} + G_{zoo}^{phy}\Phi^{zoo}$$

$$G^{dia} = G_{zoo}^{dia}\Phi^{zoo}$$

$$G^{cil} = G_{zoo}^{cil}\Phi^{zoo}$$

$$G^{bact} = G_{cil}^{bact}\Phi^{cil}$$

Table 16. Grazing Formulation.

Symbol	Description	Unit	Formulation
(1) Flagellates and Zooplankton Simulation			$G_{zoo}^{phy} = \frac{\mu^{zoo}}{E^{phy}}$
(2) Diatoms and Zooplankton Simulation			$G_{zoo}^{dia} = \frac{\mu^{zoo}}{E^{dia}}$
(3) Flagellates, Diatoms and Zooplankton Simulation			$G_{zoo}^{dia} = \rho_{zoo}^{dia}.I_{\max}^{zoo}.\Psi_{zoo}^{dia}.\Psi\left(T\right)^{zoo}$ $G_{zoo}^{phy} = \rho_{zoo}^{phy}.(I_{\max}^{zoo} - G_{zoo}^{dia}).\Psi_{zoo}^{dia}.\Psi\left(T\right)^{zoo}$
(4) Flagellates, Macrozooplankton, Microzooplankton and Bacteria			$\begin{cases} G_{zoo}^{phy} = \rho_{zoo}^{phy}.I_{\max}^{zoo}.\Psi_{zoo}^{phy}.\Psi\left(T\right)^{zoo} \\ G_{cil}^{phy} = \rho_{cil}^{phy}.I_{\max}^{cil}.\Psi_{cil}^{phy}.\Psi\left(T\right)^{cil} \end{cases}$ $G_{zoo}^{cil} = \rho_{zoo}^{cil}.(I_{\max}^{zoo} - G_{zoo}^{phy}).\Psi_{zoo}^{dia}.\Psi\left(T\right)^{zoo}$ $G_{cil}^{bact} = \rho_{cil}^{bact}.I_{\max}^{cil}.\Psi_{cil}^{bact}.\Psi\left(T\right)^{cil}$
(5) Diatoms, Macrozooplankton, Microzooplankton and Bacteria			$G_{zoo}^{dia} = \rho_{zoo}^{dia}.(I_{\max}^{zoo}).\Psi_{zoo}^{dia}.\Psi\left(T\right)^{zoo}$ $G_{zoo}^{cil} = \rho_{zoo}^{cil}.(I_{\max}^{zoo} - G_{zoo}^{dia}).\Psi_{zoo}^{cil}.\Psi\left(T\right)^{zoo}$ $G_{cil}^{bact} = \rho_{cil}^{bact}.I_{\max}^{cil}.\Psi_{cil}^{bact}.\Psi\left(T\right)^{cil}$
(6) Diatoms, Flagellates, Macrozooplankton,Microzooplankton and Bacteria Simulation			$G_{zoo}^{dia} = \rho_{zoo}^{dia}.(I_{\max}^{zoo}).\Psi_{zoo}^{dia}.\Psi\left(T\right)^{zoo}$ $\begin{cases} G_{zoo}^{phy} = \rho_{zoo}^{phy}.(I_{\max}^{zoo} - G_{zoo}^{dia}).\Psi_{zoo}^{phy}.\Psi\left(T\right)^{zoo} \\ G_{cil}^{phy} = \rho_{cil}^{phy}.I_{\max}^{cil}.\Psi_{cil}^{phy}.\Psi\left(T\right)^{cil} \end{cases}$ $G_{zoo}^{cil} = \rho_{zoo}^{cil}.(I_{\max}^{zoo} - G_{zoo}^{dia} - G_{zoo}^{phy}).\Psi_{zoo}^{cil}.\Psi\left(T\right)^{zoo}$ $G_{cil}^{bact} = \rho_{cil}^{bact}.I_{\max}^{cil}.\Psi_{cil}^{bact}.\Psi\left(T\right)^{cil}$
Ψ_Y^X	Y Grazing Limitation by X concentration	adim	$\Psi_Y^X = \begin{cases} \frac{c_Y^X.\Phi^X - \Phi_Y^{\min X}}{K_{graz}^Y + (c_Y^X.\Phi^X - \Phi_Y^{\min X})} & if\ (c_Y^X.\Phi^X - \Phi_Y^{\min X}) > 0 \\ 0 & c.c \end{cases}$

X	Predated organism	
Y	Predator organism	
μ^X	Growth rate	d-1
$\Psi(T)^X$	Temperature Limitation Factor	adim
K_{graz}^Y	Half-saturation constant for predation	[mg C/l]
c_Y^X	Y capture efficiency on X	adim
ρ_Y^X	Proportion of X in Y ingestion	adim
$\Phi_Y^{\min X}$	Minimum X concentration for Y grazing	[mgC/l]
E^X	Assimilation efficiency of X by zooplankton $(X \equiv phy, dia)$	adim
$I_{\max}^Y$	Y maximum ingestion rate	d-1

3.3 Nitrogen Biogeochemical Cycle

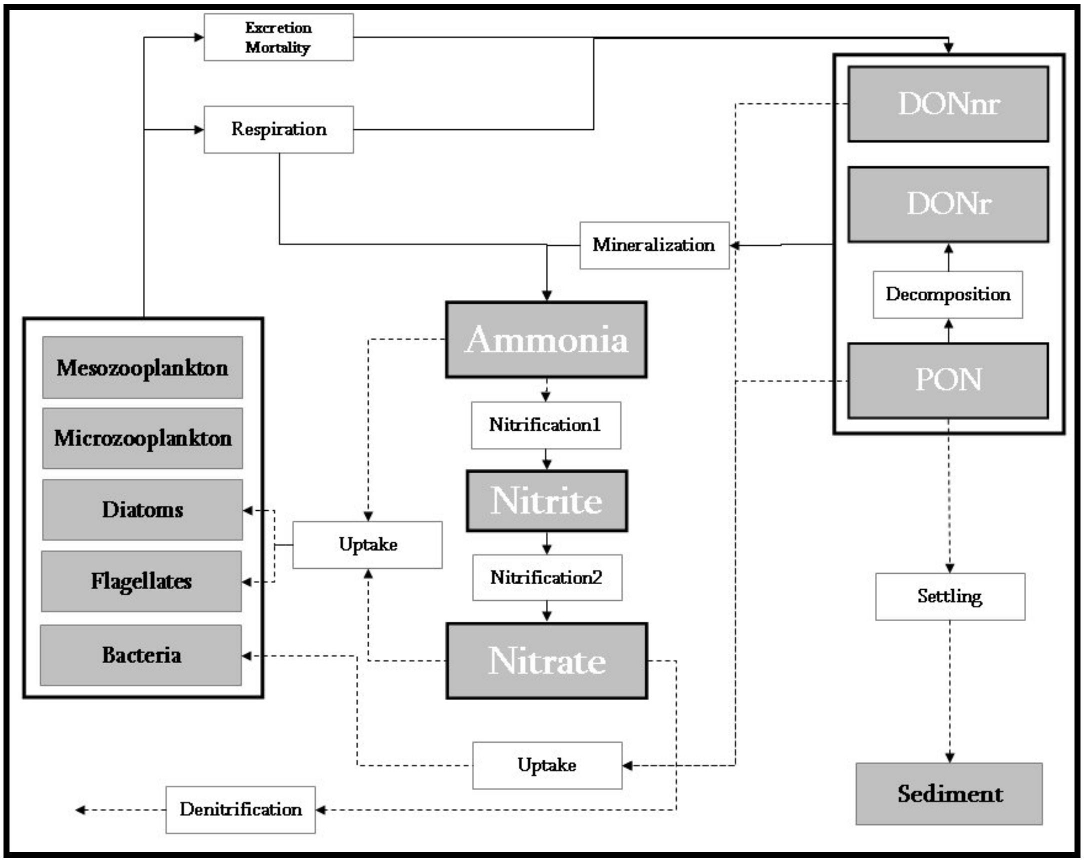

Figure 7. Nitrogen Biogeochemical Cycle.

3.3.1 Ammonia

With Bacteria:

$$
\begin{aligned}
\frac{\partial\Phi^{NH4}}{\partial t} = & \underbrace{\left[f^{phy}_{inorg}(ex^{phy} + r^{phy})\alpha^{phy}_{N:C} - \beta^{phy}_{NH_4}\mu^{phy}\alpha^{phy}_{N:C} \right]\Phi^{phy}}_{flagellates} \\
& + \underbrace{\left[f^{dia}_{inorg}(ex^{dia} + r^{dia})\alpha^{dia}_{N:C} - \beta^{dia}_{NH4}\mu^{dia}\alpha^{dia}_{N:C} \right]\Phi^{dia}}_{diatoms} \\
& + \underbrace{\left[ex^{bact}\alpha^{bact}_{N:C} - \mu^{bact}_{NH4} \right]\Phi^{bact}}_{bacteria} \\
& + \underbrace{(f^{zoo}_{inorg}ex^{cil} + r^{cil})\alpha^{cil}_{N:C}\Phi^{cil}}_{microzooplankton} \\
& + \underbrace{\left[f^{zoo}_{inorg}ex^{zoo} + r^{zoo})\alpha^{zoo}_{N:C} \right]\Phi^{zoo}}_{mesozooplankton} \\
& + \underbrace{K^{DONre}_{\min}\Phi^{DONre}}_{DONre} \\
& - \underbrace{K_{nit}\Phi^{NH4}}_{\substack{nitrification \\ step1}}
\end{aligned}
$$

Without Bacteria

$$
\begin{aligned}
\frac{\partial\Phi^{NH4}}{\partial t} = & \underbrace{\left[f^{phy}_{inorg}(ex^{phy} + r^{phy})\alpha^{phy}_{N:C} - \beta^{phy}_{NH_4}\mu^{phy}\alpha^{phy}_{N:C} \right]\Phi^{phy}}_{flagellates} \\
& + \underbrace{\left[f^{dia}_{inorg}(ex^{dia} + r^{dia})\alpha^{dia}_{N:C} - \beta^{dia}_{NH4}\mu^{dia}\alpha^{dia} \right]\Phi^{dia}}_{diatoms} \\
& + \underbrace{(f^{zoo}_{inorg}ex^{cil} + r^{cil})\alpha^{cil}_{N:C}\Phi^{cil}}_{microzooplankton} \\
& + \underbrace{\left[f^{zoo}_{inorg}(ex^{zoo} + r^{zoo})\alpha^{zoo}_{N:C} \right]\Phi^{zoo}}_{mesozooplankton} \\
& + \underbrace{K^{DONre}_{\min}\Phi_{DONre}}_{DONre} + \underbrace{K^{DONnr}_{\min}\Phi^{DONnr}}_{DONnr} + \underbrace{f^{phy}_{orgP}K^{PON}_{dec}\Phi^{PON}}_{PON} \\
& - \underbrace{K_{nit}\Phi^{NH4}}_{\substack{nitrification \\ step1}}
\end{aligned}
$$

3.3.2 Nitrite

$$\frac{\partial \Phi^{NO_2}}{\partial t} = K_{nit}\Phi^{NH_4} - K_{nit}\Phi^{NO_2}$$

3.3.3 Nitrate

$$\frac{\partial \Phi^{NO3}}{\partial t} = -\underbrace{(1-\beta_{NH_4}^{phy})\alpha^{phy}\mu^{phy}\Phi^{phy}}_{flagellates} - \underbrace{(1-\beta_{NH_4}^{dia})\alpha^{dia}\mu^{dia}\Phi^{dia}}_{diatoms} + K_{nit}\Phi^{NO_2} - K_{dnit}\Phi^{NO_3}$$

3.3.4 Particulate Organic Nitrogen

With
Bacteria

$$\begin{aligned}
\frac{\partial \Phi^{PON}}{\partial t} = & \underbrace{\left[(1-f_{inorg}^{phy})(1-f_{orgD}^{phy})(ex^{phy}+r^{phy})+m^{phy}\right]\alpha_{N:C}^{phy}\Phi^{phy}}_{flagellates} \\
& + \underbrace{\left[(1-f_{inorg}^{dia})(1-f_{orgD}^{dia})(ex^{dia}+r^{dia})+m^{dia}\right]\alpha_{N:C}^{dia}\Phi^{dia}}_{diatoms} \\
& - \underbrace{(\mu_{PON}^{bact}-m^{bact}\alpha_{N:C}^{bact})\Phi^{bact}}_{bacteria} \\
& + \underbrace{\left[(1-f_{inorg}^{zoo})(1-f_{orgD}^{zoo})ex^{cil}+m^{cil}\right]\alpha_{N:C}^{cil}\Phi^{cil}+(\delta_N^{cil}+\varphi_N^{cil})\Phi^{cil}}_{microzooplankton} \\
& + \underbrace{\left[(1-f_{inorg}^{zoo})(1-f_{orgD}^{zoo})ex^{zoo}+m^{zoo}+p^{zoo}\right]\alpha_{N:C}^{zoo}\Phi^{zoo}+(\delta_N^{zoo}+\varphi_N^{zoo})\Phi^{zoo}}_{mesozooplankton} \\
& - \underbrace{(1-f_{orgP})K_{dec}^{PON}\Phi^{PON}}_{DONre}
\end{aligned}$$

Without Bacteria

$$\begin{aligned}
\frac{\partial \Phi^{PON}}{\partial t} = & \underbrace{\left[(1-f_{inorg}^{phy})(1-f_{orgD}^{phy})(ex^{phy}+m^{phy}\right]\alpha_{N:C}^{phy}\Phi^{phy}}_{flagellates} \\
& + \underbrace{\left[(1-f_{inorg}^{dia})(1-f_{orgD}^{dia})(ex^{dia}+m^{dia}\right]\alpha_{N:C}^{dia}\Phi^{dia}}_{diatoms} \\
& + \underbrace{\left[(1-f_{inorg}^{zoo})(1-f_{orgD}^{zoo})ex^{cil}+m^{cil}\right]\alpha_{N:C}^{cil}\Phi^{cil}+(\delta_N^{cil}+\varphi_N^{cil})\Phi^{cil}}_{microzooplankton} \\
& + \underbrace{\left[(1-f_{inorg}^{zoo})(1-f_{orgD}^{zoo})(r^{zoo}+m^{zoo}+p^{zoo})\right]\alpha_{N:C}^{zoo}\Phi^{zoo}+(\delta_N^{zoo}+\varphi_N^{zoo})\Phi^{zoo}}_{mesozooplankton} \\
& - \underbrace{(1-f_{orgP})K_{dec}^{PON}\Phi^{PON}}_{DONre} \\
& - \underbrace{f_{orgP}K_{dec}^{PON}\Phi^{PON}}_{ammonia}
\end{aligned}$$

3.3.5 Non Refractory Dissolved Organic Nitrogen

With Bacteria:

$$\begin{aligned}\frac{\partial\Phi^{DONnr}}{\partial t} = {} & \underbrace{(1-f_{inorg}^{phy})f_{orgD}^{phy}(ex^{phy}+r^{phy})\alpha_{N:C}^{phy}\Phi^{phy}}_{\textit{flagellates}} \\ & +\underbrace{(1-f_{inorg}^{dia})f_{orgD}^{dia}(ex^{dia}+r^{dia})\alpha_{N:C}^{dia}\Phi^{dia}}_{\textit{diatoms}} \\ & -\underbrace{\mu_{DONnr}^{bact}\Phi^{bact}}_{\textit{bacteria}} \\ & +\underbrace{(1-f_{inorg}^{cil})f_{orgD}^{cil}ex^{cil}\Phi^{cil}}_{\textit{microzooplankton}} \\ & +\underbrace{(1-f_{inorg}^{zoo})f_{orgD}^{zoo}ex^{zoo}\alpha_{N:C}^{zoo}\Phi^{zoo}}_{\textit{mesozooplankton}}\end{aligned}$$

Without Bacteria and Microzooplankton:

$$\begin{aligned}\frac{\partial\Phi^{DONnr}}{\partial t} = {} & \underbrace{(1-f_{inorg}^{phy})f_{orgD}^{phy}(ex^{phy}+r^{phy})\alpha_{N:C}^{phy}\Phi^{phy}}_{\textit{flagellates}} \\ & +\underbrace{(1-f_{inorg}^{dia})f_{orgD}^{dia}(ex^{dia}+r^{dia})\alpha_{N:C}^{dia}\Phi^{dia}}_{\textit{diatoms}} \\ & +\underbrace{(1-f_{inorg}^{cil})f_{orgD}^{cil}ex^{cil}\Phi^{cil}}_{\textit{microzooplankton}} \\ & +\underbrace{(1-f_{inorg}^{zoo})f_{orgD}^{zoo}ex^{zoo}\alpha_{N:C}^{zoo}\Phi^{zoo}}_{\textit{mesozooplankton}} \\ & -\underbrace{K_{\min}^{DONnr}\Phi^{DONnr}}_{\textit{ammonia}}\end{aligned}$$

3.3.6 Refractory Dissolved Organic Nitrogen

$$\frac{\partial\Phi^{DONre}}{\partial t} = \underbrace{(1-f_{orgP})K_{dec}^{PON}\Phi^{PON}}_{\textit{PON}} - \underbrace{K_{\min}^{DONre}\Phi^{DONre}}_{\textit{ammonia}}$$

Table 17.Nitrogen Formulations.

Symbol	*Description*	*Unit*	*Formulation*	
$\beta^{X}_{NH_4}$	X ammonia preference factor	adim	$\beta^{X}_{NH4} = \left(\frac{\Phi^{NH4}}{K^X_N + \Phi^{NH4}}\right)\left(\frac{\Phi_{NO3}}{K^X_N + \Phi^{NO3}}\right) + \left(\frac{\Phi^{NH4}}{\Phi_{NO3} + \Phi^{NH4}}\right)\left(\frac{K^X_N}{K^X_N + \Phi^{NO3}}\right) \quad X \equiv phy, dia$	
K^{PON}_{dec}	PON decomposition Rate	d^{-1}	$K^{PON}_{dec} = K^{PON}_{dec}(T_{ref}).\theta_{dec}{}^{(T-T_{ref})}$	
$K^{DONre}_{\min}$	DONre mineralization Rate	d^{-1}	$K^{DONre}_{dec} = K^{DONre}_{\min}(T_{ref}).(\theta^{DONre}_{\min})^{(T-T_{ref})} \frac{\sum \Phi^X}{K^{phy}_r + \sum \Phi^X} \quad X \equiv phy, dia$	
$K^{DONnr}_{\min}$	DONnr mineralization Rate	d^{-1}	$K^{DONnr}_{\min} = K^{DONnr}_{\min}(T_{ref}).\theta^{DONnr(T-T_{ref})}_{\min} \frac{\sum \Phi^X}{K^{phy}_r + \sum \Phi^X} \quad X \equiv phy, dia$	
K_{nit}	Nitrification Rate	d^{-1}	$K_{nit} = K^{ref}_{nit}(T_{ref})\theta_{nit}{}^{(T-T_{ref})} \frac{\Phi^{oxy}}{K^{sat}_{nit} + \Phi^{oxy}}$	
K_{dnit}	Denitrification Rate	d^{-1}	$K_{dnit} = K^{ref}_{dnit}(T_{ref})\theta_{dnit}{}^{(T-T_{ref})} \frac{K^{sat}_{dnit}}{K^{sat}_{dnit} + \Phi^{oxy}}$	
δ^{Y}_{N}	Non-assimilated material by Y	d^{-1}	1 Phytoplankton Group 1 Zooplankton Group	$\delta^{zoo}_N = (1 - E^X)\frac{\mu^{zoo}}{E^X}\alpha^X_{N:C} \quad Y \equiv phy, dia$
			>1 Phytoplankton Group >1 Zooplankton Group	$\delta^{zoo}_N = \sum[(1 - g^X_{zoo})G^X_{zoo}\alpha^X_{N:C}] \quad Y \equiv phy, dia, cil$ $\delta^{cil}_N = \sum[(1 - g^X_{cil})G^X_{cil}\alpha^X_{N:C}] \quad Y \equiv phy, bact$
φ^{Y}_{N}	Stoichiometric food web losses	d^{-1}	1 Phytoplankton Group 1 Zooplankton Group	$\varphi^{zoo}_N = \mu^{zoo}(\alpha^{phy}_{N:C} - \alpha^{zoo}_{N:C})$
			>1 Phytoplankton Group >1 Zooplankton Group	$\varphi^{zoo}_N = \sum(\alpha^X_{N:C} - \alpha^{zoo}_{N:C})g^X_{zoo}G^X_{zoo} \quad X \equiv phy, dia, cil$ $\varphi^{cil}_N = \sum(\alpha^X_{N:C} - \alpha^{cil}_{N:C})g^X_{cil}G^X_{cil} \quad X \equiv phy, bact$

T	Water Temperature	ºC
T_{ref}	Reference Temperature	20 ºC
K^X_N	Nitrogen half-saturation constant	mg N l^{-1}
E^X	Assimilation efficiency of X by zooplankton	adim
g^X_Y	Assimilation Coefficient of X by Y	adim
G^X_Y	Y grazing on X	[d^{-1}]
$\alpha^X_{N:C}$	Nitrogen/Carbon Ratio	mg N/mgC
μ^X	Growth rate	[d^{-1}]
ex^X	Excretion Rate	[d^{-1}]
r^X	Respiration Rate	[d^{-1}]
m^X	Natural Mortality Rate	[d^{-1}]
p^{zoo}	Zooplankton predatory mortality rate: predation by higher trophic levels	[d^{-1}]
$K^{PON}_{dec}(T_{ref})$	PON decomposition rate at reference temperature	d^{-1}
θ_{dec}	PON decomposition temperature coefficient	adim
$K^{DONre}_{\min}(T_{ref})$	DONre mineralization rate at reference temperature	d^{-1}
$\theta^{DONre}_{\min}$	DONre mineralization temperature coefficient	adim
K^{phy}_r	Nutrient Regeneration Half-Saturation Constant	mgC/ l
$K^{DONnr}_{\min}(T_{ref})$	DONnr mineralization Rate at reference temperature	d^{-1}
$\theta^{DONr}_{\min}$	DONre minreralization temperature coefficient	adim
$K^{ref}_{nit}(T_{ref})$	Nitrification rate at reference temperature	adim
θ_{nit}	Nitrification temperature coefficient	adim
K^{sat}_{nit}	Nitrification half-saturation constant	mg O_2/l
$K_{dnit}(T_{ref})$	Denitrification Rate at reference temperature	d^{-1}
θ_{dnit}	Denitrification temperature coefficient	adim
f^X_{inorg}	Fraction of inorganic material excreted by X	adim
f^X_{orgD}	Dissolved organic fraction excreted by X	adim
f_{orgP}	Fraction of PON available for mineralization	adim

Table 18. Nitrogen Parameters.

Symbol	*Description*	*Unit*	*Value*	*Keyword*
$K_{dec}^{PON}(T_{ref})$	PON decomposition Rate at reference temperature	d^{-1}	0.1	NOPREF
θ_{dec}	PON decomposition temperature coefficient	adim	1.02	NOPCOEF
$K_{\min}^{DONre}(T_{ref})$	DONre mineralization Rate at reference temperature	d^{-1}	0.01	NMINR
$\theta_{\min}^{DONre}$	DONre minreralization temperature coefficient	adim	1.02	TMINR
K_r^{phy}	Nutrient Regeneration Half-Saturation Constant	mgC/ l	1	FREGSATC
$K_{nit}(T_{ref})$	Nitrification Rate at reference temperature	d^{-1}	0.06	NITRIREF
K_{nit}^{sat}	Nitrification half-saturation constant	mg O_2/l	2.0	NITSATCO
K_{dnit}^{sat}	Denitrification half-saturation constant	mg $O_{2/l}$	0.1	DENSATCO
θ_{nit}	Nitrification temperature coefficient	adim	1.08	TNITCOEF
$K_{dnit}(T_{ref})$	Denitrification Rate at reference temperature	d^{-1}	0.125	DENITREF
θ_{dnit}	Denitrification temperature coefficient	adim	1.045	TDENCOEF
$K_{\min}^{DONnr}(T_{ref})$	DONnr mineralization Rate at reference temperature	d^{-1}	0.1	NMINENR
$\theta_{\min}^{DONr}$	DONre minreralization temperature coefficient	adim	1.02	TMINNR
f_{orgP}	Fraction of PON available for mineralization	adim	0.7	PHDECOMP

3.4 Phosphorus Biogeochemical Cycle

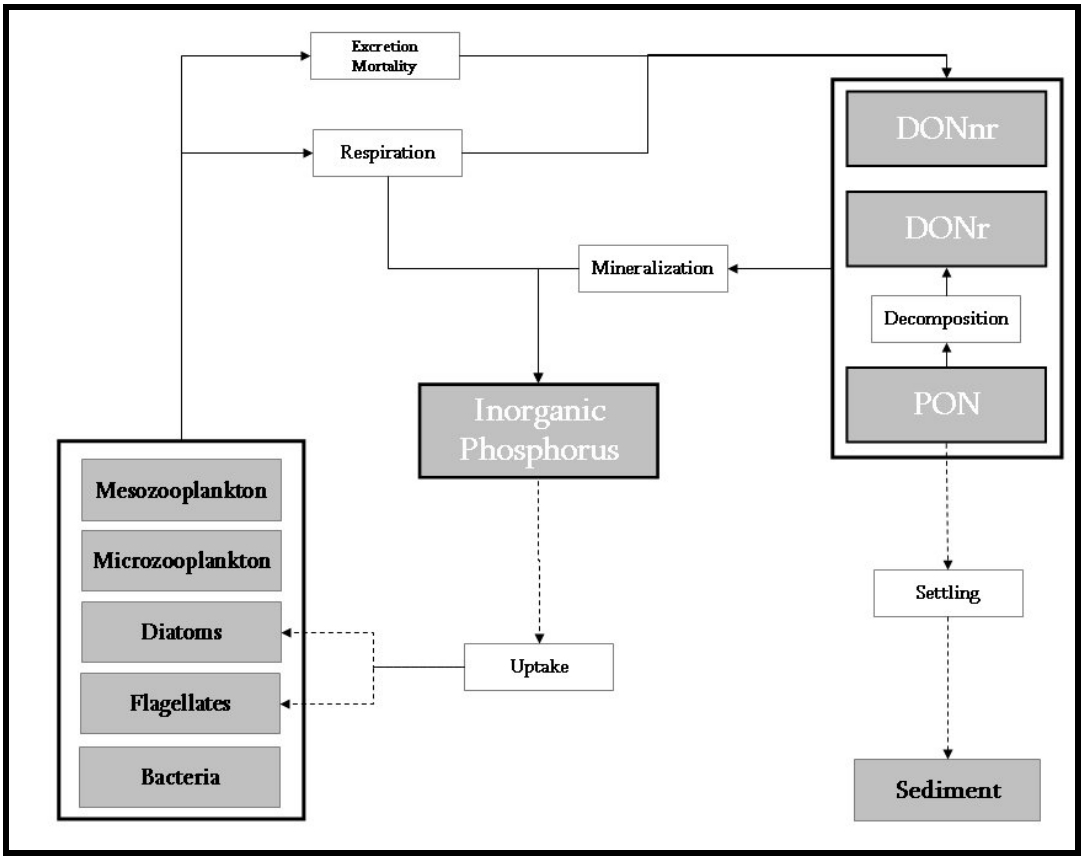

Figure 8.Phosphorus Biogeochemical Cycle.

3.4.1 Inorganic Phosphorus

$$\begin{aligned}
\frac{\partial \Phi^{IP}}{\partial t} = & \underbrace{\left[f^{phy}_{inorg} (ex^{phy} + r^{phy}) \alpha^{phy}_{P:C} - \mu^{phy} \alpha^{phy}_{P:C} \right] \Phi^{phy}}_{flagellates} \\
& + \underbrace{\left[f^{dia}_{inorg} (ex^{dia} + r^{dia}) \alpha^{dia}_{P:C} - \mu^{dia} \alpha^{dia}_{P:C} \right] \Phi^{dia}}_{diatoms} \\
& + \underbrace{[(f^{zoo}_{inorg} ex^{cil} + r^{cil}) \alpha^{cil}_{P:C}] \Phi^{cil}}_{microzooplankton} \\
& + \underbrace{\left[(f^{zoo}_{inorg} ex^{zoo} + r^{zoo}) \alpha^{zoo}_{P:C} \right] \Phi^{zoo}}_{mesozooplankton} \\
& + \underbrace{K^{DOPre}_{\min} \Phi^{DOPre}}_{DOPre} + \underbrace{K^{DOPnr}_{\min} \Phi^{DOPnr}}_{DOPnr} + \underbrace{f_{orgP} K^{POP}_{dec} \Phi^{POP}}_{POP}
\end{aligned}$$

3.4.2 Particulate Organic Phosphorus

$$\begin{aligned}
\frac{\partial \Phi^{POP}}{\partial t} = & \underbrace{\left[(1 - f^{phy}_{inorg})(1 - f^{phy}_{orgD})(ex^{phy} + r^{phy}) + m^{phy} \right] \alpha^{phy}_{P:C} \Phi^{phy}}_{flagellates} \\
& + \underbrace{\left[(1 - f^{dia}_{inorg})(1 - f^{dia}_{orgD})(ex^{dia} + r^{dia}) + m^{dia} \right] \alpha^{dia}_{P:C} \Phi^{dia}}_{diatoms} \\
& + \underbrace{\left[(1 - f^{zoo}_{inorg})(1 - f^{zoo}_{orgD}) ex^{cil} + m^{cil} \right] \alpha^{cil}_{P:C} \Phi^{cil} + (\delta^{cil}_{P} + \varphi^{cil}_{P}) \Phi^{cil}}_{microzooplankton} \\
& + \underbrace{\left[(1 - f^{zoo}_{inorg})(1 - f^{zoo}_{orgD}) ex^{zoo} + m^{zoo} + p^{zoo} \right] \alpha^{zoo}_{P:C} \Phi^{zoo} + (\delta^{zoo}_{P} + \varphi^{zoo}_{P}) \Phi^{zoo}}_{mesozooplankton} \\
& - \underbrace{(1 - f_{orgP}) K^{POP}_{dec} \Phi^{POP}}_{DONre} \\
& - \underbrace{f_{orgP} K^{POP}_{dec} \Phi^{POP}}_{IP}
\end{aligned}$$

3.4.3 Non Refractory Dissolved Organic Phosphorus

$$\begin{aligned}\frac{\partial \Phi^{DOPnr}}{\partial t} &= \underbrace{(1-f_{inorg}^{phy})f_{orgD}^{phy}(ex^{phy}+r^{phy})\alpha_{P:C}^{phy}\Phi^{phy}}_{flagellates} + \\ &+ \underbrace{(1-f_{inorg}^{dia})f_{orgD}^{dia}(ex^{dia}+r^{dia})\alpha_{P:C}^{dia}\Phi^{dia}}_{diatoms} \\ &+ \underbrace{(1-f_{inorg}^{zoo})f_{orgD}^{zoo}ex^{cil}\alpha_{P:C}^{cil}\Phi^{cil}}_{microzooplankton} \\ &+ \underbrace{(1-f_{inorg}^{zoo})f_{orgD}^{zoo}ex^{zoo}\alpha_{P:C}^{zoo}\Phi^{zoo}}_{mesozooplankton} \\ &- \underbrace{K_{\min}^{DOPnr}\Phi^{DOPnr}}_{IP}\end{aligned}$$

3.4.4 Refractory Dissolved Organic Phosphorus

$$\frac{\partial \Phi^{DOPre}}{\partial t} = \underbrace{(1-f_{orgP})K_{dec}^{POP}\Phi^{POP}}_{POP} - \underbrace{K_{\min}^{DOPre}\Phi^{DOPre}}_{IP}$$

Table 19. Phosphorus.

Symbol	*Description*	*Unit*	*Formulation*	
K_{dec}^{POP}	POP decomposition Rate	d^{-1}	$K_{dec}^{POP} = K_{dec}^{POP}(T_{ref}).\theta_{dec}^{(T-T_{ref})}$	
$K_{\min}^{DOPre}$	DONre mineralization Rate	d^{-1}	$K_{dec}^{DOPre} = K_{\min}^{DOPre}(T_{ref}).(\theta_{\min}^{DOPre})^{(T-T_{ref})} \dfrac{\sum \Phi^X}{K_r^{phy} + \sum \Phi^X} \quad X \equiv phy, dia$	
$K_{\min}^{DOPnr}$	DONre mineralization Rate	d^{-1}	$K_{\min}^{DOPnr} = K_{\min}^{DOPnr}(T_{ref}).\theta_{\min}^{DOPnr(T-T_{ref})} \dfrac{\sum \Phi^X}{K_r^{phy} + \sum \Phi^X} \quad X \equiv phy, dia$	
δ_P^Y	Non-assimilated material by Y	d^{-1}	1 Phytoplankton Group 1 Zooplankton Group	$\delta_P^{zoo} = (1-E^X)\dfrac{\mu^{zoo}}{E^X}\alpha_{P:C}^X \quad Y \equiv phy, dia$
			>1 Phytoplankton Group >1 Zooplankton Group	$\delta_P^{zoo} = \sum[(1-g_{zoo}^X)G_{zoo}^X\alpha_{P:C}^X] \quad Y \equiv phy, dia, cil$
φ_P^Y	Stoichiometric food web losses	d^{-1}	1 Phytoplankton Group 1 Zooplankton Group	$\varphi_P^{zoo} = \mu^{zoo}(\alpha_{P:C}^{phy} - \alpha_{P:C}^{zoo})$
			>1 Phytoplankton Group >1 Zooplankton Group	$\varphi_P^{zoo} = \sum(\alpha_{P:C}^X - \alpha_{P:C}^{zoo})g_{zoo}^X G_{zoo}^X \quad X \equiv phy, dia, cil$

T	Water Temperature	ºC
T_{ref}	Reference Temperature	20 ºC
K_N^X	Nitrogen half-saturation constant	mg N l^{-1}
E^X	Assimilation efficiency of X by zooplankton	adim
g_Y^X	Assimilation Coefficient of X by Y	adim
G_Y^X	Y grazing on X	[d^{-1}]
$\alpha_{P:C}^X$	Phosphorus/Carbon Ratio	mg N/mgC
p^{zoo}	Zooplankton predatory mortality rate: predation by higher trophic levels	[d^{-1}]
μ^X	Growth rate	[d^{-1}]
ex^X	Excretion Rate	[d^{-1}]
r^X	Respiration Rate	[d^{-1}]
m^X	Natural Mortality Rate	[d^{-1}]
$K_{dec}^{POP}(T_{ref})$	POP decomposition rate at reference temperature	d^{-1}
θ_{dec}	POP decomposition temperature coefficient	adim
$K_{\min}^{DOPre}(T_{ref})$	DOPre mineralization rate at reference temperature	d^{-1}
$\theta_{\min}^{DOPre}$	DOPre mineralization temperature coefficient	adim
K_r^{phy}	Nutrient Regeneration Half-Saturation Constant	mgC/ l
$K_{\min}^{DOPnr}(T_{ref})$	DOPnr mineralization Rate at reference temperature	d^{-1}
$\theta_{\min}^{DOPr}$	DOPnr minrerallization temperature coefficient	adim
f_{inorg}^X	Fraction of inorganic material excreted by X	adim
f_{orgD}^X	Dissolved organic fraction excreted by X	adim
f_{orgP}	Fraction of PON available for mineralization	adim

Table 20. Phosphorus Parameters.

Symbol	*Description*	*Unit*	*Value*	*Keyword*
$K_{dec}^{POP}(T_{ref})$	POP decomposition Rate at reference temperature	d^{-1}	0.2	PPARTMIN
θ_{dec}	POP decomposition temperature coefficient	adim	1.08	TPPARTMINCOEF
$K_{\min}^{DOPre}(T_{ref})$	DOPre mineralization Rate at reference temperature	d^{-1}	0.03	PMINR
$\theta_{\min}^{DOPre}$	DOPre minreralization temperature coefficient	adim	1.064	PMINRCOEF
$K_{\min}^{DOPnr}(T_{ref})$	DOPnr mineralization Rate at reference temperature	d^{-1}	0.1	PMINNR
$\theta_{\min}^{DOPr}$	DOPre minreralization temperature coefficient	adim	1.064	PMINNRCOEF

3.5 Silica Cycle

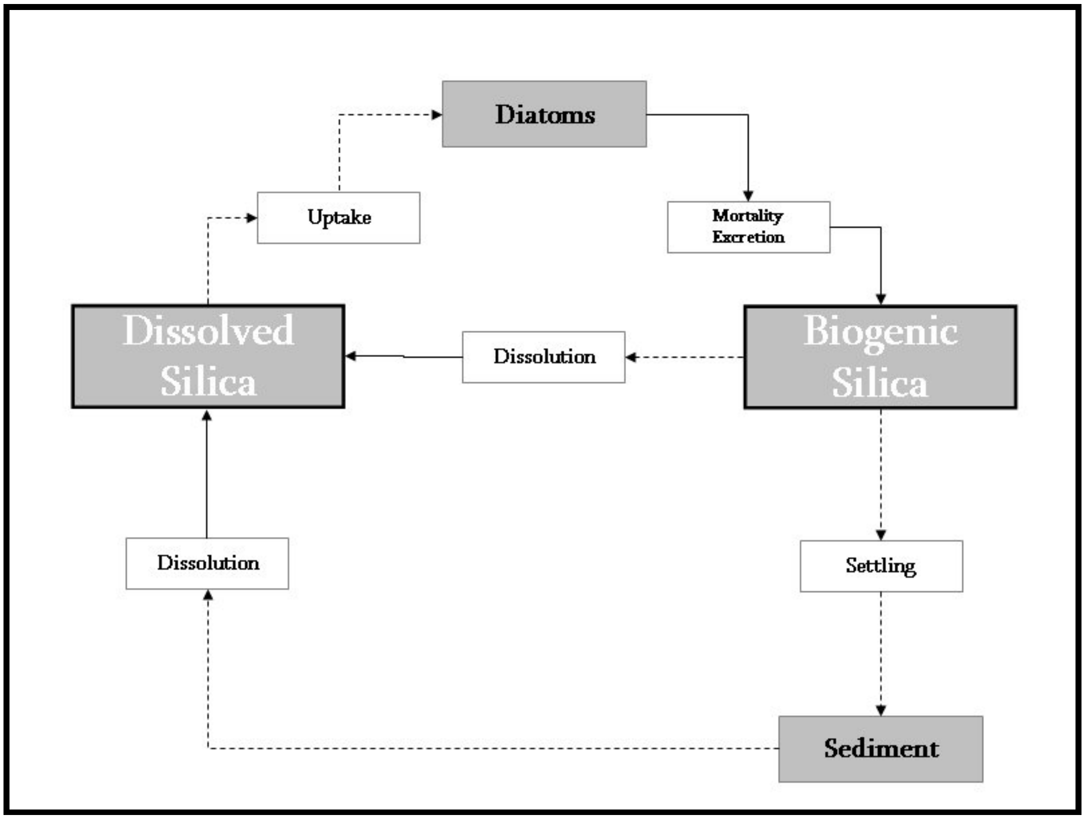

Figure 9. Silica BioGeoChemical Cycle.

3.5.1 Dissolved Silica

$$\frac{\partial \Phi^{DissSi}}{\partial t} = \underbrace{-\mu^{dia}\alpha_{Si:C}^{dia}\Phi^{dia}}_{diatoms} + \underbrace{f_{orgP}K_{dec}^{BioSi}\Phi^{BioSi}}_{BioSi}$$

3.5.2 Biogenic Silica

$$\begin{aligned}\frac{\partial \Phi^{BioSi}}{\partial t} = & \underbrace{\left[(1-f_{inorg}^{dia})(1-f_{orgD}^{dia})(ex^{dia}+r^{dia})+m^{dia}\right]\alpha_{Si:C}^{dia}\Phi^{dia}}_{diatoms} \\ & + \underbrace{G_{zoo}^{dia}\Phi^{zoo}}_{mesozooplankton} \\ & - \underbrace{f_{orgP}K_{dec}^{BioSi}\Phi^{BioSi}}_{DissSi}\end{aligned}$$

Table 21. Silica.

Symbol	Description	Unit	Formulation
K_{dec}^{BioSi}	Bio Si decomposition Rate	d^{-1}	$K_{dec}^{BioSi} = K_{dec}^{BioSi}(T_{ref}).\theta_{dec}^{BioSi(T-T_{ref})}$

T	Water temperature	ºC
T_{ref}	Reference Temperature	ºC
μ^{dia}	Diatoms growth rate	$[d^{-1}]$
ex^{dia}	Diatoms Excretion Rate	$[d^{-1}]$
r^{dia}	Diatoms Respiration Rate	$[d^{-1}]$
m^{dia}	Diatoms Natural Mortality Rate	$[d^{-1}]$
G_{zoo}^{dia}	Mesozooplankton grazing on Diatoms	$[d^{-1}]$
$\alpha_{Si:C}^{dia}$	Diatoms Silica/Carbon Ratio	mg Si/mg C
f_{orgP}	Fraction of PON available for mineralization	adim
f_{orgD}^{dia}	Dissolved organic fraction in diatoms excretions	adim
f_{inorg}^{dia}	Fraction of inorganic material in diatoms excretions	adim
$K_{dec}^{BioSi}(T_{ref})$	BioSi decomposition rate at reference temperature	d^{-1}
θ_{dec}^{BioSi}	BioSi decomposition temperature coefficient	adim

Table 22. Silica Parameters.

Symbol	*Description*	*Unit*	*Value*	*Keyword*
$K_{dec}^{BioSi}(T^{ref})$	Biogenic Sílica dissolution Rate in the Water column at the reference temperature	d^{-1}	0.03	SIKDISS
θ_{dec}^{BioSi}	Biogenic Silica dissolution temperature coefficient	adim	1.02	SIDISSTCOEF

3.6 Oxygen Cycle

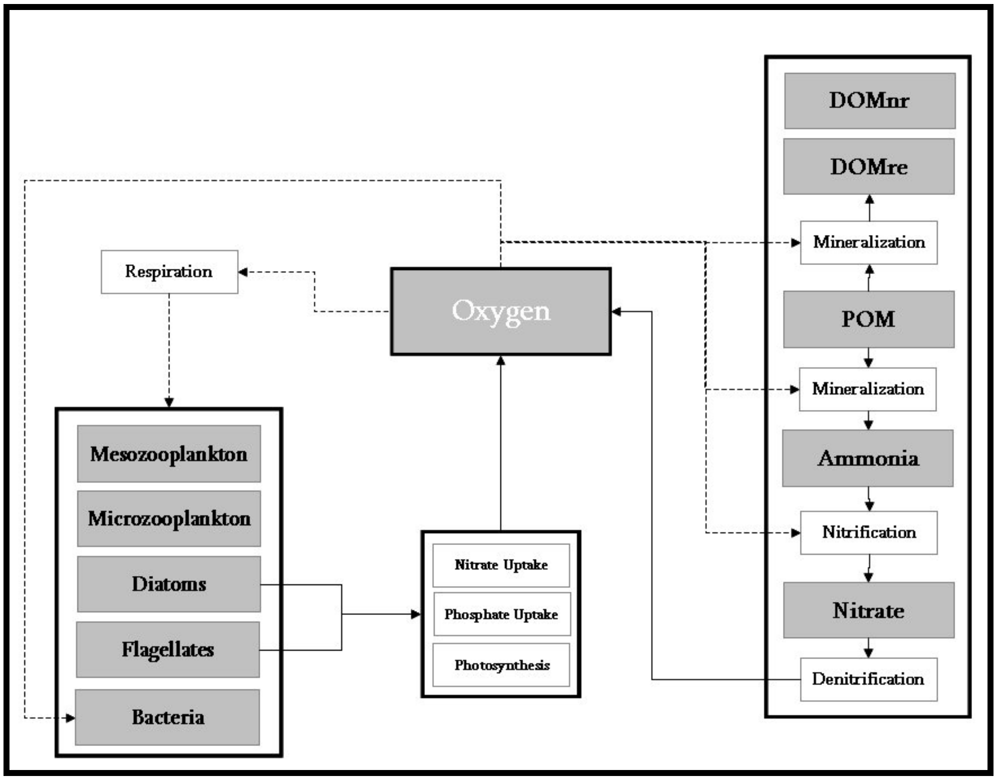

Figure 10. Oxygen Processes.

With Bacteria:

$$\begin{aligned}\frac{\partial \Phi^{oxy}}{\partial t} = {} & \underbrace{\left(\underbrace{\mu^{phy} \alpha^{photo}_{O:C}}_{photosynthesis} + \underbrace{\left(1 - \beta^{phy}_{NH4}\right) \mu^{phy} \alpha^{NO3}_{O:N} \alpha^{phy}_{N:C}}_{nitrate\ uptake} + \underbrace{\mu^{phy} \alpha^{IP}_{O:P} \alpha^{phy}_{P:C}}_{IP\ uptake} - \underbrace{r^{phy} \alpha^{plankton}_{O:C}}_{respiration} \right) \Phi^{phy}}_{flagellates} \\ & + \underbrace{\left(\underbrace{\mu^{dia} \alpha^{photo}_{O:C}}_{photosynthesis} + \underbrace{\left(1 - \beta^{dia}_{NH4}\right) \mu^{dia} \alpha^{NO3}_{O:N} \alpha^{dia}_{N:C}}_{nitrate\ uptake} + \underbrace{\mu^{dia} \alpha^{IP}_{O:P} \alpha^{dia}_{P:C}}_{IP\ uptake} - \underbrace{r^{dia} \alpha^{plankton}_{O:C}}_{respiration} \right) \Phi^{dia}}_{diatoms} \\ & + \underbrace{r^{cil} \alpha^{cil}_{O:C} \Phi^{cil}}_{microzooplankton} + \underbrace{r^{zoo} \alpha^{zoo}_{O:C} \Phi^{zoo}}_{mesozooplankton} \\ & - \underbrace{(\mu^{bact}_{PON} + \mu^{bact}_{DONnr}) \alpha^{OM}_{O:C} \Phi^{bact}}_{bacteria} \\ & - \underbrace{K^{DONre}_{\min} \alpha^{\min}_{O:N} \Phi^{DONre}}_{refractory\ organic\ nitrogen} \\ & - \underbrace{K^{POP}_{dec} \alpha^{\min}_{O:P} \Phi^{POP} - K^{DOPre}_{\min} \alpha^{\min}_{O:P} \Phi^{DOPre} - K^{DOPnr}_{\min} \alpha^{\min}_{O:P} \Phi^{DONnr}}_{organic\ phosphorus} \\ & - \underbrace{K^{oxy}_{nit} \Phi^{NH4}}_{nitrification} + \underbrace{K^{oxy}_{dnit} \Phi^{NO3}}_{denitrification}\end{aligned}$$

Without Bacteria

$$\begin{aligned}
\frac{\partial \Phi^{O}}{\partial t} = {} & \underbrace{\left(\underbrace{\mu^{phy} \alpha_{O:C}^{photo}}_{photosynthesis} + \underbrace{\left(1-\beta_{NH4}^{phy}\right) \mu^{phy} \alpha_{O:N}^{NO3} \alpha_{N:C}^{phy}}_{nitrate\ uptake} + \underbrace{\mu^{phy} \alpha_{O:P}^{IP} \alpha_{P:C}^{phy}}_{IP\, uptake} - \underbrace{r^{phy} \alpha_{O:C}^{plankton}}_{respiration} \right) \Phi^{phy}}_{flagellates} \\
& + \underbrace{\left(\underbrace{\mu^{dia} \alpha_{O:C}^{photo}}_{photosynthesis} + \underbrace{\left(1-\beta_{NH4}^{dia}\right) \mu^{dia} \alpha_{O:N}^{NO3} \alpha_{N:C}^{dia}}_{nitrate\ uptake} + \underbrace{\mu^{dia} \alpha_{O:P}^{IP} \alpha_{P:C}^{dia}}_{IP\, uptake} - \underbrace{r^{dia} \alpha_{O:C}^{plankton}}_{respiration} \right) \Phi^{dia}}_{diatoms} \\
& + \underbrace{r^{cil} \alpha_{O:C}^{cil} \Phi^{cil}}_{microzooplankton} + \underbrace{r^{zoo} \alpha_{O:C}^{zoo} \Phi^{zoo}}_{mesozooplankton} \\
& - \underbrace{K_{dec}^{PON} \alpha_{O:N}^{\min} \Phi_{PON} - K_{\min}^{DONre} \alpha_{O:N}^{\min} \Phi_{DONre} - K_{\min}^{DONnr} \alpha_{O:N}^{\min} \Phi_{DONnr}}_{organic\ nitrogen} \\
& - \underbrace{K_{dec}^{POP} \alpha_{O:P}^{\min} \Phi_{POP} - K_{\min}^{DOPre} \alpha_{O:P}^{\min} \Phi_{DOPre} - K_{\min}^{DOPnr} \alpha_{O:P}^{\min} \Phi_{DOPnr}}_{organic\ nitrogen} \\
& - \underbrace{K_{nit}^{oxy} \Phi^{NH4}}_{nitrification} + \underbrace{K_{dnit}^{oxy} \Phi^{NO3}}_{denitrification}
\end{aligned}$$

Table 23. Oxygen.

Symbol	*Description*	*Unit*	*Formulation*
$\alpha_{O:N}^{\min}$	Oxygen Consumption in Nitrogen Mineralization	mg O/mg N.d^{-1}	$\alpha_{O:N}^{\min} = \frac{1}{\alpha_{N:C}^{OM}} \times \alpha_{O:C}^{CO2} \times \frac{\Phi^{oxy}}{0.5 + \Phi^{oxy}}$
$\alpha_{O:P}^{\min}$	Oxygen Consumption in Phosphorus Mineralization	mg O/mg P.d^{-}	$\alpha_{O:P}^{\min} = \frac{1}{\alpha_{P:C}^{OM}} \times \alpha_{O:C}^{CO2} \times \frac{\Phi^{oxy}}{0.5 + \Phi^{oxy}}$
K_{nit}^{oxy}	Oxygen Consumption Rate in Nitrification	d^{-1}	$K_{nit}^{oxy} = K_{nit}.\alpha_{O:N}^{NO_3}$
K_{dnit}^{oxy}	Oxygen Consumption Rate in Denitrification	d^{-1}	$K_{dnit}^{oxy} = K_{dnit}.\alpha_{O:N}^{NO_3}$
μ^X	Growth rate	[d^{-1}]	
r^X	Respiration Rate	[d^{-1}]	
$\beta_{NH_4}^X$	Ammonia preference factor	adim	
K_{dnit}	Denitrification Rate	[d^{-1}]	
K_{nit}	Nitrification Rate	[d^{-1}]	
$\alpha_{O:C}^{CO2}$	Oxygen/Carbon Ratio in CO_2	mgO/mgC	
$\alpha_{N:C}^{OM}$	Nitrogen/Carbon ratio in Organic Matter	mgN/mgC	
$\alpha_{P:C}^{OM}$	Phosphorus/Carbon ratio in Organic Matter	mgP/mgC	
$\alpha_{O:N}^{NO3}$	Oxygen/Nitrogen Ratio in Nitrate	mgO$_2$/mgN	
$\alpha_{O:P}^{IP}$	Oxygen/Nitrogen Ratio in Phosphate	mgO$_2$/mgP	
$\alpha_{O:C}^{photo}$	Photosynthesis Oxygen:Carbon ratio	mgO$_2$/mgC	
$\alpha_{O:C}^{X}$	Oxygen/Carbon Ratio in respiration	mgO/mgC	

Table 24. Oxygen Parameters.

Symbol	*Description*	*Unit*	*Value*	*Keyword*
$\alpha_{O:C}^{CO2}$	Oxygen/Carbon Ratio in CO_2	mgO/mgC	32/12	OCRATIO
$\alpha_{O:C}^{photo}$	Photosynthesis Oxygen/Carbon ratio	mgO/mgC	32/12	PHOTOSOC
$\alpha_{O:N}^{NO3}$	Oxygen/Nitrogen Ratio in Nitrate	mgO/mgN	48/14	NITONRAT
$\alpha_{O:P}^{IP}$	Oxygen/Nitrogen Ratio in Phosphate	mgO/mgP	64/31	PHOSOPRAT
$\alpha_{O:C}^{plankton}$	Oxygen/Carbon Ratio in plankton respiration	mgO/mgC	32/12	PLANK_OC_RAT
$\alpha_{O:C}^{zoo}$	Oxygen:Carbon ratioin mesozooplankton respiration	mgO$_2$/mgC	32/12	ZOCRATIO
$\alpha_{O:C}^{cil}$	Oxygen:Carbon ratio in microzooplankton	mgO$_2$/mgC	32/12	CILOCRATIO
$\alpha_{O:C}^{bact}$	Bacteria Oxygen:Carbon Ratio	mgO$_2$/mgC	1.4	BACTRATIOOC
$\alpha_{N:C}^{OM}$	Organic Matter Nitrogen:Carbon Ratio	mgN/mgC	0.18	OMRATIONC
$\alpha_{P:C}^{OM}$	Organic Matter Phosphorus:Carbon Ratio	mgP/mgC	0.024	OMRATIOPC
$\Phi_{\min}^{O_2}$	Minimum oxygen concentration for growth	mgO$_2$/l	10e-5	MINOXYGEN