

1 The biogeochemical model of the Regional Ocean Modeling System (ROMS)

1.1 Model equations

$$\frac{\partial[NO_3]}{\partial t} = -t_{PPmax} \cdot Q_{NP} \cdot [Phyto] + Q_{nitr} \cdot [NH_4] \quad (1)$$

$$\begin{aligned} \frac{\partial[NH_4]}{\partial t} = & -t_{PPmax} \cdot Q_{RP} \cdot [Phyto] - Q_{nitr} \cdot [NH_4] + (t_{Zbmet} + Q_{excr}) \cdot [Zoo] + \\ & t_{SDremin} \cdot [SDetN] + t_{LDremin} \cdot [LDetN] \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{\partial[SDetN]}{\partial t} = & Q_{graze} \cdot (1 - AE_N) \cdot [Zoo] + t_{Pmort} \cdot [Phyto] + t_{Zmort} \cdot [Zoo] - \\ & t_{coag} \cdot ([SDetN] + [Phyto]) \cdot [SDetN] - t_{SDremin} \cdot [SDetN] + L_{vs} \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial[SDetC]}{\partial t} = & (Q_{graze} \cdot (1 - AE_N) \cdot [Zoo] + t_{Pmort} \cdot [Phyto]) \cdot r_{C:N,phyto} + \\ & t_{Zmort} \cdot [Zoo] \cdot r_{C:N,zoo} - t_{coag} \cdot ([SDetN] + [Phyto]) \cdot [SDetC] - \\ & t_{SDremin} \cdot [SDetC] + L_{vs} \end{aligned} \quad (4)$$

$$\begin{aligned} \frac{\partial[LDetN]}{\partial t} = & t_{coag} \cdot ([SDetN] + [Phyto]) \cdot ([SDetN] + [Phyto]) - t_{LDremin} \cdot [LDetN] + \\ & L_{vs} \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{\partial[LDetC]}{\partial t} = & t_{coag} \cdot ([SDetN] + [Phyto]) \cdot ([SDetC] + [Phyto] \cdot r_{C:N,phyto}) - \\ & t_{LDremin} \cdot [LDetC] + L_{vs} \end{aligned} \quad (6)$$

$$\begin{aligned} \frac{\partial[Phyto]}{\partial t} = & t_{PPmax} \cdot (Q_{NP} + Q_{RP}) \cdot [Phyto] - t_{Pmort} \cdot [Phyto] - Q_{coag} \cdot [Phyto] - \\ & Q_{graze} \cdot [Zoo] + L_{vs} \end{aligned} \quad (7)$$

$$\frac{\partial(\theta)}{\partial t} = t_{PPmax} \cdot (Q_{NP} + Q_{RP}) \cdot \left(\frac{\theta_m \cdot V_p \cdot (Q_{NP} + Q_{RP})}{\sqrt{V_p^2 + \alpha^2 \cdot \theta^2 \cdot PAR^2}} - \theta \right) + L_{vs} \quad (8)$$

$$\frac{\partial[Zoo]}{\partial t} = Q_{graze} \cdot AE_N \cdot [Zoo] - t_{Zbmet} \cdot [Zoo] - t_{Zmort} \cdot [Zoo] - Q_{excr} \cdot [Zoo] \quad (9)$$

$$\begin{aligned} \frac{\partial[O_2]}{\partial t} = & t_{PPmax} \cdot (Q_{NP} \cdot r_{O_2:NO_3} + Q_{RP} \cdot r_{O_2:NH_4}) \cdot [Phyto] - 2 \cdot Q_{nitr} \cdot [NH_4] - \\ & (t_{Zbmet} \cdot r_{O_2:NH_4} + Q_{resp}) \cdot [Zoo] - \\ & (t_{SDremin} \cdot [SDetN] + t_{LDremin} \cdot [LDetN]) \cdot r_{O_2:NH_4} + Q_{ge} * (O_{2,sat} - O_2) \end{aligned} \quad (10)$$

$$\begin{aligned} \frac{\partial[TIC]}{\partial t} = & -t_{PPmax} \cdot (Q_{NP} + Q_{RP}) \cdot [Phyto] \cdot r_{C:N,phyto} + \\ & (t_{Zbmet} \cdot r_{C:N,zoo} + Q_{resp}) \cdot [Zoo] + \\ & t_{SDremin} \cdot [SDetC] + t_{LDremin} \cdot [LDetC] + Q_{ge} * (pCO_{2,air} - pCO_2) \end{aligned} \quad (11)$$

$$\frac{\partial[TAlk]}{\partial t} = t_{PPmax} \cdot Q_{NP} \cdot [Phyto] - Q_{nitr} \cdot [NH_4] \quad (12)$$

All source terms ($Q_{...}$) are written such that they are non-dimensional. Please note that the half-saturation constants (K_{NO_3} etc.) are written here in their usual form, i.e. in concentration units, but that variables like `K_NO3` in the code are the reciprocals of the half-saturation constants.

$$Q_{NP} = \frac{([NO_3]/K_{NO_3}) \cdot I_{NH_4}}{1 + [NO_3]/K_{NO_3}} \quad (13)$$

$$Q_{RP} = \frac{[NH_4]/K_{NH_4}}{1 + [NH_4]/K_{NH_4}} \quad (14)$$

$$Q_{nitr} = t_{nitri} \cdot \left(1 - \max \left[0, \frac{PAR - I_{thNH_4}}{D_{p5NH_4} + PAR - 2 \cdot I_{thNH_4}} \right] \right) \quad (15)$$

$$Q_{graze} = t_{Zgraze} \cdot \frac{[Phyto]}{K_P + [Phyto]} \quad (16)$$

$$Q_{resp} = Q_{graze} \cdot r_{C:N,phyto} \cdot (AE_N - GGE_C) \quad (17)$$

$$Q_{excr} = Q_{graze} \cdot r_{C:N,phyto} \cdot AE_N \cdot \left(\frac{1}{r_{C:N,phyto}} - \frac{GGE_C}{AE_N \cdot r_{C:N,zoo}} \right) \quad (18)$$

The gas exchange terms Q_{ge} for O_2 and TIC affect only the top cell and are described in subsection 1.1.1.

The vertical sinking terms L_{vs} are described in subsection 1.1.2.

Variables used in source terms:

$$I_{NH_4} = \frac{1}{1 + [NH_4]/K_{NH_4}} \quad (19)$$

$$t_{PPmax} = \frac{V_p \cdot \alpha \cdot PAR \cdot \theta}{\sqrt{V_p^2 + \alpha^2 \cdot \theta^2 \cdot PAR^2}} \quad (20)$$

$$V_p = 0.59 \cdot 1.066^T \quad (21)$$

These equations represent the following changes from John Moisan's original code:

1. AE_C was replaced by AE_N in the respiration term Q_{resp} . This is necessary to preserve mass balance for the sum of these terms related to grazing: Carbon loss by phytoplankton, carbon gain by zooplankton, carbon loss by zooplankton due to excretion and respiration, carbon gain by small detritus. These terms need to add up to zero. (Usually, same values will be used for AE_N and AE_C , so that the difference in the formulation will not be apparent.)
2. The ratios $r_{O_2:NO_3}$ and $r_{O_2:NH_4}$ are newly introduced and differ in the following ways from John Moisan's formulation of Eq. 10:
 - The zooplankton metabolism term used $r_{C:N,zoo}$ (instead of $r_{O_2:NH_4}$)

- The term for the remineralization of small detritus used the $[SDetC]$ concentration with a factor of 1 (instead of the $[SDetN]$ concentration and a factor of $r_{O_2:NH_4}$)
- The term for the remineralization of large detritus used the $[LDetC]$ concentration with a factor of 1 (instead of the $[LDetN]$ concentration and a factor of $r_{O_2:NH_4}$)

The model allows to switch off the biology routine altogether by not defining BIOLOGY in the include file “cppdefs.h”. The minimum set of equations that is solved if BIOLOGY is defined comprises all N-related components (i.e. nitrate, ammonium, phytoplankton, zooplankton, small and large detritus).

If OXYGEN is defined in “cppdefs.h”, the oxygen equation is solved additionally.

If CARBON is defined in “cppdefs.h”, the equations for all C-related components (i.e. TIC, alkalinity, C content of small and large detritus) are solved additionally. *Note* that this requires defining OXYGEN as well.

Figures 1 and 2 show the fluxes of nitrogen and carbon schematically.

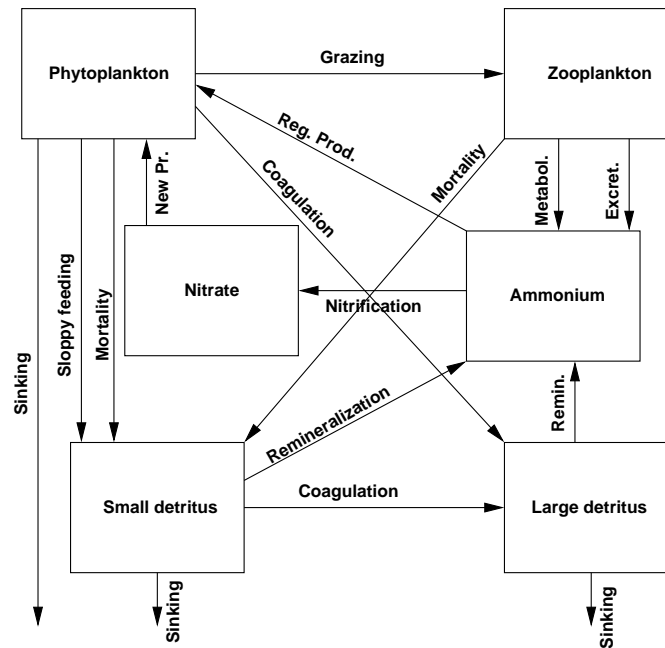


Figure 1: Schematic representation of the fluxes of nitrogen in the model.

1.1.1 Gas exchange

Gas exchange affects the O_2 and CO_2 concentrations in the top cell. It is calculated in a separate step after the biogeochemical reactions were calculated.

Oxygen

The gas exchange rate of oxygen is calculated by

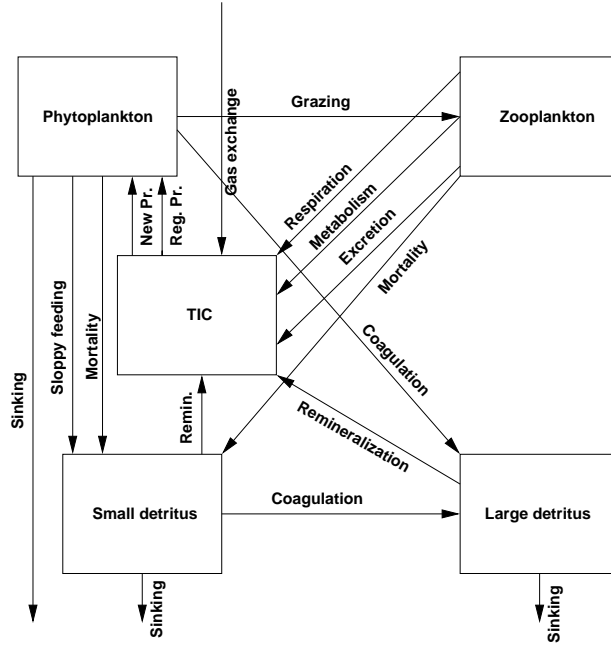


Figure 2: Schematic representation of the fluxes of carbon in the model.

$$Q_{ge,O_2} = \frac{Kv_{O_2}}{\Delta z_N} \quad (22)$$

where Δz_N is the height of the top cell and the gas transfer coefficient is calculated by

$$Kv_{O_2} = 0.31 \cdot u^2 \cdot \sqrt{\frac{660}{Sc}} \quad (23)$$

u is the average wind speed and must be given in [cm/h]. Currently the average wind speed is set to $u = 5$ m/s.

By default, the Schmidt number Sc is calculated after Wanninkhof (1992):

$$Sc = 1953.4 - 128 \cdot T + 3.9918 \cdot T^2 - 0.050091 \cdot T^3 \quad (24)$$

By defining `OCMIP_OXYGEN_SC` in the file “cppdefs.h”, an alternative formula (based on Keeling et al., Global Biogeochem. Cycles, 12, 141-163, 1998) is used:

$$Sc = 1638.0 - 81.83 \cdot T + 1.483 \cdot T^2 - 0.008004 \cdot T^3 \quad (25)$$

The saturation concentration of oxygen is calculated in a separate subroutine by using this equation:

$$O_{2,sat} = \frac{e^A \cdot \rho}{22.9316} \quad (26)$$

with

$$A = -177.7888 + \frac{25559.07}{T_K} + 146.4813 \cdot \ln\left(\frac{T_K}{100}\right) - 22.204 \cdot \frac{T_K}{100} + S \cdot \left(-0.037362 + \frac{T_K}{100} \cdot \left(0.016504 - 0.0020564 \cdot \frac{T_K}{100}\right)\right) \quad (27)$$

ρ is the density, S the salinity. T_K denotes the absolute temperature in °K.

If OCMIP_OXYGENSAT is defined in the file “cppdefs.h”, a different formula (from Garcia and Gordon, Limnology and Oceanography, 1992) is used to compute the saturation concentration of oxygen:

$$O_{2,sat} = \frac{e^A \cdot 1000}{22.9316} \quad (28)$$

with

$$A = 2.00907 + 3.22014 \cdot TS + 4.05010 \cdot TS^2 + 4.94457 \cdot TS^3 - 0.256847 \cdot TS^4 + 3.88767 \cdot TS^5 + S \cdot (-0.00624523 - 0.00737614 \cdot TS - 0.0103410 \cdot TS^2 - 0.00817083 \cdot TS^3) - 4.88682 \cdot 10^{-7} \cdot S^2 \quad (29)$$

where TS is defined by

$$TS = \ln\left(\frac{298.15 - T}{T_K}\right) \quad (30)$$

(T is in °C, T_K in °K.)

Carbon dioxide

The gas exchange rate of CO_2 is calculated by

$$Q_{ge,CO_2} = \frac{\alpha_{CO_2} \cdot K_{vCO_2}}{\Delta z_N} \quad (31)$$

The gas transfer coefficient K_{vCO_2} is calculated as in Eq. (23) with the Schmidt number for CO_2 :

$$Sc = 2073.1 - 125.62 \cdot T + 3.6276 \cdot T^2 - 0.043219 \cdot T^3 \quad (32)$$

Total inorganic carbon (TIC) comprises carbonic acid ($H_2CO_3^*$, bicarbonate (HCO_3^-), and carbonate (CO_3^{2-}). A distinction of these species for the transport calculations is not necessary. A speciation is only required for the top cell so that the partial pressure of carbon dioxide is known and the air-sea gas exchange (Eq. 11) can be calculated.

The partial pressure of CO_2 in the top cell is calculated in a separate subroutine (co2sys) with an iterative procedure. There are two alternative subroutines. By default, John Moisan’s

code (based on Ernie Lewis' BASIC program) is used. The code has various options for choosing the equilibrium constants of the carbon system. We chose the Mehrbach re-fit by Dickson and Millero (Dickson and Millero, Deep-Sea Research, 34(10):1733-1743, 1987; see also Corrigenda, Deep-Sea Research, 36:983, 1989; refit data of Mehrbach et al, Limn Oc, 18(6):897-907, 1973 on the SWS pH scale in mol/kg-SW).

If `OCMIP_CARBON` is defined in "cppdefs.h", a code from the OCMIP project is used instead. The original version of this code was based on the code by Dickson in Version 2 of "Handbook of Methods for the Analysis of the Various Parameters of the Carbon Dioxide System in Seawater", DOE, 1994 (SOP No. 3, p25-26). This subroutine (`co2calc.f`) and the routines for the iterative solution (`drtsafe.f` and `ta_iter_1.f`) as well as the previously mentioned functions for the calculation of the Schmidt number for oxygen (`sco2.f`) and the oxygen saturation concentration (`o2sato.f`) are available from the OCMIP program: <http://www.ipsl.jussieu.fr/OCMIP/phase2/simulations/Abiotic/HOWTO-Abiotic-1.html> Both subroutines (`co2sys` and `co2calc`) calculate the solubility α_{CO_2} as well.

1.1.2 VerticalSinking

Vertical sinking affects phytoplankton, small and large detritus. Chlorophyll is affected indirectly. The effect of vertical sinking is calculated at the end of each biological time step, i.e. after the biogeochemical reactions and after the gas exchange. There are three different sinking velocities, see Table 3.

The algorithm for the vertical sinking is based on the piecewise parabolic method of Colella and Woodward (1984¹).

1.1.3 Photosynthetically active radiation (PAR)

The input file with the forcings contains monthly average values of PAR at the surface. Routine `set_forces` first calculates a linearly interpolated value (between the last and the the next monthly mean) for each time step:

$$SRFLX_{\tau} = \frac{\lambda_l \cdot SRFLX_l + \lambda_n \cdot SRFLX_n}{\rho_0 \cdot C_p} \quad (33)$$

λ_l and λ_n are appropriate fractions for the temporal distance from the current time τ to the mean of the last and the next month. Note that the program uses 12 months of 30 days. ρ_0 is the average density of sea water (set to 1025 kg m^{-3}), and C_p is the specific heat of sea water (set to $3985 \text{ J kg}^{-1} \text{ K}^{-1}$).

A diurnal cycle for the insolation is superimposed:

¹P. Colella and P. R. Woodward. The piecewise parabolic method (PPM) for gas-dynamical simulations. Journal of Computational Physics, 54:174-201, 1984.

$$SRFLX = SRFLX_\tau \cdot \pi \cdot \frac{\cos(2 \cdot \pi \cdot f_d) \cdot F_1 + F_2}{\sin(\arccos(-\tan \phi \cdot \tan D)) \cdot F_1 + \arccos(-\tan \phi \cdot \tan D) \cdot F_2} \quad (34)$$

with

f_d as the fraction of the day since noon at the current time step,

$$D = -0.406 \cdot \cos(f_a \cdot \pi/180) \quad (35)$$

(f_a is the fraction of the year since January 1 at the current time step),

$$F_1 = \cos D \cdot \cos(\phi \cdot \pi/180) \quad (36)$$

$$F_2 = \sin D \cdot \sin(\phi \cdot \pi/180) \quad (37)$$

(ϕ is the latitude in degrees).

Finally, if the calculated surface radiation is negative, 0 is used instead:

$$SRFLX = \max[0, SRFLX] \quad (38)$$

If the surface radiation is 0, no production of phytoplankton will take place during this time step, i.e. $Q_{NP} = Q_{RP} = 0$ instead of Equations (13) and (14).

Within the biology routine, the PAR for each cell is successively calculated. The loop starts at the top cell. For each cell, the PAR in the center of the cell is calculated with

$$PAR_k = PAR_{k+1} \cdot e^{-0.5 \cdot (k_{water} + k_{Chla}) \cdot [Chla]_k \cdot \Delta z_k} \quad (39)$$

k is the cell index (from 1 at the bottom to N at the top). PAR_{N+1} is the surface PAR, k_{water} and k_{Chla} are attenuation coefficients for water and chlorophyll, $[Chla]$ is the chlorophyll concentration in this cell, and Δz_k is the height of the cell.

After the calculation of the new and regenerated production, PAR_k is multiplied again with the same attenuation factor.

This procedure is repeated for each cell. Since the chlorophyll concentrations are different for all cells, the attenuation coefficients will be different as well.

1.2 Initial conditions

Tables 1 and 2 list the initial conditions for all components. The depth dependent initial conditions (IC) are calculated after the following formula:

$$IC = C_1 + C_2 \cdot z + C_3 * e^{z/C_4} + C_5 * e^{z/C_6} \quad (40)$$

Since C_1 and C_2 are negative for oxygen, the term $C_1 + C_2 \cdot z$ will be replaced with 0 if it is negative.

| Component | C_1 | C_2 | C_3 | C_4 | C_5 | C_6 | Unit |
|-------------|--------|-----------------------|-------|-------|-------|-------|---------------------|
| Temperature | 5 | $1.475 \cdot 10^{-3}$ | 5.65 | 100 | 5 | 500 | [C] |
| Salinity | 34.28 | $-1.75 \cdot 10^{-4}$ | -0.8 | 200 | -0.2 | 400 | [PSU] |
| NO_3 | 1.48 | $3.2 \cdot 10^{-3}$ | -48 | 250 | 0 | - | [$mmolNm^{-3}$] |
| O_2 | -0.767 | $-1.23 \cdot 10^{-3}$ | 5 | 230 | 1 | 220 | [$mmolO_2m^{-3}$] |

Table 1: Initial conditions of those components with depth dependence.

| Component | Value | Unit |
|------------------|---|--------------------|
| NH_4 | 0.1 | [$mmolNm^{-3}$] |
| Chlorophyll | 0.1 | [$mgChlam^{-3}$] |
| Phytoplankton | $\frac{0.1}{r_{C:N,phyto} \cdot 12 \cdot \theta_m}$ | [$mmolNm^{-3}$] |
| Zooplankton | 0.06 | [$mmolNm^{-3}$] |
| Small detritus N | 0.04 | [$mmolNm^{-3}$] |
| Large detritus N | 0.02 | [$mmolNm^{-3}$] |
| TIC | 1988.5 | [$mmolCm^{-3}$] |
| Alkalinity | 2214.0 | [$mmolCm^{-3}$] |
| Small detritus C | 0.265 | [$mmolCm^{-3}$] |
| Large detritus C | 0.1325 | [$mmolCm^{-3}$] |

Table 2: Initial conditions of those components without depth dependence. $r_{C:N,phyto}$ and θ_m are described in subsection 1.3.

1.3 Parameters for the biogeochemical model

The parameters listed in Table 3 are from John Moisan's code:

| Variable | Description | Value | Unit |
|-----------------|---|-----------|------------------------------|
| k_{water} | light attenuation due to sea water | 0.04 | $[m^{-1}]$ |
| k_{Chla} | light attenuation by chlorophyll | 0.025 | $[(m^2mgChla)^{-1}]$ |
| α | initial slope of the P-I curve | 4 | $[mgC(mgChlaWm^{-2}d)^{-1}]$ |
| $r_{C:N,phyto}$ | C:N ratio for phytoplankton | 6.625 | $[molC(molN)^{-1}]$ |
| $r_{C:N,zoo}$ | C:N ratio for zooplankton | 5 | $[molC(molN)^{-1}]$ |
| θ_m | maximum cellular chlorophyll:C Ratio | 0.053 | $[mgChla(mgC)^{-1}]$ |
| K_{NO3} | half-saturation for phyto. NO3 uptake | 1.0 / 0.5 | $[mmolNm^{-3}]$ |
| K_{NH4} | half-saturation for phyto. NH4 uptake | 1.0 / 0.5 | $[mmolNm^{-3}]$ |
| t_{Pmort} | Phyt mortality to SDetN rate | 0.07 | $[d^{-1}]$ |
| t_{Zgraze} | Zoo-specific maximum grazing rate | 0.75 | $[d^{-1}]$ |
| AE_N | Zoo assimilation efficiency for N | 0.75 | $[-]$ |
| AE_C | Zoo assimilation efficiency for C | 0.75 | $[-]$ |
| GGE_C | Zoo gross growth efficiency for C | 0.65 | $[-]$ |
| K_P | Zoo half-saturation const. for ingestion | 1 | $[mmolNm^{-3}]$ |
| t_{Zbmet} | Zoo specific excretion rate | 0.1 | $[d^{-1}]$ |
| t_{Zmort} | Zoo quadratic mortality to Detritus | 0.1 | $[d^{-1}(mmolNm^{-3})^{-1}]$ |
| $t_{SDremin}$ | Small Detrital breakdown to NH4 rate | 0.01 | $[d^{-1}]$ |
| t_{coag} | Specific (per unit Phyt+SDetN) aggregation rate | 0.01 | $[(mmolNm^{-3})^{-1}d^{-1}]$ |
| $t_{LDremin}$ | Specific rate of LDetN recycling to NH4 | 0.01 | $[d^{-1}]$ |
| w_{SD} | Sinking velocity for SDetN | 0.1 | $[md^{-1}]$ |
| w_{LD} | Sinking velocity for LDetN | 10 | $[md^{-1}]$ |
| w_{Phyto} | Sinking velocity for Phyt | 0.1 | $[md^{-1}]$ |
| t_{nitri} | Nitrification of NH4 to NO3 | 0.1 | $[d^{-1}]$ |
| I_{thNH4} | threshold PAR for nitrification inhib. | 0.0095 | $[Wm^{-2}]$ |
| D_{p5NH4} | 0.5 dose for nitrification inhibition | 0.036 | $[Wm^{-2}]$ |

Table 3: John Moisan's parameters for the biogeochemical model

With the parameters listed above, the zooplankton excretion term becomes negative:

$$\left(\frac{1}{r_{C:N,phyto}} - \frac{GGE_C}{AE_N \cdot r_{C:N,zoo}} \right) = \left(\frac{1}{6.625} - \frac{0.65}{0.75 \cdot 5} \right) = -0.0224 \quad (41)$$

This leads to an unrealistic behavior: Zooplankton ingests ammonium and carbon dioxide. To remedy this, CN_Z was changed to 6.625 so that this term becomes positive.

Table 4 shows the parameters that were taken from the ROMS3D model without carbon (only the differences are shown).

| Variable | Description | Value | Unit |
|---------------|---|------------|------------------------------|
| k_{Chla} | light attenuation by chlorophyll | 0.024 | $[(m^2mgChla)^{-1}]$ |
| α | initial slope of the P-I curve | 1 | $[mgC(mgChlaWm^{-2}d)^{-1}]$ |
| θ_m | max. cellular chlorophyll to C Ratio | 0.053478 | $[mgChla(mgC)^{-1}]$ |
| K_{NO_3} | half-sat. for phyto. NO_3 uptake | 1.0 / 0.75 | $[mmolNm^{-3}]$ |
| t_{Pmort} | Phyt mortality to SDetN rate | 0.072 | $[d^{-1}]$ |
| t_{Zgraze} | Zoo-specific maximum grazing rate | 0.6 | $[d^{-1}]$ |
| K_P | Zoo half-saturation for ingestion | 3 | $[mmolNm^{-3}]$ |
| t_{Zmort} | Zoo quadratic mortality to Detritus | 0.025 | $[d^{-1}(mmolNm^{-3})^{-1}]$ |
| $t_{SDremin}$ | Small Detrital breakdown to NH_4 rate | 0.03 | $[d^{-1}]$ |
| t_{coag} | Specific (per unit Phyt+SDetN) aggregation rate | 0.005 | $[(mmolNm^{-3})^{-1}d^{-1}]$ |
| w_{SD} | Sinking velocity for SDetN | 1.0 | $[md^{-1}]$ |
| w_{Phyto} | Sinking velocity for Phyt | 0.5 | $[md^{-1}]$ |
| t_{nitri} | Nitrification of NH_4 to NO_3 | 0.05 | $[d^{-1}]$ |

Table 4: Revised parameters for the biogeochemical model (only those parameters that differ from John Moisan's are listed)