

Regulated Ecosystem Model with two phytoplankton classes REcoM-2

The Regulated Ecosystem Model, version 2, (REcoM-2) describes the biogeochemistry in the ocean with a relatively simple ecological model including two phytoplankton functional types (diatoms and non-diatoms), one zooplankton and one detritus compartment, and inorganic and organic forms of the main nutrients (Figure 1). Some emphasis is put on phytoplankton physiology, which is described in a way that allows for changes in cellular stoichiometry (N:C:Chl:Si for diatoms and N:C:Chl for non-diatoms, respectively). All in all, the model solves mass balance equations for 21 tracers, which are described by equations of the type

$$\frac{\partial A}{\partial t} = -(\mathbf{U} + \mathbf{w}) \cdot \nabla A + \nabla \cdot (\kappa \nabla A) + S(A) \quad (1)$$

where A is the volumetric concentration of a tracer, \mathbf{U} is the three-dimensional advection velocity and κ is the diffusivity, both supplied by the physical circulation model. The sinking velocity of particles $\mathbf{w} = (0, 0, w)$ increases linearly with depth for detritus and has a constant value for phytoplankton and diatoms. $S(A)$ are the biogeochemical sources or sinks of the tracer A and are described in detail, for any of the tracers, in the following.

1 Carbonate chemistry

Dissolved inorganic carbon (DIC) The balance of DIC is affected by a number of processes; sources for DIC are respiration by nanophytoplankton (*phy*), diatoms (*dia*) and heterotrophs (*het*), remineralization of dissolved organic carbon (DOC) and dissolution of calcitic detritus (*det*). Sinks are carbon fixation by primary producers and the formation of calcium carbonate (Z). In addition, sea-air flux of CO_2 (F_C) leads to an exchange of carbon with the atmosphere, depending on the partial pressure difference of CO_2 between ocean and atmosphere. This exchange is treated separately as boundary condition in

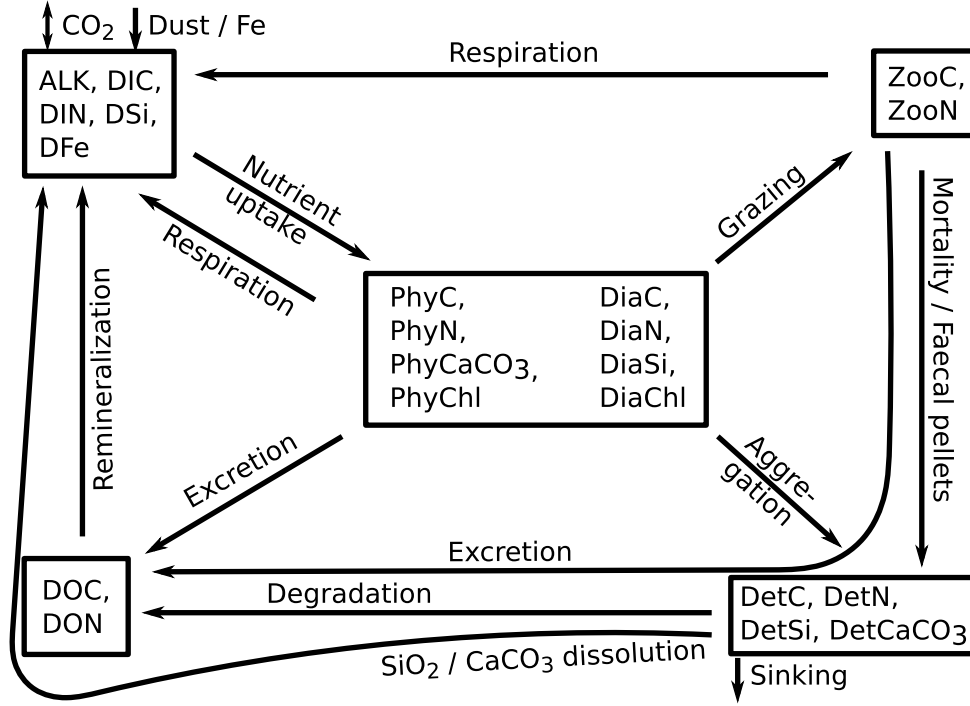


Figure 1: Schematic sketch of the ecosystem model REcoM-2. The 21 tracers can be grouped (indicated by boxes) into dissolved nutrients and carbonate system parameters (upper left), phytoplankton (center), zooplankton (upper right), detritus (lower right), and dissolved organic material (lower left). Source and sink terms are depicted by arrows, short arrows denote exchange with atmosphere and sediments. Not shown: sediments also release alkalinity, inorganic nutrients and dissolved organic matter.

section 7.

$$\begin{aligned}
 S(\text{DIC}) = & (r_{phy} - p_{phy}) \cdot C_{phy} + (r_{dia} - p_{dia}) \cdot C_{dia} \\
 & + r_{het} \cdot C_{het} + \rho_{\text{DOC}} \cdot f_T \cdot \text{DOC} \\
 & + \lambda \cdot \text{CaCO}_3_{det} - Z
 \end{aligned} \tag{2}$$

See section 3 for details on photosynthesis (p) and phytoplankton respiration (r) rates. C_{phy} , C_{dia} and C_{het} refer to carbon biomass of nanophytoplankton, diatoms and heterotrophs, respectively. See section 4 for the formulation of the heterotrophic respiration rate (r_{het}) and section 6 for the DOC remineralization term ($\rho_{\text{DOC}} \cdot f_T \cdot \text{DOC}$). The calcite dissolution rate (λ) is defined in Eq. 50 and the calcification flux (Z) in Eq. 37.

Total Alkalinity (TA) The alkalinity balance is determined by processes co-occurring with primary production and remineralization of dissolved organic matter. Alkalinity is increased by nitrogen assimilation and reduced by remineralization of dissolved organic nitrogen (DON). The contribution of phosphate assimilation and remineralization to alkalinity is taken into account by assuming a constant Redfield ratio (16:1) relating DON to dissolved organic phosphorous (DOP). Further, alkalinity is reduced during calcification

and increased during dissolution of CaCO_3 .

$$S(\text{TA}) = \left(1 + \frac{1}{16}\right) \cdot (a_{phy}^N \cdot C_{phy} + a_{dia}^N \cdot C_{dia} - \rho_{\text{DON}} \cdot f_T \cdot \text{DON}) + 2 (\lambda \cdot \text{CaCO}_{3det} - Z) \quad (3)$$

See section 3 for details on the nitrogen assimilation rates (a_{phy}^N and a_{dia}^N), and section 6 for the DON remineralization term ($\rho_{\text{DON}} \cdot f_T \cdot \text{DON}$). The calcification flux (Z) is defined in Eq. 37 and the dissolution rate of CaCO_3 (λ) in Eq. 50.

2 Nutrients

Dissolved Inorganic Nitrogen (DIN) DIN in the model is the sum of the concentrations of nitrate, nitrite and ammonia. The DIN pool in the water column is reduced when nanophytoplankton and diatoms take up DIN and build it into their cells. Remineralization of DON is a source for DIN.

$$S(\text{DIN}) = -a_{phy}^N \cdot C_{phy} - a_{dia}^N \cdot C_{dia} + \rho_{\text{DON}} \cdot f_T \cdot \text{DON} \quad (4)$$

See section 3 for details on the nitrogen assimilation rates (a_{phy}^N and a_{dia}^N) and section 6 for an explanation of the temperature dependent DON remineralization.

Dissolved Silicate (DSi) Silicon cycles between dissolved silicic acid, or silicate DSi, and the biogenic silica in diatoms Si_{dia} and detritus (Si_{det}). Silicate in the water column is drawn down by silicate assimilation and returned via degradation of detritus silica.

$$S(\text{DSi}) = -a_{dia}^{Si} \cdot C_{dia} + \rho_{Si}^T \cdot \text{Si}_{det} \quad (5)$$

See section 3 for the definition of the silicate assimilation rate (a_{dia}^{Si}). The temperature-dependent dissolution rate of silica ρ_{Si}^T is defined in Eq. 48.

Dissolved Iron (DFe) Dissolved iron is treated in the model like in *Parekh et al.* (2004), i.e. it is considered the sum of the concentrations of “free” (i.e. inorganically bound) iron Fe' and organically complexed iron FeL . The partitioning into these two types is assumed to be in chemical equilibrium always, and is calculated at each timestep by solving the law of mass action for a reaction $\text{Fe}' + \text{L} \rightleftharpoons \text{FeL}$ with L being the free ligand concentration, assuming both a constant conditional stability constant $K_{FeL} = \text{Fe}' \cdot \text{L} / \text{FeL}$ and total ligand concentration $\text{L}_T = \text{L} + \text{FeL}$.

Dissolved iron is drawn down in concert with photosynthesis by nanophytoplankton and diatoms and by scavenging of free Fe. For the scavenging we assume that it is proportional to detritus carbon, which we take as a proxy for the mass of sinking particles. Iron is released during respiration of phytoplankton and heterotrophs, remineralization of DOC, and excretion of heterotrophs. Degraded iron is directly remineralized to dissolved iron.

For all these processes, we assume a constant iron:carbon ratio (q^{Fe}).

$$S(\text{DFe}) = q^{Fe} \cdot ((r_{phy} - p_{phy}) \cdot C_{phy} + (r_{dia} - p_{dia}) \cdot C_{dia} + (r_{het} + \epsilon_{het}^C) \cdot C_{het} + \rho_{\text{DOC}} \cdot f_T \cdot \text{DOC}) - \kappa_{Fe}^{scav} \cdot C_{det} \cdot \text{Fe}' \quad (6)$$

See section 3 for an explanation of phytoplankton photosynthesis (p) and respiration (r) rates and section 4 for the heterotrophic respiration (r_{het}) and carbon excretion rate (ϵ_{het}^C). The DOC remineralization term is described in section 6.

3 Phytoplankton

The equations for the two classes of phytoplankton are based on a slightly modified version of the physiological model by *Geider et al.* (1998) that has been amended by non-physiological mortality terms, namely grazing and aggregation loss to sinking detritus (*Schartau et al.*, 2007). For diatoms an additional equation describing the formation and loss of biogenic silica in the diatom frustule has been added by *Hohn* (2009).

All physiological rates, such as the photosynthesis and assimilation rates depend on cell quota in the formulation of *Geider et al.* (1998). These are defined as the intracellular ratios of N:C, Chl:C and Si:C:

$$q = \frac{\text{N}}{\text{C}}; \quad q^{Si} = \frac{\text{Si}}{\text{C}}; \quad q^{Chl} = \frac{\text{Chl}}{\text{C}}; \quad (7)$$

In addition quota are used to convert biomass in terms of carbon or nitrogen to Fe, Si, Chl or CaCO_3 :

$$q^{Fe} = \frac{\text{Fe}}{\text{C}} \quad q^{Si:N} = \frac{\text{Si}}{\text{N}}; \quad q^{Chl:N} = \frac{\text{Chl}}{\text{N}}; \quad q^{CaCO_3:N} = \frac{\text{CaCO}_3}{\text{N}}; \quad (8)$$

Nitrogen pool (N_{phy} and N_{dia}) The nitrogen pool in nanophytoplankton and diatoms is built up by the assimilation of nitrogen, which is assumed proportional to carbon biomass. Metabolic processes lead to excretion of biogenic nitrogen to the DON pool. At high intracellular N:C ratios (q), we assume that this excretion is downregulated. Aggregation and grazing by zooplankton transfer nitrogen to the detritus and zooplankton pools:

$$S(N_{phy}) = a_{phy}^N \cdot C_{phy} - (\epsilon_{phy}^N \cdot f_{phy}^{lim} + g) \cdot N_{phy} - G_{phy} \quad (9)$$

$$S(N_{dia}) = a_{dia}^N \cdot C_{dia} - (\epsilon_{dia}^N \cdot f_{dia}^{lim} + g) \cdot N_{dia} - G_{dia} \quad (10)$$

See section 4 for a description of the grazing formulation (G_{phy} and G_{dia}). The carbon-specific nitrogen uptake rate depends on the maximum photosynthetic rate (p_{phy}^{max} and p_{dia}^{max} , Eq. 21, Eq. 22), which is converted to nitrogen units by multiplication with an optimal N:C uptake ratio (σ_{phy}^N and σ_{dia}^N). Nitrogen uptake rates are further affected by the intracellular nitrogen status q through f_{phy}^{lim} and f_{dia}^{lim} , (see Eq. 14 and Eq. 15) and by extracellular nitrogen concentrations through an assumed Michaelis-Menten uptake

kinetics.

$$a_{phy}^N = p_{phy}^{max} \cdot \sigma_{phy}^N \cdot f_{phy}^{lim} \cdot \left(\frac{DIN}{DIN + K_{phy}^N} \right) \quad (11)$$

$$a_{dia}^N = p_{dia}^{max} \cdot \sigma_{dia}^N \cdot f_{dia}^{lim} \cdot \left(\frac{DIN}{DIN + K_{dia}^N} \right) \quad (12)$$

As in the model by *Geider et al.* (1998), both the limiting functions (f_{phy}^{lim} and f_{dia}^{lim}) for nitrogen assimilation and excretion rates ϵ_{phy}^N and ϵ_{dia}^N are treated as functions of the intracellular nitrogen status (i.e., N:C ratios q).

The mathematical form of how this regulation is described has no specific basis in physiology. In a slight change against the model by *Geider et al.* (1998) we use a uniform general limitation function for all types of quota regulation, which is given by

$$f(q_1, q_2, \theta) = \begin{cases} 1 - \exp(-4\theta(q_1 - q_2)^2) & \text{if } q_1 < q_2 \\ 0 & \text{if } q_1 \geq q_2 \end{cases} \quad (13)$$

This regulation function is close to one for $q_1 \ll q_2$, but tends to zero for $q_1 \rightarrow q_2$; θ is a dimensionless constant that determines how close q_1 and q_2 have to be for a significant decrease of f .

With this function we can now formulate the functions limiting nitrogen assimilation as

$$f_{phy}^{lim} = f(q_{phy}, q_{phy\ max}, \theta_{max}) \quad (14)$$

and

$$f_{dia}^{lim} = f(q_{dia}, q_{dia\ max}, \theta_{max}) \quad (15)$$

The aggregation rate (g) is assumed to be proportional to the abundance of phytoplankton and detritus:

$$g = \phi_{phy} \cdot N_{phy} + \phi_{phy} \cdot N_{dia} + \phi_{det} \cdot N_{det} \quad (16)$$

The constants ϕ_{phy} and ϕ_{det} are specific aggregation rates (i.e. per unit biomass per unit time) of phytoplankton and detritus, respectively, which reflect the roles of phytoplankton and detritus in the aggregation processes.

Carbon pool (C_{phy} and C_{dia}) The carbon biomass of nanophytoplankton and diatoms increases as a result of carbon assimilation during photosynthesis. Loss terms include excretion (ϵ) of DOC, which is limited by the availability of proteins as in the nitrogen pool, respiration (r), aggregation (g), and grazing (G).

$$S(C_{phy}) = (p_{phy} - \epsilon_{phy}^C \cdot f_{phy}^{lim} - r_{phy} - g) \cdot C_{phy} - \frac{1}{q_{phy}} \cdot G_{phy} \quad (17)$$

$$S(C_{dia}) = (p_{dia} - \epsilon_{dia}^C \cdot f_{dia}^{lim} - r_{dia} - g) \cdot C_{dia} - \frac{1}{q_{dia}} \cdot G_{dia} \quad (18)$$

Grazing (G) is calculated on the basis of nitrogen biomass and converted to carbon using the intracellular N:C ratio (q_{phy} , q_{dia}). See section 4 for the grazing formulation, Eq. 16 for the aggregation rate g and Eq. 14 and Eq. 15 for the limiter functions for the carbon excretion rates ϵ_{phy}^C and ϵ_{dia}^C .

The photosynthetic rate (p_{phy} and p_{dia}) is a saturating function of the photosynthetically active radiation (PAR). The saturating light level is affected by the internal chlorophyll status of the cells. The initial slope of the photosynthesis-irradiance-curve is obtained by multiplication of the light harvesting efficiency per chlorophyll (α) with the intracellular chlorophyll to carbon ratio (q^{Chl}).

$$p_{phy} = p_{phy}^{max} \cdot (1 - \exp(-\alpha_{phy} \cdot q_{phy}^{Chl} \cdot PAR/p_{phy}^{max})) \quad (19)$$

$$p_{dia} = p_{dia}^{max} \cdot (1 - \exp(-\alpha_{dia} \cdot q_{dia}^{Chl} \cdot PAR/p_{dia}^{max})) \quad (20)$$

The apparent maximum photosynthetic rates (p_{phy}^{max} and p_{dia}^{max}) are based on the true constant maximum photosynthetic rates μ_{phy}^{max} and μ_{dia}^{max} , but vary with the metabolic state of the cell, external dissolved Fe concentration and temperature:

$$p_{phy}^{max} = \mu_{phy}^{max} \cdot f_T \cdot \min(l_{phy}^{Fe}, l_{min}^N) \quad (21)$$

$$p_{dia}^{max} = \mu_{dia}^{max} \cdot f_T \cdot \min(l_{dia}^{Fe}, l_{min}^N, l_{min}^{Si}) \quad (22)$$

Growth, as most metabolic processes is faster at higher temperatures. We parameterize this by multiplication of the maximum growth rate with an Arrhenius function f_T of the local temperature (T in Kelvin), relative to a reference temperature T_{ref} :

$$f_T = \exp\left(-4500 \cdot \left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \quad (23)$$

Growth-limitation by iron is represented by a Michaelis-Menten term

$$l_{phy}^{Fe} = \frac{DFe}{DFe + K_{phy}^{Fe}}, \quad l_{dia}^{Fe} = \frac{DFe}{DFe + K_{dia}^{Fe}} \quad (24)$$

while nitrogen limitation of nanophytoplankton and diatoms is modeled as a function of the intracellular nitrogen quota q , with growth ceasing completely at a minimum quota q_{min}

$$l_{min}^N = f(q_{min}, q, \theta_{min}) \quad (25)$$

For diatoms, photosynthesis is also downregulated if the cellular Si:C ratio (q^{Si}) approaches a minimum ratio q_{min}^{Si}

$$l_{min}^{Si} = f(q_{min}^{Si}, q^{Si}, \theta_{min}^{Si}) \quad (26)$$

θ_{min} and θ_{min}^{Si} are dimensionless constants which regulate the steepness of the quota-growth

relation (see Eq. 13).

The respiration rates (r_{phy} and r_{dia}) represent the sum of maintenance metabolic losses and the costs of biosynthesis, which are proportional to the rates of nutrient assimilation:

$$r_{phy} = \eta_{phy} \cdot f_{phy}^{lim} + \zeta^N \cdot a_{phy}^N \quad (27)$$

$$r_{dia} = \eta_{dia} \cdot f_{dia}^{lim} + \zeta^N \cdot a_{dia}^N + \zeta^{Si} \cdot a_{dia}^{Si} \quad (28)$$

See Eq. 14 and Eq. 15 for the limiting functions f^{lim} of the constant maintenance respiration rates η_{phy} and η_{dia} . ζ denotes the cost for nutrient uptake and synthesis of cellular machinery in mol carbon per mol of nitrogen and silicon, respectively. See Eq. 11, Eq. 12 and Eq. 34 for details of the nutrient assimilation rates.

Chlorophyll (Chl_{phy} and Chl_{dia}) Chlorophyll synthesis is modeled as a function of irradiance and of nitrogen assimilation. Chlorophyll is degraded with a fixed rate (d^{Chl}), and lost via aggregation (g) and grazing (G).

$$S(Chl_{phy}) = s_{phy} \cdot C_{phy} - (d_{phy}^{Chl} + g) \cdot Chl_{phy} - G_{phy} \cdot q_{phy}^{Chl:N} \quad (29)$$

$$S(Chl_{dia}) = s_{dia} \cdot C_{dia} - (d_{dia}^{Chl} + g) \cdot Chl_{dia} - G_{dia} \cdot q_{dia}^{Chl:N} \quad (30)$$

See Eq. 16 for the aggregation rate (g). The grazing flux G in terms of nitrogen biomass is converted to chlorophyll using the intracellular Chl:N ratio ($q^{Chl:N}$).

The chlorophyll synthesis rate s is assumed to be proportional to the nitrogen assimilation rate, as nitrogen is required for the synthesis of chlorophyll, for light harvesting and in the photosynthetic apparatus:

$$s_{phy} = a_{phy}^N \cdot q_{phy}^{Chl:N} \cdot \min \left(1, \frac{p_{phy}}{\alpha_{phy} \cdot q_{phy}^{Chl} \cdot PAR} \right) \quad (31)$$

$$s_{dia} = a_{dia}^N \cdot q_{dia}^{Chl:N} \cdot \min \left(1, \frac{p_{dia}}{\alpha_{dia} \cdot q_{dia}^{Chl} \cdot PAR} \right) \quad (32)$$

The carbon-specific nitrogen assimilation rates (a_{phy}^N and a_{dia}^N , see Eq. 11 and 12) are converted to chlorophyll units by multiplication with a constant maximum Chl:N ratio ($q_{phy}^{Chl:N}$ and $q_{dia}^{Chl:N}$). The regulation term $\min(1, p_{phy}/(\alpha_{phy} \cdot q_{phy}^{Chl} \cdot PAR))$ reflects the ratio of energy assimilated to energy absorbed; it increases under low irradiance and declines as photosynthesis becomes light saturated and/or nutrient limited. See Eq. 19 and Eq. 20 for the descriptions of photosynthesis rate p_{phy} and p_{dia} .

Diatom silica pool (Si_{dia}) The silica frustule of diatoms is built through silicate assimilation. Any term that leads to a decrease in N-biomass through excretion, grazing or aggregation, on the other hand, leads to a corresponding transfer of silica to the detritus silica pool.

$$S(Si_{dia}) = a_{dia}^{Si} \cdot C_{dia} - (\epsilon_{dia}^N \cdot f_{dia}^{lim} + g) \cdot Si_{dia} - G_{dia} \cdot q_{dia}^{Si:N} \quad (33)$$

The intracellular Si:N ratio $q_{dia}^{Si:N}$ is used to convert the grazing flux G_{dia} (Eq. 42) to the corresponding loss in biogenic silica. See Eq. 16 for the aggregation rate (g) and Eq. 15 for the function (f_{dia}^{lim}) limiting the excretion rate (ϵ_{dia}^N).

Silicate assimilation is treated as a relatively independent metabolic pathway. Here, silicon uptake is formulated as Michaelis-Menten kinetics. The maximum silicon uptake rate is calculated from the constant maximum photosynthesis rate (μ_{dia}^{max}) by multiplying it with a constant maximum Si:C uptake ratio (σ_{dia}^{Si}), and is regulated by intracellular N:C and Si:C ratios (f_{dia}^{lim} and f_{dia}^{Si}) and temperature (f_T). Silicon uptake is reduced when cellular Si:C ratios (q^{Si}) approach the maximum Si:C ratio (q_{max}^{Si}). θ_{max}^{Si} is a dimensionless constant which is used to regulate the slope.

$$a_{dia}^{Si} = \mu_{dia}^{max} \cdot \sigma_{dia}^{Si} \cdot f_T \cdot f_{dia}^{lim} \cdot f_{dia}^{Si} \cdot \left(\frac{DSi}{DSi + K_{dia}^{Si}} \right) \quad (34)$$

$$f_{dia}^{Si} = f(q^{Si}, q_{max}^{Si}, \theta_{max}^{Si}) \quad (35)$$

Iron limitation shows an indirect influence on silicate assimilation via variable intracellular Si:N:C ratios by affecting the assimilation of nitrogen and carbon. See Eq. 15 for the description of the limiting function f_{dia}^{lim} and Eq. 23 for the definition of the temperature dependence f_T .

Calcite pool ($CaCO_{3phy}$) In REcoM-2, the formation of biogenic calcium carbonate is limited to phytoplankton (i.e. coccolithophorids) which are assumed to form a constant fraction of the non-diatom phytoplankton. Formation of $CaCO_3$ by heterotrophs, such as foraminifera or pteropods is neglected. Biogenic $CaCO_3$ is transformed into detritus $CaCO_3$ along with organic matter excretion, respiration, aggregation and grazing.

$$S(CaCO_{3phy}) = Z - (\epsilon_{phy}^C \cdot f_{phy}^{lim} + r_{phy} + g) \cdot CaCO_{3phy} - G_{phy} \cdot q_{phy}^{CaCO_3:N} \quad (36)$$

Calcification (Z) is proportional to gross carbon fixation by nanophytoplankton:

$$Z = \psi \cdot p_{phy} \cdot C_{phy} \quad (37)$$

ψ is the calcite production ratio that incorporates the ratio of calcium carbonate producers to total nanophytoplankton and the $CaCO_3$:POC ratio in coccolithophorids. The latter is assumed to be 1.

See Eq. 14 for the function f_{phy}^{lim} limiting the excretion rate ϵ_{phy}^C . Nanophytoplankton photosynthesis (p_{phy}) respiration (r_{phy}) and aggregation (g) rates are defined in Eq. 19, Eq. 27 and Eq. 16, respectively. The grazing flux G_{phy} (Eq. 41) is calculated in units of nitrogen biomass and converted to $CaCO_3$ using the intracellular $CaCO_3$:N ratio ($q_{phy}^{CaCO_3:N}$).

4 Heterotrophs

Nitrogen pool (N_{het}) Heterotrophic zooplankton increase their nitrogen pool via grazing, and loose nitrogen through excretion of DON and a quadratic mortality term:

$$S(N_{het}) = G \cdot \gamma - m_{het} \cdot N_{het}^2 - \epsilon_{het}^N \cdot N_{het} \quad (38)$$

A quadratic term is used for the mortality of heterotrophs ($m_{het} \cdot N_{het}^2$), and the excretion rate ϵ_{het}^N transfers heterotrophic nitrogen directly to the DON pool. The grazing efficiency γ determines how much of the grazed phytoplankton is built into heterotrophic biomass. We assume that sloppy feeding and the formation of feces transfer the remainder of the grazed phytoplankton directly to detritus.

The grazing on nanophytoplankton and diatoms is defined as:

$$G = \xi \cdot \frac{(N_{phy} + N'_{dia})^2}{\varphi_1 + (N_{phy} + N'_{dia})^2} \cdot f_T \cdot N_{het} \quad (39)$$

The grazing rate is calculated from a constant maximum grazing rate (ξ) by multiplication with a sigmoidal dependency of nutritional intake to resource density with half-saturation constant φ_1 . It depends on temperature following the same relationship as for phytoplankton growth (f_T). N'_{dia} encompasses a preference term for grazing on diatoms, relative to that on nanophytoplankton:

$$N'_{dia} = \tau \cdot \frac{N_{dia}^2}{\varphi_2 + N_{dia}^2} \cdot N_{dia} \quad (40)$$

Here, τ is the maximum diatom preference and is smaller than one, which implies that zooplankton grazes preferably on nanophytoplankton; the effective grazing preference is allowed to vary with diatom biomass, with φ_2 being the half saturation parameters for grazing preference of diatoms. $\varphi_2 = 0$ implies a constant preference.

The relative contributions of grazing on nanophytoplankton and on diatoms to the total grazing flux are calculated by their respective proportion to the total zooplankton food resource.

$$G_{phy} = G \cdot \frac{N_{phy}}{N_{phy} + N'_{dia}} \quad (41)$$

$$G_{dia} = G \cdot \frac{N'_{dia}}{N_{phy} + N'_{dia}} \quad (42)$$

Carbon pool (C_{het}) The heterotrophic carbon biomass is a balance between carbon uptake via grazing and carbon loss via mortality, carbon excretion and respiration.

$$S(C_{het}) = \left(\frac{1}{q_{phy}} \cdot G_{phy} + \frac{1}{q_{dia}} \cdot G_{dia} \right) \cdot \gamma - \frac{1}{q_{het}} \cdot m_{het} \cdot N_{het}^2 - \epsilon_{het}^C \cdot C_{het} - r_{het} \cdot C_{het} \quad (43)$$

The grazing flux in terms of nitrogen biomass is converted to carbon biomass using the respective intracellular N:C ratios (q_{phy} and q_{dia}). Sloppy feeding causes some of the grazed phytoplankton to be transferred directly to the detritus pool, as determined by the grazing efficiency γ . The remainder is built into heterotrophic biomass. The quadratic mortality flux ($m_{het} \cdot N_{het}^2$), which causes carbon to be lost to the detritus compartment, is converted to carbon using the intracellular heterotrophic N:C ratio (q_{het}). When the C:N ratio in heterotrophs ($q_{het}^{C:N} = 1/q_{het}$) exceeds the Redfield ratio, heterotrophic respiration is assumed to drive the ratio back towards Redfield, with a time-scale κ_{het} :

$$r_{het} = \begin{cases} f_T \cdot (q_{het}^{C:N} - q_{Redfield}^{C:N}) / \kappa_{het} & \text{if } q_{het}^{C:N} > q_{Redfield}^{C:N} \\ 0 & \text{if } q_{het}^{C:N} \leq q_{Redfield}^{C:N} \end{cases} \quad (44)$$

5 Detritus

Nitrogen pool (N_{det}) Losses of phytoplankton nitrogen due to aggregation, mortality and sloppy feeding have to pass the N_{det} compartment before being degraded to DON, which is the only loss term for detrital nitrogen.

$$S(N_{det}) = G \cdot (1 - \gamma) + g \cdot (N_{phy} + N_{dia}) + m_{het} \cdot N_{het}^2 - \rho_{PON} \cdot f_T \cdot N_{det} \quad (45)$$

See section 4 for a definition of the grazing flux G , the grazing efficiency γ and the zooplankton mortality flux ($m_{het} \cdot N_{het}^2$). The aggregation rate g is defined in Eq. 16. Degradation of N_{det} to DON is based on a constant degradation rate (ρ_{PON}) and a temperature dependency (f_T , Eq. 23).

Carbon pool (C_{det}) The C_{det} compartment is balanced by carbon sources associated with sloppy feeding, aggregation of phytoplankton, mortality of heterotrophs and degradation of C_{det} to DOC as the only loss term.

$$S(C_{det}) = \left(\frac{1}{q_{phy}} \cdot G_{phy} + \frac{1}{q_{dia}} \cdot G_{dia} \right) \cdot (1 - \gamma) + g \cdot (C_{phy} + C_{dia}) + \frac{1}{q_{het}} \cdot m_{het} \cdot N_{het}^2 - \rho_{POC} \cdot f_T \cdot C_{det} \quad (46)$$

The grazing and the quadratic mortality flux (see section 4), which are calculated in terms of N biomass, are converted to carbon biomass via the respective intracellular N:C ratios (q_{phy} , q_{dia} and q_{het}). The sloppy feeding part of the grazing flux is transferred to the C_{det} compartment, while the main grazing flux is built into heterotrophic biomass, as determined by the grazing efficiency γ . The degradation term consists of a constant degradation rate ρ_{POC} and takes into account a temperature dependency f_T (see Eq. 23).

Silica pool (Si_{det}) The detrital silica budget consists of aggregation, grazing and excretion fluxes from diatoms to detritus and silica dissolution, which shifts silicon from Si_{det}

to dissolved silicate.

$$S(\text{Si}_{det}) = (g + \epsilon_{dia}^N \cdot f_{dia}^{lim}) \cdot \text{Si}_{dia} + G_{dia} \cdot q_{dia}^{Si:N} - \rho_{Si}^T \cdot \text{Si}_{det} \quad (47)$$

See section 3 for definitions of the aggregation (g) and excretion (ϵ) fluxes and section 4 for the grazing fluxes (G).

The silica dissolution rate ρ_{Si}^T follows the temperature dependence of *Kamatani* (1982), until it exceeds the maximum dissolution rate ρ_{Si}

$$\rho_{Si}^T = \min(1.32 \cdot 10^{16} \cdot \exp(\frac{-11200}{T}), \rho_{Si}) \quad (48)$$

Calcium carbonate pool (CaCO_3_{det}) Nanophytoplankton loses CaCO_3 to the detrital CaCO_3 compartment via excretion, respiration, aggregation and grazing. Dissolution of CaCO_3 leads to an increase in DIC and alkalinity (see section 1).

$$S(\text{CaCO}_3_{det}) = (\epsilon_{phy}^C \cdot f_{phy}^{lim} + r_{phy} + g + G_{phy} \cdot q_{phy}^{CaCO_3:N}) \cdot \text{CaCO}_3_{phy} - \lambda \cdot \text{CaCO}_3_{det} \quad (49)$$

The nanophytoplankton excretion term (ϵ_{phy}^C) is regulated by intracellular quota as defined in Eq. 14. Refer to section 3 for a definition of the respiration (r_{phy}) and the aggregation (g) rates. The grazing flux is calculated in terms of nitrogen biomass (Eq. 41) and is converted to CaCO_3_{det} by multiplication with the intracellular $\text{CaCO}_3:N$ ratio ($q_{phy}^{CaCO_3:N}$).

Detrital calcite decreases exponentially with water depth with a vertical length scale of 3500 m according to *Yamanaka and Tajika* (1996). The dissolution rate λ [d^{-1}] depends on the sinking speed of detritus, so that

$$\lambda = \frac{w_{det}}{3500 \text{ m}} \quad (50)$$

where w_{det} increases with depth according to

$$w_{det} = 20 \text{ m s}^{-1} + 0.0288 \text{ s}^{-1} \cdot \text{depth}(m) \quad (51)$$

6 Dissolved Organic Matter (DOM)

Dissolved Organic Nitrogen (DON) DON is produced via N excretion by nanophytoplankton, diatoms and heterotrophs, and by degradation of detrital N. It is turned into DIN by remineralization.

$$S(\text{DON}) = \epsilon_{phy}^N \cdot f_{phy}^{lim} \cdot N_{phy} + \epsilon_{dia}^N \cdot f_{dia}^{lim} \cdot N_{dia} + \epsilon_{het}^N \cdot N_{het} + \rho_{PON} \cdot f_T \cdot N_{det} - \rho_{DON} \cdot f_T \cdot \text{DON} \quad (52)$$

The constant excretion rates of phytoplankton (ϵ_{phy}^N and ϵ_{dia}^N) are reduced if the N:C ratio is larger than a threshold (see Eq. 14 and Eq. 15). Heterotrophic nitrogen excretion ($\epsilon_{het}^N \cdot N_{het}$) depends only on the heterotrophic biomass. Degradation of N_{det} to DON and remineralization from DON to DIN is temperature dependent, so that the constant

degradation (ρ_{PON}) and remineralization (ρ_{DON}) rates are multiplied with the Arrhenius function (f_T , see Eq. 23).

Dissolved Organic Carbon (DOC) DOC sources are carbon excretion by nanophytoplankton, diatoms and heterotrophs, and degradation of C_{det} . Remineralization of DOC leads to a transfer of carbon from DOC to DIC.

$$S(\text{DOC}) = \epsilon_{phy}^C \cdot f_{phy}^{lim} \cdot C_{phy} + \epsilon_{dia}^C \cdot f_{dia}^{lim} \cdot C_{dia} + \epsilon_{het}^C \cdot C_{het} + \rho_{POC} \cdot f_T \cdot C_{det} - \rho_{DOC} \cdot f_T \cdot \text{DOC} \quad (53)$$

Metabolic excretion of organic matter by phytoplankton is determined by a constant excretion rate and cell quota (ϵ_{phy}^C and ϵ_{dia}^C , see section 3). The heterotrophic excretion rate per heterotrophic biomass is constant (ϵ_{het}^C). The constant degradation (ρ_{POC}) and remineralization (ρ_{DOC}) rates that determine the fluxes from C_{det} to DOC and from DOC to DIC are altered following the Arrhenius function (f_T , Eq. 23).

7 Boundary conditions and early diagenesis

In its present version, REcoM-2 considers neither riverine input of nutrients, carbon and alkalinity, nor permanent burial of organic matter, calcium carbonate and silica in the sediment. At the sea surface, we assume no normal flux of tracers, except for DIC that can exchange with the atmospheric reservoir of CO_2 . This surface boundary condition can be written as

$$\kappa \frac{\partial A}{\partial z} \Big|_{z=\eta} = \begin{cases} 0 & \text{for } A \neq \text{DIC} \\ F_C & \text{for } A = \text{DIC} \end{cases} \quad (54)$$

where η is the sea surface elevation, and the air-sea flux of carbon F_C (positive for flux out of the ocean) is calculated from DIC, TA, atmospheric $p\text{CO}_2$, temperature, salinity and wind speed, following OCMIP protocols. Likewise, we assume no horizontal flux of tracers at lateral boundaries.

At the bottom of the ocean, the sinking flux of particulates (nanophytoplankton, diatoms and detritus) is directed into a homogeneous sediment layer, where POC and PON are degraded and instantaneously remineralized and calcium carbonate and silica are dissolved with fixed rates. The corresponding equations are

$$\begin{aligned} \frac{\partial \text{POC}_{sed}}{\partial t} &= w_{det} \cdot C_{det} - d^C \cdot \text{POC}_{sed} \\ \frac{\partial \text{PON}_{sed}}{\partial t} &= w_{det} \cdot N_{det} - d^N \cdot \text{PON}_{sed} \\ \frac{\partial \text{Si}_{sed}}{\partial t} &= w_{det} \cdot \text{Si}_{det} - d^{Si} \cdot \text{Si}_{sed} \\ \frac{\partial \text{CaCO}_3_{sed}}{\partial t} &= w_{det} \cdot \text{CaCO}_3_{det} - d^{CaCO_3} \cdot \text{CaCO}_3_{sed} \end{aligned} \quad (55)$$

where POC_{sed} , PON_{sed} , Si_{sed} , and CaCO_3_{sed} are vertically integrated concentrations in the sediment layer, i.e. they have the unit mol m^{-2} . d^C , d^N , d^{Si} , and d^{CaCO_3} are the degradation or dissolution rates for POC, PON, Si and CaCO_3 , respectively.

The nutrients and alkalinity released during the degradation/remineralization and dissolution are directly returned into the water as a flux, i.e. the boundary condition at the ocean bottom is

$$\kappa \frac{\partial A}{\partial z} \Big|_{z=-H} = \begin{cases} d^C \cdot \text{POC}_{sed} + d^{CaCO_3} \cdot \text{CaCO}_{3sed} & \text{for } A = \text{DIC} \\ d^N \cdot \text{PON}_{sed} & \text{for } A = \text{DIN} \\ (1 + 1/16) \cdot d^N \cdot \text{PON}_{sed} + 2d^{CaCO_3} \cdot \text{CaCO}_{3sed} & \text{for } A = \text{TA} \\ d^{Si} \cdot \text{Si}_{sed} & \text{for } A = \text{DSi} \\ q^{Fe} \cdot d^C \cdot \text{POC}_{sed} & \text{for } A = \text{DFe} \\ 0 & \text{for all other tracers} \end{cases} \quad (56)$$

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Table 1: Model coefficients and their standard values

Symbol	Value	Unit	Parameter
T_{ref}	288.15	K	reference temperature
ψ	0.02	dimensionless	calcite production ratio
q^{Fe}	0.005	$\mu\text{mol Fe (mmol C)}^{-1}$	Fe:C ratio
κ_{Fe}^{scav}	0.0156	$(\text{mmol C m}^{-3})^{-1} \text{d}^{-1}$	Fe scavenging rate
α_{phy}	0.14	$\text{mmol C (mg Chl)}^{-1} (\text{W m}^{-2} \text{d})^{-1}$	initial slope of P-I curve
α_{dia}	0.19	$\text{mmol C (mg Chl)}^{-1} (\text{W m}^{-2} \text{d})^{-1}$	diatom initial slope of P-I curve
μ_{phy}^{max}	3.0	d^{-1}	maximum photosynthesis rate
μ_{dia}^{max}	3.5	d^{-1}	diatom maximum photosynthesis rate
ϵ_{phy}^N	0.05	d^{-1}	excretion rate of nitrogen
ϵ_{dia}^N	0.05	d^{-1}	diatom excretion rate of nitrogen
ϵ_{phy}^C	0.10	d^{-1}	excretion rate of carbon
ϵ_{dia}^C	0.10	d^{-1}	diatom excretion rate of carbon
σ_{phy}^N	0.20	$\text{mol N (mol C)}^{-1}$	N:C uptake ratio
σ_{dia}^N	0.20	$\text{mol N (mol C)}^{-1}$	diatom N:C uptake ratio
σ_{dia}^{Si}	0.20	$\text{mol Si (mol C)}^{-1}$	diatom Si:C uptake ratio
K_{phy}^N	0.55	mmol N m^{-3}	half-saturation constant N uptake
K_{dia}^N	1.0	mmol N m^{-3}	diatom half-saturation constant N uptake
K_{phy}^{Fe}	0.02	$\mu\text{mol Fe m}^{-3}$	half-saturation constant Fe uptake
K_{dia}^{Fe}	0.12	$\mu\text{mol Fe m}^{-3}$	diatom half-saturation constant Fe uptake
K_{dia}^{Si}	4.0	mmol Si m^{-3}	diatom half-saturation constant Si uptake
$q_{phy max}$	0.20	$\text{mol N (mol C)}^{-1}$	maximum N:C ratio
$q_{dia max}$	0.20	$\text{mol N (mol C)}^{-1}$	diatom maximum N:C ratio
q_{max}^{Si}	0.80	$\text{mol Si (mol C)}^{-1}$	diatom maximum Si:C ratio
q_{min}	0.04	$\text{mol N (mol C)}^{-1}$	minimum N:C ratio
q_{min}^{Si}	0.04	$\text{mol Si (mol C)}^{-1}$	minimum Si:C ratio
$q_{phy max}^{Chl:N}$	3.15	$\text{mg Chl (mmol N)}^{-1}$	nanophytoplankton maximum Chl:N ratio
$q_{dia max}^{Chl:N}$	4.2	$\text{mg Chl (mmol N)}^{-1}$	diatom maximum Chl:N ratio
θ_{max}	1000	dimensionless	regulation slope
θ_{min}	50	dimensionless	regulation slope
θ_{min}^{Si}	1000	dimensionless	regulation slope
θ_{max}^{Si}	1000	dimensionless	regulation slope
ζ^N	2.33	$\text{mol C (mol N)}^{-1}$	C cost of N assimilation
ζ^{Si}	0	$\text{mol C (mol Si)}^{-1}$	C cost of Si assimilation
ϕ_{phy}	0.015	$(\text{mmol N m}^{-3})^{-1} \text{d}^{-1}$	phytoplankton specific aggregation rate
ϕ_{det}	0.0165	$(\text{mmol N m}^{-3})^{-1} \text{d}^{-1}$	detritus specific aggregation rate
η_{phy}	0.01	d^{-1}	maintenance respiration rate
η_{dia}	0.01	d^{-1}	diatom maintenance respiration rate
d_{phy}^{Chl}	0.3	d^{-1}	chlorophyll degradation rate
d_{dia}^{Chl}	0.3	d^{-1}	diatom chlorophyll degradation rate
γ	0.4	dimensionless	grazing efficiency

Table 2: Model coefficients and their standard values

Symbol	Value	Unit	Parameter
m_{het}	0.05	$(\text{mmol N m}^{-3})^{-1} \text{ d}^{-1}$	quadratic mortality rate
ϵ_{het}^N	0.15	d^{-1}	zooplankton N excretion rate
ϵ_{het}^C	0.15	d^{-1}	zooplankton C excretion rate
φ_1	0.35	$(\text{mmol N m}^{-3})^2$	half-saturation constant for grazing
φ_2	0	$(\text{mmol N m}^{-3})^2$	half-saturation constant for diatom grazing preference
ξ	2.4	$\text{mmol N m}^{-3} \text{ d}^{-1}$	maximum grazing rate
τ	0.5	dimensionless	maximum preference for grazing on diatoms
$q_{Redfield}^{C:N}$	6.625	$\text{mol C (mol N)}^{-1}$	Redfield ratio of C:N
κ_{het}	0.01	d	time-scale for restoring towards Redfield
ρ_{PON}	0.165	d^{-1}	PON degradation rate
ρ_{POC}	0.15	d^{-1}	POC degradation rate
ρ_{DON}	0.11	d^{-1}	DON remineralisation rate
ρ_{DOC}	0.1	d^{-1}	DOC remineralisation rate
ρ_{Si}	0.02	d^{-1}	maximum Si dissolution rate
L_T	1	$\mu\text{mol m}^{-3}$	total ligand concentration
K_{FeL}	100	$\text{m}^3 \mu\text{mol}^{-1}$	ligand stability constant
d^C	0.005	d^{-1}	POC degradation rate in sediment
d^N	0.005	d^{-1}	PON degradation rate in sediment
d^{Si}	0.005	d^{-1}	Si degradation rate in sediment
d^{CaCO_3}	0.005	d^{-1}	CaCO_3 degradation rate in sediment

Table 3: Name and symbols of model coefficients

Symbol	Model code	Parameter
T_{ref}	recom_Tref	reference temperature
ψ	calc_prod_ratio	calcite production ratio
q^{Fe}	Fe2C	Fe:C ratio
κ_{Fe}^{scav}	kScavFe	Fe scavenging rate
α_{phy}	alpha	initial slope of P-I curve
α_{dia}	alpha_d	diatom initial slope of P-I curve
μ_{phy}^{max}	P_cm	maximum photosynthesis rate
μ_{dia}^{max}	P_cm_d	diatom maximum photosynthesis rate
ϵ_{phy}^N	lossN	excretion rate of nitrogen
ϵ_{dia}^N	lossN_d	diatom excretion rate of nitrogen
ϵ_{phy}^C	lossC	excretion rate of carbon
ϵ_{dia}^C	lossC_d	diatom excretion rate of carbon
σ_{phy}^N	NCuptakeRatio	N:C uptake ratio
σ_{dia}^N	NCuptakeRatio_d	diatom N:C uptake ratio
σ_{dia}^{Si}	SiCuptakeRatio	diatom Si:C uptake ratio
K_{phy}^N	k_din	half-saturation constant N uptake
K_{dia}^N	k_din_d	diatom half-saturation constant N uptake
K_{phy}^{Fe}	k_fe	half-saturation constant Fe uptake
K_{dia}^{Fe}	k_fe_d	diatom half-saturation constant Fe uptake
K_{dia}^{Si}	k_si	diatom half-saturation constant Si uptake
$q_{phy max}$	NCmax	maximum N:C ratio
$q_{dia max}$	NCmax_d	diatom maximum N:C ratio
q_{max}^{Si}	SiCmax	diatom maximum Si:C ratio
q_{min}	NCmin	minimum N:C ratio
q_{min}^{Si}	SiCmin	minimum Si:C ratio
$q_{phy max}^{Chl:N}$	CHL_N_max	nanophytoplankton maximum Chl:N ratio
$q_{dia max}^{Chl:N}$	CHL_N_max_d	diatom maximum Chl:N ratio
θ_{max}	NMaxSlope	regulation slope
θ_{min}	NMinSlope	regulation slope
θ_{min}^{Si}	SiMinSlope	regulation slope
θ_{max}^{Si}	SiMaxSlope	regulation slope
ζ^N	biosynth	C cost of N assimilation
ζ^{Si}	biosynthSi	C cost of Si assimilation
ϕ_{phy}	agg_PP	phytoplankton specific aggregation rate
ϕ_{det}	agg_PD	detritus specific aggregation rate
η_{phy}	res_phy	maintenance respiration rate
η_{dia}	res_phy_d	diatom maintenance respiration rate
d_{phy}^{Chl}	deg_CHL	chlorophyll degradation rate
d_{dia}^{Chl}	deg_CHL_d	diatom chlorophyll degradation rate
γ	grazEff	grazing efficiency

Table 4: Name and symbols of model coefficients

Symbol	Model code	Parameter
m_{het}	loss_het	quadratic mortality rate
ϵ_{het}^N	lossN_z	zooplankton N excretion rate
ϵ_{het}^C	lossC_z	zooplankton C excretion rate
φ_1	epsilon	half-saturation constant for grazing
φ_2	sdiasq	half-saturation constant for diatom grazing preference
ξ	graz_max	maximum grazing rate
τ	pzdia	maximum preference for grazing on diatoms
$q_{Redfield}^{C:N}$	redfield	Redfield ratio of C:N
κ_{het}	res_het	time-scale for restoring towards Redfield
ρ_{PON}	reminN	PON degradation rate
ρ_{POC}	reminC	POC degradation rate
ρ_{DON}	rho_N	DON remineralisation rate
ρ_{DOC}	rho_C1	DOC remineralisation rate
ρ_{Si}	reminSi	maximum Si dissolution rate
L_T	totalLigand	total ligand concentration
K_{FeL}	ligandStabConst	ligand stability constant
d^C	decayRateBenN	POC degradation rate in sediment
d^N	decayRateBenC	PON degradation rate in sediment
d^{Si}	decayRateBenSi	Si degradation rate in sediment
d^{CaCO_3}	decayRateBenCa	CaCO ₃ degradation rate in sediment