

Supplements

I. Model equations

i. Hypothesis 0: Neglecting N₂ fixation

As a starting hypothesis, we test whether a model without nitrogen fixing can reproduce the observed distribution of inorganic nutrients. We test this model with and without allowing a sediment denitrification flux, denoted as H0 and H0', respectively. Therefore, H0 fully neglects N₂ fixation, while H0' implicitly assumes that N₂ fixation inputs and N₂ denitrification are balanced.

This model (H0) tracks the changes of 8 state-variables: nitrate (NO₃), ammonium (NH₄), dissolved inorganic phosphorus (DIP), non-fixing phytoplankton (Phy), zooplankton (Zoo), "small" detritus (D_S), "large" detritus (D_L), and oxygen (O₂). Model equations correspond to those described in Fennel et al., 2006 and 2013. Changes in phytoplankton and zooplankton biomass are measured in nitrogen units only, which implies a constant N:P ratio for these functional groups. The stoichiometry of non-fixing phytoplankton and zooplankton is set to the Redfield ratio ($R_{N:P}^{nf}=16$), and their biomass changes according to:

$$\frac{\partial Phy}{\partial t} = \mu_{Phy} Phy - gZoo - m_{Phy} Phy - w_{Phy} \frac{\partial Phy}{\partial z} \quad (1)$$

$$\frac{\partial Zoo}{\partial t} = g\beta Zoo - l_{BM} Zoo - l_E \frac{Phy^2}{k_{Phy} + Phy^2} \beta Zoo - m_{Zoo} Zoo^2 \quad (2)$$

Phytoplankton growth (equ. 1) depends on light and nutrient supply according to: $\mu_{Phy} = \mu_{Phy}^{max} f(I) \min(L_{NO_3} + L_{NH_4}, L_{DIP})$. This formulation assumes that growth is limited by light and nutrient availability using a multiplicative effect. In terms of nutrient limitation, it follows Liebig's Law of the minimum, as growth is limited by the scarcest nutrient resource of either nitrogen or phosphorus. The maximum non-fixing phytoplankton growth rate, μ_{Phy}^{max} , varies with temperature using a Q₁₀ formulation according to $\mu_{Phy}^{max}(T) = \mu_{Phy}^0 1.88^{T/10^\circ C}$ (Eppley, 1972), where μ_{Phy}^0 is the assumed maximum growth rate at T = 0°C. The light limitation function is equal to $f(I) = \frac{\alpha_{Phy} I}{\sqrt{(\mu_{Phy}^{max})^2 + \alpha_{Phy}^2 I^2}}$ (Smith, 1936), where I is the depth varying photosynthetically active radiation, and α_{Phy} is the initial slope of the photosynthetic reaction. The value of I decreases exponentially with depth (z) according to $I(z) = I_0(1 - \phi)e^{-z k_w - \int_0^z k_{chl} Chl_{Phy} dz}$,

where the coefficients $\phi=0.62$ and $k_w = 0.05 \text{ m}^{-1}$ are set for oceanic clear waters according to Jerlov's type IA (Paulson and Simpson, 1977), and the coefficient $k_{chl} = 0.04 \text{ m}^{-1}$ represents light attenuation due to chlorophyll concentrations (*Chl*). I_0 is the surface solar radiation recorded at the IUI station.

Non-fixing phytoplankton is grazed by zooplankton at a density dependent rate $g = g_{Phy}^{max} \frac{Phy^2}{k_{Zoo}^{Phy} + Phy^2}$, with only a fraction β being assimilated into zooplankton growth. The last two terms in equation 1 represent non-fixing phytoplankton mortality and sinking, which occur at a rate of m_{Phy} and a speed of w_{Phy} , respectively. In equation 2, l_{BM} , l_E , and m_Z represent the zooplankton base metabolic, excretion and mortality rates.

Changes in nutrient concentrations are defined by the following set of equations:

$$\frac{\partial NO_3}{\partial t} = -\mu_{Phy}^{max} f(I)L_{NO_3}Phy + nNH_4 \quad (3)$$

$$\begin{aligned} \frac{\partial NH_4}{\partial t} = & -\mu_{Phy}^{max} f(I)L_{NH_4}Phy + l_{BM}Zoo + l_E \frac{Phy^2}{k_P + Phy^2} \beta Zoo + r_{D_S}D_{S(N)} + r_{D_L}D_{L(N)} \\ & - nNH_4 \end{aligned} \quad (4)$$

$$\begin{aligned} \frac{\partial DIP}{\partial t} = & \frac{1}{R_{N:P}^{nf}} \left(-\mu_{Phy}^{max} f(I)L_{DIP}Phy + l_{BM}Zoo + l_E \frac{Phy^2}{k_P + Phy^2} \beta Zoo \right) + r_{D_S(P)}D_{S(P)} \\ & + r_{D_L}D_{L(P)} \end{aligned} \quad (5)$$

Equations 3, 4, and 5 represent the changes in nitrate, ammonium, and dissolved inorganic phosphorus, respectively. In these equations, nutrient uptake by non-fixing phytoplankton is modulated by the maximum non-fixing phytoplankton growth rate μ_{Phy}^{max} , the light limitation function $f(I)$, and the corresponding nutrient limitation factor (L_{NO_3} , L_{NH_4} , or L_{DIP}). The nutrient limitation factors for ammonium and dissolved inorganic phosphorus in the form of phosphate are Michaelis-Menten (1913) functions:

$$L_{NH_4} = \frac{NH_4}{k_{Phy}^{NH_4} + NH_4} \quad (6)$$

$$L_{DIP} = \frac{DIP}{k_{Phy}^{DIP} + DIP} \quad (7)$$

The nitrate limitation factor is also a Michaelis – Menten (1913) function, but is modified by the availability of NH_4 , which inhibits NO_3 uptake:

$$L_{NO_3} = \frac{NO_3}{k_{Phy}^{NO_3} + NO_3} \frac{1}{\left(1 + NH_4/k_{Phy}^{NH_4}\right)} \quad (8)$$

Both NH_4 and DIP receive contributions from zooplankton metabolic and excretion losses, and from the degradation of small and large detritus. The parameters l_{BM} , l_E are the metabolic loss and mortality rates of zooplankton. Degradation rates for small and large detritus are represented by r_{D_S} and r_{D_L} , respectively. Both the nitrogen and phosphorus fractions of the two detritus groups are tracked, for which we use the subscripts “(N)” and “(P)” correspondingly. The last terms in equations 3 and 4 represent the transformation of NH_4 into NO_3 via nitrification at rate n .

The model also estimates non-fixing phytoplankton chlorophyll content (Chl_{Phy}):

$$\frac{\partial Chl_{Phy}}{\partial t} = \rho_{Chl_{Phy}} \mu_{Phy} Phy - g_{Zoo} \frac{Chl_{Phy}}{Phy} - m_{Phy} Chl_{Phy} - w_{Phy} \frac{\partial Chl_{Phy}}{\partial z} \quad (9)$$

where the factor $\rho_{Chl_{Phy}}$ represents a variable chlorophyll-to-biomass ratio. This factor accounts for the photoacclimation effect of increased chlorophyll production under low light conditions and is determined following Geider et al., (1997):

$$\rho_{Chl_{Phy}} = \frac{\theta_{Phy}^{max} \mu_{Phy} Phy}{\alpha_{Phy} I Chl_{Phy}} \quad (10)$$

The two fractions of detritus aim to represent small-suspended particles of non-living organic matter (D_S) that can aggregate to form larger sinking particles (D_L). “Small” detritus (eq. 11) is formed from the unassimilated fraction of zooplankton grazing (i.e., sloppy feeding), and from dead phytoplankton and zooplankton. The small detritus pool suffers losses from coagulation and degradation. “Large” detritus (eq. 12) is produced through the coagulation D_S , and is removed by degradation and sinking at a w_{D_L} speed. The sinking speed of large detritus is assumed to be faster than for non-fixing phytoplankton (w_{Phy}).

$$\frac{\partial D_S}{\partial t} = g(1 - \beta) Zoo + m_Z Zoo^2 + m_{Phy} Phy - r_{D_S} D_S \quad (11)$$

$$\frac{\partial D_L}{\partial t} = \tau D_S^2 - r_{D_L} D_L - w_{D_L} \frac{\partial D_L}{\partial z} \quad (12)$$

Oxygen (eq. 13) is produced during photosynthesis and consumed by zooplankton metabolism, and the degradation of dissolved organic matter and detritus, as in Fennel et al. (2013):

$$\frac{\partial O_2}{\partial t} = \mu_{Phy}^{max} f(I) (L_{NO_3} R_{O_2:NO_3} + L_{NH_4} R_{O_2:NH_4}) Phy - 2 nNH_4 - R_{O_2:NH_4} (l_{BM} Zoo + r_{D_S} D_S - r_{D_L} D_L) \quad (13)$$

where $R_{O_2:NO_3} = \frac{138 \text{ mol } O_2}{16 \text{ mol } NO_3}$ and $R_{O_2:NH_3} = \frac{106 \text{ mol } O_2}{16 \text{ mol } NH_3}$ represent stoichiometric ratios corresponding to the oxygen produced during photosynthesis per mole of nitrate and ammonium consumed.

At the ocean surface, oxygen concentrations are modified by the air-sea gas exchange $F_{air-sea}$:

$$F_{air-sea} = \frac{vk_{O_2}}{\Delta Z} (O_{sat} - O_2) \quad (14)$$

such that a flux of oxygen into the top layer of thickness Δz occurs when its oxygen concentration is lower than the oxygen saturation value (O_{sat}), and a flux into the atmosphere occurs if it is higher. The formulation of O_{sat} is based on García and Gordon (1992), and the gas exchange coefficient for oxygen, vk_{O_2} , is parameterized following Wanninkhof et al., (2011) as:

$$vk_{O_2} = 0.28 u_{10}^2 \sqrt{\frac{660}{S_{CO_2}}}, \quad (15)$$

where u_{10} is the wind speed 10 m above the sea surface, and S_{CO_2} is the Schmidt number.

We assume that organic matter reaching the bottom is instantaneously remineralized into ammonium. Sediment oxygen consumption is represented as in Fennel et al. (2013). This model was tested with and without allowing a denitrification flux (H_0 and H_0' , respectively). When present, the denitrification flux follows Fennel et al. (2013) with a loss fraction 6 mol N_2 per mol of organic matter remineralized.

ii. Hypothesis 1: Generic autotrophic N_2 fixers

In model version H1, we introduce the state variable G_F , which represents a group of generic autotrophic N_2 fixers:

$$\frac{\partial G_F}{\partial t} = \mu_F G_F - m_F G_F - l_F G_F - \tau (D_S + G_F) G_F \quad (16)$$

The growth of the fixing organisms is limited by light and DIP only (i.e., an obligate autotrophic diazotroph). The parameters m_F , l_F , τ represent a mortality rate, an excretion rate, and the coagulation rate, respectively. An accompanying chlorophyll equation is also introduced, and

total chlorophyll becomes the sum of the non-fixing and fixing autotrophic organisms: $Chl = Chl_{Phy} + Chl_{G_F}$. All other state variable equations are modified accordingly. That is, uptake of DIP by G_F is included as a sink in the DIP equation (Eq. 5), G_F excretion becomes an additional source of ammonium in Eq. 4, G_F mortality becomes a source of D_S in Eq. 11, and G_F coagulated aggregates become a source of D_L in Eq. 12. The stoichiometry of diazotrophs is set to $R_{N:P}^f = 45$ (Fennel et al., 2002; Letelier and Karl, 1996).

iii. Hypothesis 2: Unicellular and colonial N_2 fixers

In model version H2, we replace the generic autotrophic diazotroph group with two different groups that represent colonial and unicellular cyanobacteria:

$$\frac{\partial U_F}{\partial t} = \mu_{U_F} U_F - m_{U_F} U_F - l_{U_F} U_F - g_{U_F} Zoo \quad (17)$$

$$\frac{\partial C_F}{\partial t} = \mu_{C_F} C_F - m_{C_F} C_F - l_{C_F} C_F - \tau(D_S + C_F) C_F \quad (18)$$

The group of colonial N_2 fixers, C_F , represents *Trichodesmium* spp. A minimum temperature limit for the growth of *Trichodesmium* spp. is imposed by setting the maximum growth rate to 0 when temperature is below 20°C, based on the inability to culture this type of organism below this temperature (Breitbarth et al., 2007). The unicellular cyanobacteria group, U_F , overall follows the same formulation as the generic diazotroph, except that no coagulation term is included in this equation as they represent picoplanktonic free-living cells that do not form large colonies. Instead, this group is grazed by zooplankton similar to grazing on non-fixing phytoplankton. This is based on evidence that *Trichodesmium* spp. colonies may be less palatable and harder to digest due to toxins and that grazing is not a major fate of this group (O'Neil and Roman, 1994). Moreover, it has been suggested that colonies represent an evolutionary adaptation that allows a decreased grazing pressure (Nielsen 2006). As in the previous model version, other equations are modified where necessary.

iv. Hypothesis 3: Heterotrophic N_2 fixers

In model version H3 we introduce an additional heterotrophic diazotroph group H_F , so that this ecosystem model includes three types of N_2 fixers. The formulation of H_F follows:

$$\frac{\partial H_F}{\partial t} = \mu_{H_F} H_F - m_{H_F} H_F - l_{H_F} H_F \quad (18)$$

These organisms are not limited by light availability and grow by consuming both dissolved inorganic and organic phosphorus from D_S , following $\mu_{HF} = \psi_{DIP} \frac{DIP}{k_{HF}^{DIP} + DIP} + \psi_{DS} \frac{D_{S(P)}}{k_{HF}^{DS} + D_{S(P)}}$.

The coefficients ψ_{DIP} and ψ_{DS} represent preferences, which are set as equal ($\psi_{DIP} = \psi_{DS} = 0.5$).

II. Model sensitivity to physical nudging

Effect of physical nudging on temperature and density fields estimated from a model run with nudging minus a model run without nudging. The dashed vertical line marks the simulation period used as a model spin-up.

