BSEM equations and parameters

The general form of equations governing the biogeochemical model is expressed by

$$\frac{\partial A}{\partial t} + \nabla(\vec{u}.A) = F_A + R(A) \qquad \text{(S1)}$$

where A denotes each of the state variables, $\vec{u}$ is the three dimensional fluid velocity vector, F_A denotes the sum of horizontal and vertical diffusion terms, $R(A)$ refers the local rates of change of the 12 model compartments. Except $R(A)$, the mathematical forms of all terms in the differential equation above and their numerical solution procedures are similar to those of the temperature and salinity transport equations in the GETM/GOTM [1]. GETM and GOTM modules solve 3D transport equations for 12 non-conservative substances that BSEM involves. Detailed representation of source-sink terms is described below for each model compartment.

S.1. The autotrophs

The biological source-sink term $R(P)$ for the phytoplankton include the phytoplankton growth that is reduced by overall limitation function, Ψ_X, grazing by different zooplankton groups, and physiological mortality (Eq. S2). Temporal variations of the large (P_L) and small (P_S) phytoplankton biomass are governed by the biological source-sink terms and settling velocity of the form

$$R(P_X) = \sigma_X.\Psi_X.P_X - \sum GR(P_X).Z_Y - m_{PX}.P_X - w_P\frac{\partial P_X}{\partial z}, \qquad \text{(S2)}$$

where

$$\Psi_X = f_X(N_n, N_a, PO).f_X(I).f_X(T) \qquad \text{(S3)}$$

represents the total limitation function of the primary production, and the subscript X denotes either L for the large or S for the small size group, while Y denotes S, L or N, for small- , large zooplankton or *Noctiluca*, respectively; w_P is the settling velocity of the phytoplankton ($w_P = 0$ for the small phytoplankton and $w_P = w_{PL}$ for large); and z is the depth. The phytoplankton growth is modelled as

the product of the maximum specific growth rate, σ_X, total limitation function, Ψ_X, and phytoplankton

biomass P_X. The function $f_X(N_n, N_a, PO)$ is parameterised assuming that either nitrogen or phosphorus

controls phytoplankton growth [2]. This function represents the nutrient uptake expressed as the

minimum of total nitrogen (sum of nitrate and ammonium) limitations $f_X(N_n, N_a) = f_X(N_n) + f_X(N_a)$

and phosphorus limitation $f_X(PO)$.

Thus the function Ψ_X, that limits the primary production is defined by

$$\Psi_X = f_X(I).f_X(T).min\{f_X(N_n) + f_X(N_a), f_X(PO) \}. \qquad \text{(S4)}$$

The limiting functions in equation (S4) are expressed by the Monod-type hyperbolic functions

involving a saturation response at high resource concentrations.

$$f_X(N_a) = \left[\frac{N_a}{K_{AX}+N_a}\right], \quad f_X(N_n) = \left[\frac{N_n}{K_{NX}+N_n}\right].e^{-\lambda.N_a}, \quad f_X(PO) = \left[\frac{PO}{K_{POX}+PO}\right], \qquad \text{(S5)}$$

where

$$K_{NX} = a + bP_X, K_{AX} = 0.1\, K_{NX} \text{ and } K_{POX} = K_{NX}/np \qquad \text{(S6)}$$

are the corresponding half saturation functions of nitrate, ammonium and phosphate uptakes. They are

parameterised following [3]. Values of the constants a, b and λ are given in Table S2, and the

denominator np represents the $N{:}P$ ratio. The nitrogen limitation function $f_X(N_n)$ (Eq. S5) is based on

[4] and accounts for the inhibition of nitrate uptake in the presence of ammonium. Following Liebig's

law of the minimum, the nutrient uptake rate is thus limited by either total nitrogen or phosphorus.

The growth is also subject to simultaneous limitations by the photosynthetically available radiation

$f_X(I)$, and temperature $f_X(T)$. Using a spectrally unresolved model, the light limitation is parameterized

by [5]

$$f_X(I) = [\tanh(\alpha_X I)].e^{-\beta_X I} , \qquad \text{(S7)}$$

where α_X is a parameter controlling slope of the photosynthesis-irradiance curve at low values of the photosynthetically available irradiance (PAR) whose intensity I is calculated by the hydrodynamic model, β_X is the photoinhibition parameter to reduce the growth at high irradiance conditions.

The silicate control on the diatom growth is neglected as the available data does not yield evidence for the prevailing role of silicate limitation although its input from major rivers tends to decline during the last two decades [6]. The temperature controls of the growth, $f_X(T)$ for the large and small phytoplankton are assumed to be

$$f_L(T) = Q10^{(12-T)/12} \quad \text{and} \quad f_S(T) = Q10^{(T-20)/10}. \tag{S8}$$

In this way the large phytoplankton group can grow faster at low temperatures, while the small phytoplankton grows faster above 20° C. Weak temperature control is imposed for the small phytoplankton group, however the lower growth rate of the large phytoplankton group gives indirectly the small phytoplankton group a growth advantage.

Phytoplankton biomass decreases due to grazing by the zooplankton (Z_S and Z_L) and heterotrophic dinoflagellate species *Noctiluca* (Z_N), and phytoplankton mortality (second and third terms in the right-hand side of Eq. S2). The expressions $GR(P_X)$, used to model the grazing term is given in the next paragraph, where the ingestion of the heterotrophs and carnivores are presented. Coefficients of the phytoplankton mortality rates, m_{PX}, are given in Table S2.

S.2. The heterotrophs and carnivores

Changes in the zooplankton biomass are controlled by ingestion, predation, excretion, and mortality which are expressed by

$$R(Z_Y) = \varphi\left[\sum_i GR_j(A_i).Z_Y\right] - \sum_W GR_W(Z_Y).Z_W - \mu_Y.Z_Y - m_{ZY}.Z_Y^2, \tag{S9}$$

where Z_Y and $Z_W \neq Z_Y$ (Y or W denote either S, L, N or G); φ is the coefficient of assimilation efficiency, μ_Y and m_{ZY} are, respectively, the excretion rate and the natural mortality rate expressed in the quadratic form.

The ingestion terms $GR_j(A_i)$ in Eq. (S9) are represented by the Michaelis-Menten (the so-called Holling type II) functional form for jth predator on ith prey, in terms of the maximum rate g_j, the temperature limitation function $f_j(T)$, and the food capture efficiency coefficient $b_{j,i}$ for the food item A_i.

$$GR_j(A_i) = g_j \cdot f_j(T) \cdot \frac{b_{j,i} \cdot A_i}{K_j + [\sum_i b_{j,i} \cdot A_i]}, \qquad b_{j,i} = \frac{a_{j,i} \cdot A_i}{\sum_i a_{j,i} \cdot A_i}, \qquad \text{(S10)}$$

where the terms within the square bracket in the denominator refer to the total food available for the consumption of any zooplankton group; K_j denotes its half-saturation value; $a_{j,i}$ denotes the constant food preference coefficient specified externally as in Table S1. According to the above equations, when a food type declines, its grazing preference decreases [7]. In this case, zooplankton select an alternative food type having higher biomass. Thus, grazing preferences may switch from one prey to another depending on local conditions and the predator may select temporally and spatially most favourable food types.

The temperature control of the growth, $f_j(T)$, is introduced in the form

$$f_S(T) = 1 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(S11a)}$$

$$f_L(T) = 1 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(S11b)}$$

$$f_N(T) = Q10^{(T-12)/8} \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(S11c)}$$

$$f_G(T) = 4.5 - 1/(T-15) \quad \text{for} \quad T > 16 \quad \text{and} \quad f_G(T) = 1 \quad \text{otherwise.} \qquad \text{(S11d)}$$

According to the observations, *Noctiluca* can maintain its growth at a wide temperature range of 12-30ºC [8]. Eq. S11c supresses the *Noctiluca* growth at low temperatures but favours it in spring and summer months when the surface mixed layer starts warming up. Eq. S11d imposes the growth advantage of *Mnemiopsis* and *Beroe Ovata* population at high temperatures during July-August and strong decline at the end of the year [9]. The mortality rate of Z_G is increased four times in November-

December in order to maintain Z_G peaks until October. The mortality rate of the large zooplankton, m_{ZL}, is controlled by the temperature, so, $m_{ZL} = m_{0ZL}Q10^{(T-20)/10}$ and m_{0ZL} is a constant listed in Table S2.

S.3. Particulate organic nitrogen and phosphorus

It is assumed that the dissolved organic nitrogen and phosphorus pool is controlled by the egestion and sloppy feeding (i.e. unassimilated part of the food grazed), phytoplankton and zooplankton mortalities, its consumption by zooplankton groups within the water column (the third term), the transformation into the dissolved organic nitrogen and phosphorus pool at a rate $\varepsilon(DO)$ and the sinking rate of detritus, w_D (Eq. S12). As in [10], 70% of particulate organic nitrogen is assumed to decompose directly into ammonium and phosphorus.

$$R(D) = (1 - \varphi).Graz + Mort - \varphi.Cons - \varepsilon_n.D - w_D\frac{\partial D}{\partial z}, \qquad (S12)$$

$$Graz = GR_S(P_S).Z_S + [GR_L(P_L) + GR_L(Z_S) + GR_L(Z_N)].Z_L + [GR_N(P_L) + GR_N(Z_S)].Z_N + [GR_G(Z_S) + GR_G(Z_L) + GR_G(Z_N)].Z_G, \qquad (S13)$$

$$Mort = \sum_X m_{PX}.P_X + \sum_Y m_{ZY}.Z_Y^2, \qquad (S14)$$

$$Cons = GR_L(D).Z_L + GR_N(D).Z_N. \qquad (S15)$$

$$\varepsilon_n = \varepsilon(DO).f_D(T), \text{ where } f_D(T) = e^{d_o T}, \qquad (S16)$$

$$\varepsilon(DO) = \begin{cases} 1 & \text{for } DO > 250 \text{ mmol } O_2 \text{ m}^{-3} \\ \left\{1 + \frac{K_{DO}}{K_{DO}+DO}\right\} & \text{for } 250 \text{ mmol } O_2 \text{ m}^{-3} \geq DO \geq DO_l \\ 0.25 & \text{for } DO < DO_l \end{cases} \qquad (S17)$$

The detritus decomposition rate depends on oxygen and temperature (Eq. S16). Eq. S17 parameterises the higher decomposition rate in the oxygen deficient part of the water column due to more active bacterial processes with respect to the surface aerobic layer. The decomposition processes continue even in an absence of oxygen due to bacterial activities employing electron acceptors other than oxygen [11].

S.4. Dissolved inorganic nitrogen and phosphorus

The changes in ammonium, nitrate and phosphate concentrations are expressed by

$$R(N_a) = \frac{1-np}{np}\{\lambda.\varepsilon_n.D + \sum_Y \mu_{ZY}.Z_Y\} - \sum_X[\sigma_X.f_X(N_a).f_X(I).f_X(T).P_X] - r_n.\frac{I_n}{I_n+I}.N_a -$$

$$r_a.N_n.N_a, \tag{S18}$$

$$R(N_n) = r_n.\frac{I_n}{I_n+I}.N_a - \sum_X[\sigma_X.f_X(N_n).f_X(I).f_X(T).P_X] - \frac{3}{5}r_a.N_n.N_a - \frac{4}{53}r_s.HS.N_n, \tag{S19}$$

$$R(PO) = \{\varepsilon_n.D + \sum_Y \mu_{ZY}.Z_Y - \sum_X[\sigma_X.f_X(PO).f_X(I).f_X(T).P_X]\}/np \tag{S20}$$

In Eq. S18, the first and second terms represent ammonium sources due to decomposition of detritus (remineralisation) and zooplankton excretion, respectively. The source terms are multiplied by the expression of np, which represents the phytoplankton and zooplankton $N:P$ stoichiometry. This is because the detritus represents both dissolved organic nitrogen and phosphorus, and zooplankton excretions contain both nitrogen and phosphorus, as well [12]. $1/np$ part of detritus remineralisation and zooplankton excretion is assumed to be source of PO and the rest is the source of N_a. The third term represents its uptake during the primary production and the last two terms are the ammonium oxidation by oxygen (nitrification) and by nitrate in the absence of oxygen. The light dependent nitrification rate is applied.

Nitrification is the only internal (reaction) source of nitrate (Eq. S19). According to Eq. S19 nitrate is consumed due to its uptake by the phytoplankton (the second term), anaerobic particulate matter remineralization (the third term) that applies at oxygen concentrations less than 10 mmol O_2 m^{-3}, the oxidations of ammonium and hydrogen sulphide taking place at oxygen concentrations less than 10 mmol O_2 m^{-3} following the reaction equations in [13].

The phosphate sources (Eq. S20) are the same as for the ammonium divided by the parameter np, which represents the phytoplankton and zooplankton $N:P$ stoichiometry. The third term represents its uptake during the primary production

S.5. Dissolved oxygen and hydrogen sulphide

Dissolved oxygen concentration is altered by a balance between its photosynthetic production by the autotrophs and the consumption due to the pelagic decomposition of organic matter (Eq. S12). The excretion of zooplankton as well as the oxidation of ammonium within the oxygenated parts of the water column ($DO > DO_l$) and oxidation of hydrogen sulphide near the anoxic interface is given by

$$R(DO) = 8.125[\sum_X \Psi_X. P_X] - 6.625[\varepsilon_n. D + \sum_Y \mu_{ZY}. Z_Y] - 2 \, r_a. N_a - \frac{1}{2} r_o. HS. DO \quad (S21)$$

The air-sea exchanges of surface dissolved oxygen concentration is given by the model of [14] (see also in [15]).

The reaction kinetics governing temporal changes of hydrogen sulphide concentration are given by

$$R(HS) = 0.5 \, \varepsilon_n. D - r_o. HS. DO - r_s. HS. N_n , \qquad\qquad (S22)$$

where the first term represents hydrogen sulphide production by the process of sulphate based anaerobic organic matter decomposition, the second and third terms express the oxidation reactions of H₂S by nitrate and oxygen (Eqs. S19 and S21). The coefficients are given in Table S2.

Table S1. Food preference coefficients of the predator groups on the prey groups.

	Z_S	Z_L	Z_N	Z_G
P_L	--	1.0	0.5	--
P_S	1.0	--	0.5	--
D	--	0.5	1.0	--
Z_S	--	0.5	0.25	1.0
Z_L	--	--	--	0.5
Z_N	--	0.25	--	0.3

Table S2. BSEM input parameters.

Parameter	Value	Unit	Definition
α_L	0.18	$W^{-1} m^2$	Initial slope of P-I curve for P_L
α_S	0.12	$W^{-1} m^2$	Initial slope of P-I curve for P_S
β_L	0.001	$W^{-1} m^2$	Photo inhibition parameter for P_L
β_S	0.035	$W^{-1} m^2$	Photo inhibition parameter for P_S
γ_{ZL}	0.5	d^{-1}	Maximum grazing rate of Z_L
γ_{ZS}	0.8	d^{-1}	Maximum grazing rate of Z_S
γ_{ZN}	0.5	d^{-1}	Maximum grazing rate of Z_N
γ_{ZG}	0.15	d^{-1}	Maximum grazing rate of Z_G
ε_n	0.2	d^{-1}	Default remineralisation rate of D
λ	3.0	$(mmol \, N)^{-1}$	N_a inhibition parameter

Parameter	Value	Unit	Definition
μ_{ZL}	0.05	d^{-1}	Excretion rate of Z_L
μ_{ZS}	0.06	d^{-1}	Excretion rate of Z_S
μ_{ZN}	0.06	d^{-1}	Excretion rate of Z_N
μ_{ZG}	0.08	d^{-1}	Excretion rate of Z_G
σ_L	2.5	d^{-1}	Maximum growth rate P_L
σ_S	2.0	d^{-1}	Maximum growth rate P_S
φ	0.7	-	Assimilation efficiency
a	0.5	mmol N m^{-3}	Half-saturation constant in Eq. S3
b	0.5	-	Half-saturation constant in Eq. S3
d_o	0.15	°C^{-1}	Temperature factor of mineralisation
DO_l	10	mmol O$_2$ m^{-3}	Minimum oxygen concentration Eqs. S6c and d
K_{DO}	150	mmol O$_2$ m^{-3}	Oxygen half-saturation constant for D remineralisation
K_{ZL}	0.5	mmol N m^{-3}	Half-saturation constant for grazing of Z_L
K_{ZS}	0.4	mmol N m^{-3}	Half-saturation constant for grazing of Z_S
K_{ZN}	0.4	mmol N m^{-3}	Half-saturation constant for grazing of Z_N
K_{ZG}	0.25	mmol N m^{-3}	Half-saturation constant for grazing of Z_G
I_n	10	W m^{-2}	Limiting value of light attenuation (Eq. S7a)
m_{PL}	0.04	d^{-1}	Mortality rate of P_L
m_{PS}	0.02	d^{-1}	Mortality rate of P_S
m_{0ZL}	0.25	d^{-1}	Default mortality rate of Z_L
m_{ZS}	0.1	d^{-1}	Mortality rate of Z_S
m_{ZN}	0.15	d^{-1}	Mortality rate of Z_N
m_{ZG}	0.04	d^{-1}	Mortality rate of Z_G
np	16	-	Redfield ratio
Q_{10}	2.0	-	Factor of temperature control
r_a	0.01	d^{-1}	Default oxidation rate of N_a by N_n
r_n	0.1	d^{-1}	Default nitrification rate
r_o	0.01	d^{-1}	Default oxidation rate of HS by DO
r_s	0.01	d^{-1}	Default oxidation rate of HS by N_n
w_D	5.0	m d^{-1}	Detritus sedimentation rate
w_{PL}	0.5	m d^{-1}	P_L sedimentation rate

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