Responses to the interactive comments on the model description paper "ERSEM 15.06: a generic model for marine biogeochemistry and the ecosystem dynamics of the lower trophic level" by M. Butenschön et al.

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1 Answers to Referee P. Wallhead

1.1 On the general comments

Phil Wallhead:

ERSEM is an important and well-known model in marine biogeochemistry and ecosystem modelling. This manuscript provides a detailed description of the latest version and demonstrates its application in several contexts, including 1D and 3D coupled hydrodynamic models as well as new drivers for 0D simulations ("ERSEM Aquarium") and individual parameterization analysis (Python framework). The new version is a significant update since Blackford et al. (2004) and is presented in unprecedented detail. This, combined with the new drivers for implementation and testing, ensures that the manuscript and its supplement constitute a novel and useful contribution to the marine modelling community. Given the scope and complexity of the model the authors have done an admirable job describing it in such detail within a reasonable number of pages. The manuscript is surprisingly readable: I was able to read it through closely over a few sessions, and can imagine that it could be read fairly quickly by a modeller shopping around for a new model. I can therefore see it functioning both as a reference and as an introduction for potential new users. The example implementations and figures towards the end are particularly useful in this latter regard." Where I think there is the most room for improvement is in the explanation and justification of the model. The model structure and formulation represents a large number of modelling choices: the more these can be explained/justified on rational or empirical grounds, the more useful will be this paper, I believe. Citation is a good way of doing this, but in lieu of that even modelling anecdotes could be helpful. The overall ratio (citations : modelling choices) is acceptable in the present manuscript, but I think it could be higher, and there are a few places where I feel that more explanation is clearly needed. I have indicated some places where more explanation is desirable or needed in my specific comments. Overall, I am pleased to recommend this manuscript for publication subject to minor revisions.

Thank you very much for these comments, we are glad to read that the perceived scope of the manuscript matches our intentions. We agree with you that there is space for more detailed information on the choices and background of the model formulations and aim to provide these in the revised version of the manuscript.

1.2 On the specific comments

Phil Wallhead:

p7068, Eqn 1. The last term is not explained. If it is already covered by the fluxes across the sea floor (p7069, l3) then the term should be deleted. If it represents some biogeochemical transformations of pelagic state variables which are particular to the bottom layer and not covered by the \mathcal{F} s, this should be explained here.

The last term would represent indeed the fluxes across the sea floor and should indeed not be there. It is a remainder of a previous notation, which was abandoned as these fluxes are in fact boundary conditions of the pelagic system and should not appear in the general equation for the interior. This equation now reads:

$$\frac{\partial c_{\mathsf{p}}}{\partial t} + \vec{u} \cdot \frac{\partial c_{\mathsf{p}}}{\partial \vec{x}} + \overset{c_{\mathsf{p}}}{w_{\mathsf{sed}}} \frac{\partial c_{\mathsf{p}}}{\partial z} = \nu \frac{\partial^2 c_{\mathsf{p}}}{\partial \vec{x}^2} + \left. \frac{\partial c_{\mathsf{p}}}{\partial t} \right|_{\mathsf{bgc}}$$

Phil Wallhead:

Section 2.2 is a nice addition, very useful for work on coupling ERSEM to physical models.

Thank you.

Phil Wallhead:

p7074, Eqn 4. Might be worth explaining the basis for neglecting nutrient excretion by phytoplankton (e.g. Puyo-Pay et al., 1997).

The formulation of nutrient uptake is based on the main function of phytoplankton, photosynthesis (which is seen as an assimilation of carbon and based on the assumption that nutrients and not carbon are the limiting resource, see also the reply to the following comment). Therefore excretion is focused on the release of excess carbon, while we consider the excretion of nutrients largely negligible. However, the model allows for small releases of nutrients to regulate the internal stochiometry when the actual quota exceeds the storage capacity of the cells and respiration exceeds photosynthesis. In fact the uptake terms (Eq. 5) may turn negative when rest respiration exceeds the assimilated rate or the internal nutrient content exceeds the storage capacity (p7078 first paragraph). This approach is in line with findings that nutrient excretion plays a minor role in the phytoplankton physiology. (Puyo-Pay et al. 1997).

In order to clarify these concepts we have rephrased the corresponding paragraph in the manuscript and expicitly split the uptake term in Eq. 5 in uptake and release:

Nutrient uptake of nitrogen, phosphorus and iron is regulated by the nutrient demand of the phytoplankton group, limited by the external availibility. Excretion is modelled as the disposal of non-utilisable carbon in photosynthesis while the release of nutrients is limited to the regulation of the internal stochiometric ratio. This approach is consistent with observations that nutrient excretion plays a minor role in the phytoplankton fluxes (Pujo-Pay et al., 1997). Consequently, demand of nutrients may be positive or negative in sign in relation to the levels of the internal nutrient storages and the balance between photosynthesis and carbon losses, so that:

$$\frac{\partial \overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{upt} = \begin{cases} \min\left(\left. \mathcal{F}_{demand} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}, \left. \mathcal{F}_{avail} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} \right) & \text{if} \quad \mathcal{F}_{demand} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} > 0 \\ 0 & \text{if} \quad \mathcal{F}_{demand} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} < 0 \\ \frac{\partial \overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{rel} = \begin{cases} 0 & \text{if} \quad \mathcal{F}_{demand} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} > 0 \\ \mathcal{F}_{demand} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} > 0 & \text{if} \quad \mathcal{F}_{demand} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} < 0 \end{cases}$$

The nutrient demand (with the exception of silicate) is computed from assimilation demand at maximum quota $\overset{\chi}{q}_{\max_{\mathbb{N},\mathbb{P},\mathbb{F}:\mathbb{C}}}$ complemented by a regulation term relaxing the internal quota towards the maximum quota and compensating for rest respiration:

$$\begin{aligned} \mathcal{F}_{demand} \Big|_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\chi} = & \overset{\chi}{\mathcal{S}}_{gpp} \left(1 - \overset{\chi}{\mathcal{Q}}_{excr} \right) \left(1 - \overset{\chi}{q}_{aresp} \right) \overset{\chi}{q}_{max_{\mathbb{N},\mathbb{P},\mathbb{F};\mathbb{C}}} \quad \overset{\chi}{\mathcal{P}}_{\mathbb{C}} \\ & + r_{nlux} \left(\overset{\chi}{q}_{max_{\mathbb{N},\mathbb{P},\mathbb{F};\mathbb{C}}} \quad \overset{\chi}{\mathcal{P}}_{\mathbb{C}}' - \mathscr{P}'_{\mathbb{N},\mathbb{P},\mathbb{F}} \right) - \overset{\chi}{r}_{resp} \quad \mathscr{P}'_{\mathbb{N},\mathbb{P},\mathbb{F}} \end{aligned}$$

where r_{nlux} is the rate of nutrient luxury uptake towards the maximum quota.

Note, that these terms may turn negative when rest respira-

tion exceeds the effective assimilation rate $\overset{\chi}{\mathcal{S}}_{\mathsf{gpp}}\left(1-\overset{\chi}{\mathcal{Q}}_{\mathsf{excr}}\right)\left(1-\overset{\chi}{q}_{\mathsf{aresp}}\right)\overset{\chi}{P}_{\mathbb{C}}$

or the internal nutrient content exceeds the maximum quota resulting in nutrient release in dissolved inorganic from. The maximum quota for nitrogen and phosphorus may exceed the optimal quota allowing for luxury storage while it is identical to the optimum quota for iron and silicate.

The uptake is capped at the maximum achievable uptake depending on the nutrient affinities $r_{aff_{PEna}}^{\chi}$ and the external dis-

solved nutrient concentrations:

$$\begin{split} \mathcal{F}_{\text{avail}} |_{\mathcal{N}_{\mathbb{P},\mathbb{F}}}^{\tilde{\mathcal{P}}_{\mathbb{P},\mathbb{F}}} = \overset{\chi}{r}_{\text{aff}_{\mathbb{P},\mathbb{F}}} \mathcal{N}'_{\mathbb{P},\mathbb{F}} \stackrel{\chi}{\mathcal{P}_{\mathbb{C}}}, \\ \mathcal{F}_{\text{avail}} |_{\mathcal{N}_{\mathbb{N}}}^{\chi} = \begin{pmatrix} \chi & \text{ox} & \lambda'_{\mathbb{N}} + \chi & \lambda'_{\text{aff}_{a}} \\ \mathcal{N}'_{\mathbb{N}} + \chi & \mathcal{N}'_{\mathbb{N}} \end{pmatrix} \overset{\chi}{\mathcal{P}_{\mathbb{C}}} \end{split}$$

where the nitrogen need is satisfied by uptake in oxidised and reduced form in relation to the respective affinities and external availability.

Phil Wallhead:

p7074, Eqn 5. It seems that the ERSEM treatment of nutrient limitation departs from Geider et al., 1997, 1998 and Fasham-type models (Fasham et al., 1990) in another important sense. In ERSEM, nitrogen and phosphorus limitation do not impact the gross primary production (as do silicate and iron limitation) but instead increase the rate of excretion and lysis, and also limit chlorophyll synthesis (Eqns 6, 7, 10). This seems to be a key structural difference and presumably has a physiological/experimental basis — I would like some more explanation/references for this difference in the treatment of limitation by different nutrients. A consequence seems to be that ERSEM phytoplankton in nitrogen-limited regimes, such as the surface waters of the subtropical gyres in summer, will go on happily converting DIC to DOC. Might this help to explain the "paradoxical" summer drawdown of DIC at BATS? Other aspects that may deserve explanation/references: 1) Eqn 5 uses a negative exponential form for the saturation of photosynthesis with irradiance, consistent with target theory / a Poisson process (Sakshaug et al., 1991); 2) Eqn 5 predicts that carbon fixation becomes insensitive to temperature and nutrient limitation at low light (physiological justification?).

The formulation in fact combines the form originally presented with ERSEM II in Baretta-Bekker et al. 1997 for the balance of carbon assimilation, excretion and respiration with the negative exponential light harvesting model based on Jassby and Plat 1976, Platt et al. 1982 and Geider et al. 1997 and describes the total specific carbon fixation (total GPP, Eq. 5). In this formulation the gross carbon assimilation is assumed to be not depending on nitrogen and phosphorus. Total GPP is assumed to be composed of a fraction which is assimilated (cellular GPP) through photosynthesis and a fraction which is not utilisable, e.g. due to nutrient limitation, and excreted (dissolved extracellular GPP, Eq. 6). A similar approach can be found in Falkowski and Raven (Aquatic Photosynthesis, pg.

315, Eq. 8.16) although that equation includes also respiration which we describe separately in Eq. 12. In ERSEM, nitrogen and phosphorus limitation is assumed to alter the partition of fixed carbon between cellular and extracellular (dissolved) GPP. The idea behind this assumption is that nutrient limitation (nitrogen and phosphorus) affects more the assimilation of newly fixed carbon into cellular biomass (assimilation) than the photosynthesis itself. It should be noted that by reducing the amount of fixed carbon going into cellular biomass nutrient limitation (although not affecting the specific GPP) does affect GPP indirectly. This means that in a fully nutrient limited environement it will lead to a short continuation of conversion of DIC to DOC which will in any case decay gradually with the phytoplankton biomass. This dissolved (extracellular) component of gross primary production is not considered in Geider et al 1997 or 1998.

We have rephrased this answer into a paragraph that we have added in the begining of the section on primary producers:

The formulation of photosynthesis combines the form originally presented in Baretta-Bekker et al. (1997) for the balance of carbon assimilation, excretion and respiration with the negative exponential light harvesting model based on Jassby and Plat (1976), Platt et al. (1982) and Geider et al. (1997) in order to describe the total specific carbon fixation. In this formulation the gross carbon assimilation is assumed to be not depending on nitrogen and phosphorus. Total gross primary production (GPP) is assumed to be composed of a fraction which is assimilated (cellular GPP) through photosynthesis and a fraction which is not utilisable, e.g. due to nutrient limitation, and excreted. A similar approach can be found in Falkowski and Raven (2007). The idea behind this assumption is that nutrient (or specifically nitrogen and phosphorus) limitation affects more the assimilation of newly fixed carbon into cellular biomass (assimilation) than the photosynthesis itself.

As for the temperature nutrient dependence of the phytoplankton carbon assimilation at low light, note that the metabolic temperature response in form of the Q10 function I_{τ} is not limited to the exponent of the light harvesting, but also included as a proportional factor to the gross carbon assimilation and by that regulates the activity level of phytoplankton at any light level in the same way. Similarly, the internal nutrient limitation will reduce relative carbon assimilation by the same amount at any light level. (In addition nutrient limitation enhaces lysis so affects the organism also at rest.)

Phil Wallhead:

p7076, Eqns 9-10. I think it may be better swap the order here. For me, the "acclimated quota" is really defined by Eqn 10, and then parameterized by Eqn 9. Also, I find the term "acclimated quota" confusing — perhaps a better term would be "nutrient-replete ratio of chlorophyll synthesis to carbon uptake". The word "acclimated" is confusing here because it would seem to imply a ratio under conditions of balanced growth, when C:Chl ratio has adjusted to the ambient light levels. Equation 9 rather seems to parameterize the non-acclimated ratio (cf. Eqn 4 in Geider et al. 1997). Under acclimated conditions, the Chl:C ratio in the denominator might be related to E_{PAR} (cf. Eqn 5 in Geider et al., 1997).

We agree, we have swapped the equations and rephrased accordingly. The corresponding passage now reads:

The synthesis rate of chlorophyll *a* is given by:

$$\left. \frac{\partial \stackrel{\chi}{\mathcal{P}}_{\mathcal{C}}}{\partial t} \right|_{\mathsf{gpp}} = \stackrel{\chi}{l}_{\langle \mathbb{NP} \rangle} \stackrel{\chi}{\varphi} \stackrel{\chi}{\mathcal{S}}_{\mathsf{gpp}} \stackrel{\chi}{\mathcal{P}}_{\mathbb{C}},$$

where $\overset{\lambda}{\varphi}$ is the ratio of chlorophyll *a* synthesis to carbon fixation under nutrient replete conditions. It is given by:

$$\overset{\chi}{arphi} = \left(\overset{\chi}{q}_{arphi \mathsf{max}} - q_{\mathsf{min}_{\mathcal{C}:\mathbb{C}}}
ight) rac{\overset{\chi}{\mathcal{S}_{\mathsf{gpp}}}}{\overset{\chi}{lpha_{\mathsf{PI}}} \mathcal{E}_{\mathsf{PAR}} \stackrel{\chi}{q}_{\mathcal{C}:\mathbb{C}}} + q_{\mathsf{min}_{\mathcal{C}:\mathbb{C}}} \, ,$$

where $\overset{\chi}{q}_{\varphi \max}$ are the maximum achievable chlorophyll *a* to carbon quota for each type, $q_{\min_{c:c}}$ is the minimum chlorophyll *a* to carbon quota.

This formulation differs from the original formulation of Geider et al. (1997) in its asymptotic limit of the carbon to chlorophyll *a* synthesis at high PAR. In the original formulation the ratio is unbound, while in this formulation it is bound by the inverse minimum chlorophyll *a* to carbon ratio $q_{\min_{c:c}}$ in order to avoid excessive quotas not observed in nature.

Phil Wallhead:

p7076-7077, Eqns 11-13. It is not obvious to me that the loss rates from excretion, respiration, and lysis should be the same for both carbon

and chlorophyll. Can these assumptions be justified? For example Geider et al. (1997) do not immediately assume that the chlorophyll respiration rate equals the carbon respiration rate.

While we have implemented a modulation of the chlorophyll a dynamics in photosynthesis regulated by light and nutrient supply, we have simply assumed the loss processes to be proportional to the carbon pool. This is clearly a first order approximation in absense of better knowledge. However, as a side note, also Geider et al. in their 1998 paper in the end assign the specific losses to the same value (eq. 9 of their paper), even if they formally maintain two separate parameters for carbon and chlorophyll a losses. In any case, the ratio of chlorophyll a to carbon seems to be modelled sensibly considering the results of Pina et al. 2015 (figure 3 panel c) and figure 8 of our paper.

Phil Wallhead:

p7077-7078, Eqns 15-18. Again I think a change in order would make for easier reading, so that the reader is not left wondering why "nutrient demand" should be calculated at all. I would start with Eqn 18 to calculate nutrient uptake, then explain that this is limited by internal cellular "demand" and an upper limit imposed by the capacity to actively take up nutrient at the cell surface (here termed "availability", but maybe "max uptake" would be better?). Might also help to remind that the affinities have units [carbon $^{-1}$ time $^{-1}$] unlike the other "r"s. On a scientific note, surely the assumption of a linear dependence of (maximum) uptake rate on external nutrient concentration deserves some comment/references (e.g. Aksnes and Egge, 1991; Franks, 2009)? When a nutrient starved cell is suddenly exposed to a very high external nutrient concentration, it seems likely that the cell-surface uptake capacity would be saturated, which is inconsistent with the linear formulation of Eqns 16, 17. However, internal constraints on nutrient uptake rate (via S_{gpp} and r_{nlux}) would then presumably limit the realized nutrient uptake rate to realistic levels, such that a saturation parameter for uptake at the cell surface might be redundant. . .?

Thanks, we have changed the order of equations accordingly (see answer to comment on 7074, Eq. 4 above for the revised formulation if the manuscript) and added a footnote clarifying the units. As for the nutrient uptake capacity, the formulation is indeed formulated as proportional to the affinity, and thus purely linear, rather than limited by a saturation assumption of Michaelis-Menten type (Aknes-Egge 1991). This is justifyable as our model treats phytoplankton in pools of functional groups, rather than individual species with defined saturation characteristics (Franks 2009). We have rephrased this explanation for the manuscipt in the following paragraph:

This purely linear formulation of maximum uptake proportional to the affinity is in contrast to the more widely used saturation assumption of Michaelis-Menten type (Aksnes and Egge, 1991). It is justified here as ERSEM treats phytoplankton in pools of functional groups, rather than individual species with defined saturation characteristics (Franks, 2009).

Phil Wallhead:

p7079, Eqns 21-23. Should explain why silicate gets this special treatment. Something to do with lack of internal storage...?

The variability of the internal silicate quota of diatoms reported in literature is small and there's little or no evidence of luxury uptake capacity for this element (Brzesinzky, 1985; Moore 2013). These factors combined with the large uncertainties in the silicate cycle have led us to this simplified description of the pelagic silicate dynamics. We have added this clarification to the revised manuscript in the form

The variability of the internal silicate quota of diatoms reported in literature is small and there's little evidence of luxury uptake capacity for this element (Brzesinzky, 1985; Moore 2013). The silicate dynamics of diatoms are therefore modelled by a simple relaxation towards the optimal quota given by the equations: ...

Phil Wallhead:

p7080-7081, Eqns 27-31. Again it would be good to briefly explain where this more elaborate multi-source feeding parameterization comes from. As far as I can tell, it is equivalent to a Fasham-type Michaelis-Menten formulation (Fasham et al., 1990, Eqns 8, 9) with the feeding preference constants multiplied by Michaelis-Menten type "detectability ratios". But it is not clear to the reader what extra is gained by the f_{min} parameters. Chasing down the reference I find that the ERSEM parameterization is a "Class 2D passive switching model" (Gentleman et al., 2003, Table 3a). But can we say anything about why this particular choice was made for ERSEM, among the many possibilities?

The formulation is since the original ERSEM versions (Broekhuizen et al. 1995;Heath et al. 1997) based indeed on a functional response of type

II (Chesson, 1983). The additional parameter f_{min} represents an attempt to include sub-scale processes by adding a detection restriction for an individual prey type on top of the uptake limitation for total prey. In the water volume of a single cell (which within the underlying continuum hypothesis may be consiedered large with respect to prey individuals and small patches) prey, particularly when it is scarce, may be distributed in separate patches. Consequently, if one prey type is scarce while another one is more abundant, the limitation should consider the distinct prey which is achieved here by the additional Michaelis-Menten terms for individual preys.

We have inserted the following paragraph after the zooplankton uptake equations:

This formulation is similar to the approach used in Fasham et al. (1990), but introduces additional Michaelis-Menten terms for inidividual prey types. The purpose here is to include subscale effects of pooling as preys of different types can be assumed to be distributed in separate patches in the comparatively large cell volume. Consequently, individual prey patches below a certain size are less likely to be grazed upon compared

to the larger patches, which is expressed by the h_{\min}^{χ} parameter.

Note, that in response to Referee M. Baird we have relabeld the f_{min} parameters by h_{min} .

Phil Wallhead:

p7082, Eqns 32-34. The parameterization of trophic transfer appears to be a large source of sensitivity/uncertainty in biogeochemical models (Anderson et al., 2013). Can anything be said about how ERSEM developers arrived at this particular formulation?

The formulation goes back to the original ERSEM version I (Broekhuizen et al. 1995) which, based on the standard organism layout (Baretta 1995), uses a fixed assimilation efficiency with a constant fraction lost in faeces. These are accompanied by the activity costs in form of activity respiration, again as a constant fraction of uptake. While there is other approaches to model the trophic transfer, there is no clear indication as too which is the most adequate one (Anderson, 2013).

We rephrased this paragraph in order to include these concepts in the following way:

The ingestion and assimilation of food by the predators is subject to inefficiencies that, given the wide diversity of uptake mechanisms within the zooplankton pools, is for simplicity taken as a fixed proportion of the gross uptake $1 - \frac{\chi}{q_{eff}}$. These losses are attributed to the excretion of faeces as a constant fraction ($\frac{\chi}{q_{excr}}$) and activity costs in form of enhanced respiration ($1 - \frac{\chi}{q_{excr}}$).

The excretion term in Eq. 25 is then given by:

$$\frac{\partial \overset{\chi}{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \Bigg|_{\text{excr}} = \left(1 - \overset{\chi}{q}_{\text{eff}}\right) \overset{\chi}{q}_{\text{excr}} \left. \frac{\partial \overset{\chi}{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{upt}}$$

Respiration losses are composed of the activity costs and a basal respiration term required for maintenance and hence proportional to the current biomass by the constant factor \tilde{r}_{resp} multiplied with the metabolic temperature response (Eq. 231):

$$\frac{\partial Z_{\mathbb{C}}^{\chi}}{\partial t}\bigg|_{\mathsf{resp}} = \left(1 - \overset{\chi}{q}_{\mathsf{eff}}\right) \left(1 - \overset{\chi}{q}_{\mathsf{excr}}\right) \left.\frac{\partial Z_{\mathbb{C}}^{\chi}}{\partial t}\bigg|_{\mathsf{upt}} + \overset{\chi}{r}_{\mathsf{resp}} \overset{\chi}{h}_{\mathsf{T}} \overset{\chi}{Z'}_{\mathbb{C}}$$

This simple formulation of assimilation losses is closely related to the phytoplankton losses described in the previous section following the concept of the standard organism (Baretta 1995) pending a better undestanding of the underlying physiological mechanisms (Anderson et al. 2013).

Phil Wallhead:

p7086, Eqns 45-46. Why is the maximum uptake flux of *R* by bacteria capped at a value of *rR*? What does this represent ecologically? I would have expected a maximum flux proportional to bacterial biomass (*B*), in which case no capping would be needed...

The formulation actually switches from a mode that is proportional to bacteria concentration (when substrate concentrations are sufficiently large with respect to the bacteria concentration) to a mode that is proportional to the substrate biomass (when substrate is scarce compared to bacteria), regulated by the bacteria/substrate ratio. The reasoning behind this approach is that bacteria uptake would be determined by the substrate available up to a certain limit when the individual bacteria uptake is saturated and uptake will become proportional to the bacteria biomass. We have changed the description in the manuscript as follows:

Bacterial uptake of DOM is given by a substrate mass specific turn-over rate r_{lab}^{B} for labile dissolved organic matter when substrate is scarce and by a maximum bacteria mass specific potential uptake regulated by temperature and limited by nutrient and oxygen conditions when substrate is abundant and the uptake per bacteria is saturated , regulated by the ratio of bacteria over substrate biomass:

$$\begin{split} & \overset{B}{\mathcal{S}}_{upt} = \min\left(r_{lab}^{B}, \begin{array}{c} \overset{B}{g} & \overset{B}{max} \end{array} \overset{B}{h_{T}} \overset{B}{l_{0}} \min\left(\overset{B}{l_{P}}, \overset{B}{l_{N}} \right) \frac{B_{\mathbb{C}}}{\frac{lab}{R_{\mathbb{C}}^{\prime}}} \right), \\ & \frac{\partial B_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{upt} = \overset{B}{\mathcal{S}}_{upt} \begin{array}{c} \overset{lab}{R'_{\mathbb{C},\mathbb{N},\mathbb{P}}}, \end{array} \end{split}$$

`

Phil Wallhead:

p7092, I7-15. This is not entirely clear. For example: Does the small POM receive iron input directly from the grazing fluxes of all zooplankton on nano- and picophytoplankton?

That is correct, for the iron component of grazing the size class of particulate matter is given by the prey it derives from, while for silicate it is given by the predator that ingests the material. We have clarified the related description:

In the case of silicate the particulate organic matter types are determined by the predator that ingested the prey and directly releases the silicate contained in the frustule. They are consequently distributed analogous to the zooplankton excretion:

•••

For iron, on the contrary, the size of particulate iron is given by the prey size class and taken analogous to phytoplankton lysis reflecting the assimilation of iron into the cytoplasm:

•••

Phil Wallhead:

p7098. What about aragonite dynamics?

The parameterisation of calcification adopted is undoubtely simple with respect to the complexity of the processes, the diversity of calcifiers and of the minerals (aragonite, calcite, high Mg calcite) involved. Given the limited knowledge of the physiological constraint of calcification, and the need to constrain the number of state variables included in the model (see response to Mark Baird as well), we adopted an implicit parametersation of calcification based on the concept of the rain ratio, i.e. of the CaCO3:POC ratio in the sedimenting flux, where no distinction is made on the type of calcium carbonate.

We have added the following phrase to the manuscript for clarification:

Since the rain ratio has been defined for the sinking fluxes and calcite is the more resistant mineral, we limit the description to calcite in this part of the model, neglecting aragonite.

As a side note, the choice to consider only calcite is common to many biogeochemical models (e.g. PISCES (Gehlen et al., 2007), MEDUSA (Yool et al., 2013), Moore et al., 2002)). In any case, when the carbonate system is solved, saturation state of both forms of CaCO3 are given.

Phil Wallhead:

p7099, Eqn 92. This makes me uneasy about mass conservation. Sedimentation redistributes the living phytoplankton biomass (Eqn 1). But here the sedimentation flux divergence of living phytoplankton contributes directly to the calcite dynamics without any biogeochemical transformation. Wouldn't this "create" carbon from nothing in the lower levels? Doesn't it duplicate the sedimentation term in Eqn 1 applied to calcite?

In the leading paragraph of the section we have alluded to the reasoning of the calcification module that is not a prognostic model based on the actual processes generating calcite. In this approach the amount of calcification in a given time-step is semi-diagnostically derived from a postulated rain-ratio that is approximated from environmental conditions (based on the limitation state of nanopytoplankton, temperature and the current calcite saturation level). To achieve this rain-ratio the local change (and not only production) of particulate carbon is accompanied by a corresponding change in dissolved inorganic calcite. The actual processes of calcification are not modelled here. Nevertheless, the carbon mass is conserved by this description as all the calcite added based on the description mentioned is taken out from DIC (see Eq.s 114, 115). We have added the following phrase towards the end of the calcification section:

Note, that while the calcification rates are implicitly derived from the rain-ratio and not directly modelled processes, this formulation is still conservative as all sources and sinks of calcite are balanced by DIC (see Eq.s 114 and 115).

Phil Wallhead:

p7103, Eqn 111. It's not obvious to me why the remineralization flux of dissolved organic iron might be assumed proportional to the grazing flux from medium POM to mesozooplankton. What exactly is the sequence of events that is being parameterized here? Wouldn't it be better related to zooplankton excretion fluxes?

In general, the dissolution of particulate organic iron to dissolved inorganic iron by bacterial remineralisation is described implicitly in Eq. 64, 65 (see also Vichi et al. 2007). The assumption here is that the feeding activity of zooplankton increases the bio-availability of the particles and accelerates the conversion into dissolved inorganic iron. In addition, there was a minor mistake in the formula as the second term shouldn't have had the *C*, *N* and *P* components, so this passage now reads.

$$\frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\text{remin}} = \mathcal{F}\Big|_{\substack{Z \\ R}}^{\text{MESO}} \quad \substack{\text{med} \\ R'} \quad R'_{\mathbb{F}} + \frac{\partial \overset{\chi}{R}_{\mathbb{F}}}{\partial t}\Big|_{\text{decomp}}$$

It is assumed here that the feeding activity of scavenging zooplankton increases the bio-availability and accelerates the decomposition of particulate iron.

Phil Wallhead:

p7104, I5. Would be nice to have a reference for silicate remineralization being confined to the benthos.

We have added the phrase:

This neglection of silicate conversion into inorganic form in the water column is based on observations that the recycling of this element in particulate form while sinking down the water column is much lower than for the other nutrients, such that most of its remineralisation is confined to the sea-floor (Broecker and Peng, 1982; Dugdale 1995). Nevertheless, we are aware that this is an oversimplification at least in parts of the open ocean and are currently working on an implementation of remineralisation of silicate in the water column that will be added to the next model release.

Phil Wallhead:

p7105, Eqn 125. How is the calcium ion concentration calculated? From salinity?

In the current form it is assumed constant at the oceanic mean concentration based on the lack of relieable data. The calcium ion concentration is fairly constant in seawater (Kleypas et al., 1999), with a little increase in deep oceans and locally strong decreases towards river water. Consequently a salinity regression as suggested would be desirable, but there is few evidence for a robust formulation of such a relationship and the impact of such a formulation would be minor with the exception of major riverine outflows. We have added the following phrase to the manuscript in order to clarify:

The variability of this ratio is dominated by $c_{[CO_3^{2-}]}$ as $c_{[Ca^{2+}]}$ is nearly constant in sea water (Kleypas et al., 1990) and therefore fixed in the model at the oceanic mean value of 0.01028 mol kg⁻¹.

Phil Wallhead:

p7111, l21. If I have understood correctly from reading further, the benthic state variables describe the total content per square metre of all three layers combined (corresponding to the c_b in Eqn 138), so there is strictly no explicit vertical resolution, even between the three layers. When it is necessary to account for layer-specific habitat and predation ranges, the individual layers contents are calculated from the total content and an implicit vertical resolution model (Eqn 151), and a vertical line is used to denote the restriction. However, only the unrestricted total contents are evolved dynamically. Please add something at this point and/or later to clarify this to the reader.

This is correct. We have amended the core paragraph of the introductory Sec. 4.1 to make this concept clearer in the revised manuscript.

The model includes the functional types of aerobic and anaerobic bacteria as decomposers of organic material, three types of benthic predators (suspension feeders, deposit feeders and meiobenthos), dissolved organic matter and three forms of particulate detritus classified according to their availability and decomposition time scales into degradable, available refractory and buried refractory matter.

Benthic state variables are vertically integrated contents (in mass per area) whose vertical distributions are constrained by the following simplifying assumptions: Three distinct layers are considered in the model, a top, aerobic layer that is oxygenated and delimited by the horizon of dissolved oxygen, an intermediate oxidised layer with no free oxygen, but oxidised nitrogen available (also referred to as denitrification layer) and delimited by the horizon of oxidised nitrogen and a completely anoxic deep sediment layer. Given its very shallow penetration into the sediments, for simplicity, also dissolved organic matter is assumed to be restricted to the aerobic layer. Below these layers, limited by the total depth horizon of the model, no biogeochemical processes take place and only buried refractory matter exists.

The chemical components of the types are identical to the pelagic part consisting of carbon, nitrogen, phosphorus, silicate and iron; the silicate and iron cycles are simplified, bypassing the living functional types, in a similar manner to the pelagic part of the model. The silicate contained in detritus is remineralised implicitly into inorganic form in the sediments, while the iron in detritus is directly recycled and returned to the water column.

The vertical distribution of dissolved inorganic and particulate organic matter is crucial in determining the availability of food and resources to the benthic organisms. It is implicitly resolved assuming near-equilibrium conditions for the inorganic components determining the diffusion rate with the overlying water body for the inorganic forms and assumes exponentially decaying distributions for particalute organic mattter. The vertical dynamics of these distributions are described by dedicated state variables that describe the structure of the sediments. These are given by the oxygen horizon (the lower limit of the oxygenated layer and the upper limit of the denitrification layer), the oxidised nitrogen horizon (the lower limit of the denitrification layer and the upper limit of the strictly anoxic layer) and the mean penetration depths for available refractory carbon, nitrogen and phosphorus and degradable carbon, nitrogen, phosphorus and silicate.

Phil Wallhead:

p7113, Eqn 139. I assume this comes from parameterizing the physical exchange as a linear mixing flux and setting the overall tendency to zero? A little more explanation might help.

p7113, Eqn 140. Please explain where this comes from, and why a different equation is needed when $c_p > c_b$. Moreover, why do we care about c_{bed} ?

The change of concentration between cell centre of the pelagic bottom layer and sediment interface is indeed approximated by a linearisation of the diffusive mixing given the equilibrium flux condition at the sediment interface neglecting all other fluxes. The different formulations for positive and negative fluxes are necessary to guarantee positive concentrations. A standard linearisation would risk to generate negative concentrations at the sea-bed when $c_p < \left| p_{\text{vmix}} \frac{\partial c_b}{\partial t} \right|_{\text{bgc}} \right|$. Instead we have opted to use the Patanka scheme here (Patanka, 1980, Sec. 7.2-2; Burchard et al., 2003), which for the case of a net sink in the sediments uses the approximation

$$c_{\text{bed}} = c_p + p_{\text{vmix}} \left. \frac{\partial c_b}{\partial t} \right|_{\text{bgc}} \frac{c_{bed}}{c_p} = c_p \frac{c_p}{c_p - p_{\text{vmix}} \left. \frac{\partial c_b}{\partial t} \right|_{\text{bgc}}}.$$

The concentration at the sea bed c_{bed} is needed as boundary condition for the steady state production-diffusion balance in Eq. 138. We have amended this section as follows:

The sediment surface concentration c_{bed} required as a boundary condition to the production-diffusion balance above is generally not equal to the concentration at the centre of the lowest pelagic discretisation cell c_p , as diffusion across the sediment surface will be attenuated by the bottom boundary layer. In the simplest case the difference between cell centre and sediment surface concentrations can be estimated assuming a linear diffusive flux as positively proportional to the biogeochemical net change in the sediments. However, a problem arises for this formulation when the sediments act as net sink, as the calculated differences may exceed the cell centre concentration suggesting negative concentrations at the sediment interface. Therefore, for negative net sinks in the sediments the formulation suggested by Patankar (1980); Burchard et al. (2003) is applied, leading to the equation:

$$c_{\text{bed}} = \begin{cases} c_{\text{p}} + p_{\text{vmix}} \frac{\partial c_{\text{b}}}{\partial t} \Big|_{\text{bgc}} & \text{if} & \frac{\partial c_{\text{b}}}{\partial t} \Big|_{\text{bgc}} > 0 \\ c_{\text{p}} \frac{c_{\text{p}}}{c_{\text{p}} - p_{\text{vmix}} \frac{\partial c_{\text{b}}}{\partial t} \Big|_{\text{bgc}}} & \text{if} & \frac{\partial c_{\text{b}}}{\partial t} \Big|_{\text{bgc}} < 0 \end{cases}$$

where p_{vmix} is an inverse mixing velocity constant.

Phil Wallhead:

p7114-7115, Eqns 144-147. I would start by assuming Eqn 147 but with a general e-folding depth (say λ). The total c_b is then given by Eqn 144 with D replaced by λ . I think Eqn 145 actually only applies for $d \gg \lambda$ (note the "uv" term $= -\lambda de^{-d/\lambda}$ when integrating by parts). So then we can say that in the limit $d \gg \lambda$, the mean penetration depth $D \approx$ the e-folding scale λ . Eqn 144 as written then follows.

This makes the derivation indeed a lot clearer, thanks. We have rephrased as:

The penetration of organic matter type ψ into the sediments is assumed as exponential decay of a concentration $\overset{\psi}{c}(\zeta)$ from a sediment surface value $\overset{\psi}{c_0}$ as a function of the e-folding depth λ :

$$\overset{\psi}{c}(\zeta) = \overset{\psi}{c}_0 e^{-rac{\zeta}{\lambda}}$$
 .

Total content $\overset{\psi}{c}_{b}$ is then given by the integral

$$\overset{\psi}{c}_{\mathsf{b}} = \overset{\psi}{c}_0 \int_0^{d_{\mathsf{tot}}} e^{-\frac{\zeta}{\lambda}} \mathsf{d}\zeta$$

and the penetration depth $\stackrel{\psi}{D}$ of matter ψ is defined accordingly as

$$\overset{\psi}{D}=rac{1}{arphi}\overset{\psi}{c_{\mathsf{b}}} \int_{0}^{d_{\mathsf{tot}}} \zeta e^{-rac{\zeta}{\lambda}}\mathsf{d}\zeta$$

For $\mathit{d}_{tot}
ightarrow \infty$ the two integrals of Eq.s 2 and 3 yield

$$\lambda = \overset{\psi}{D} = \frac{\overset{\psi}{c_{\mathsf{b}}}}{\overset{\psi}{c_{\mathsf{0}}}}$$

i.e. the mean penetration depth is given by the *e*-folding depth of the distribution function:

$$\overset{\psi}{c}(\zeta) = \overset{\psi}{c}_0 e^{-rac{\zeta}{\psi}}_{D} = rac{\overset{\psi}{c}_{\mathsf{b}}}{\overset{\psi}{\psi}} e^{-rac{\zeta}{\psi}}_{D} \ .$$

Phil Wallhead:

p7115, Eqns 148-150. I'm afraid you lost me here. What is the basis for Eqn 148? Eqn 149 appears to relate a function of depth on the LHS to a constant on the RHS. How does this lead to Eqn 150?

We should indeed have been more explicit. Based on the formulas 144-147 the change of penetration depth due to vertically distributed sources and sinks $f(\zeta)$ can then be calculated by the formula:

$$rac{\mathrm{d}D}{\mathrm{d}t} = \int_0^\infty \left(\zeta - D
ight) rac{f\left(\zeta
ight)}{c_\mathrm{b}} \mathrm{d}\zeta \,.$$

(This can be proven by using Eq.s 145 and 146:

$$dD = D(c(\zeta) + fdt) - D(c(\zeta)) = \frac{c_0 \int_0^\infty \zeta(c(\zeta) + f(\zeta) dt) d\zeta}{c_0 \int_0^\infty (c(\zeta) + f(\zeta) dt) d\zeta} - D$$
$$= \frac{c_0 \int_0^\infty \zeta c(\zeta) d\zeta + \int_0^\infty \zeta f(\zeta) d\zeta dt}{c_0 \int_0^\infty c(\zeta) d\zeta + c_0 \int_0^\infty f(\zeta) d\zeta dt} - D$$
$$= \frac{c_0 \int_0^\infty \zeta c(\zeta) d\zeta + \int_0^\infty \zeta f(\zeta) d\zeta dt - c_0 \int_0^\infty Dc(\zeta) d\zeta - \int_0^\infty Df(\zeta) d\zeta dt}{c_0 \int_0^\infty c(\zeta) d\zeta + c_0 \int_0^\infty f(\zeta) d\zeta dt}$$
$$= \int_0^\infty (\zeta - D) \frac{f(\zeta)}{c_b} d\zeta dt.$$

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As the model is not vertically explicit, but based on the model assumptions, processes can be attributed to layers (e.g. activity of aerobic bacteria to the aerobic layer), the changes \mathcal{F}_i caused in a given layer can be attributed to discrete depth levels being the centre of the layer ζ_i , so that

$$\frac{\mathrm{d}D}{\mathrm{d}t} = \sum_{i} \left(\zeta_{i} - D\right) \frac{\mathcal{F}_{i}}{c_{\mathsf{b}}}.$$

This is complemented by movement of sediment material in bioturbation that smoothes the concentration gradient and is therefore implemented as diffusive flux proportional to the difference in concentrations between 0 and a bioturbatation length scale δ_{bturb} .

However, there was a typo in Eq. 149 which has obscured this step, the correct form is

$$\left. rac{\partial D}{\partial t}
ight|_{ ext{bturb}} = rac{
u_{ ext{bturb}}}{rac{\psi}{c_{ ext{b}}}} (rac{\psi}{c_0} - rac{\psi}{c}(\delta_{ ext{bturb}})) \,,$$

Eq. 150 is then simply the result of inserting the vertical profile of Eq. 147 into this equation. We have amended the corresponding section of the manuscript as follows:

The change of penetration depth due to vertically distributed sources and sinks $f(\zeta)$ can then be calculated by the formula:

$$rac{\mathrm{d}D}{\mathrm{d}t} = \int_0^\infty \left(\zeta - D
ight) rac{f\left(\zeta
ight)}{c_\mathrm{b}} \mathrm{d}\zeta\,.$$

As the model is not vertically explicit, but, based on the model assumptions, processes can be attributed to layers (e.g. activity of aerobic bacteria to the aerobic layer), the changes \mathcal{F}_i caused in a given layer can be attributed to discrete depth levels being the centre of the layer ζ_i .

The changes of penetration depth due to source and sink terms are complemented by the physical displacement of organic matter by the process of bioturbation, so that the total change is given by the equation:

$$\frac{\partial \overset{\psi}{D}}{\partial t} = \sum_{i} (d_{i} - \overset{\psi}{D}) \frac{f_{i}}{\overset{\psi}{C}_{b}} + \left. \frac{\partial \overset{\psi}{D}}{\partial t} \right|_{\text{bturk}}$$

Bioturbation smoothes the concentration gradient and is therefore implemented as diffusive flux proportional to the difference in concentrations between 0 and a bioturbatation length scale δ_{bturb}

$$\left. rac{\partial D}{\partial t}
ight|_{ ext{bturb}} = rac{
u_{ ext{bturb}}}{\psi} (\stackrel{\psi}{c_0} - \stackrel{\psi}{c} (\delta_{ ext{bturb}})) ,$$

where ν_{bturb} is the bioturbation diffusivity of particulate matter (Eq. 210). Still assuming that $\overset{\psi}{D} \ll d_{\text{tot}}$, this takes the form

$$\left. \frac{\partial D}{\partial t} \right|_{\text{bturb}} = \frac{\nu_{\text{bturb}}}{D} \left(1 - e^{-\frac{\delta_{\text{bturb}}}{\psi}} \right) \,. \tag{1}$$

Phil Wallhead:

p7117, I13-14. Reference to support exclusive feeding on particulates by anaerobic bacteria?

The exclusive feeding on particulates by anaerobic bacteria is a consequence of the vertical strucure of the model design which assumes for simplicity that dissolved matter is confined to the aerobic layer as the reduced solubility in the lower layers doesn't allow organic material in dissolved form. This should have been included in the introduction to the benthic form and is now included in the amended introduction quoted above in the reponse to the comment on p7111, l21. Consequently the anaerobic bacteria can not obtain dissolved matter.

Phil Wallhead:

p7117, l15-17. Reference to support preferential uptake of organic nitrogen/phosphate?

We have provided a reference:

The uptake of organic nitrogen and phosphorus is enhanced by a nutrient preference factor $\stackrel{\chi}{p}_{nup}$ supported by observations that the relative nutrient content of benthic DOM decreases under bacteria production (van Duylet al., 1993). It is complemented by the uptake of inorganic forms when organic matter is nutrient-poor with respect to the fixed bacterial stoichiometric ratio.

Phil Wallhead:

p7118, l8. Anaerobic bacteria really only excrete particulate matter? Please provide a reference.

This is again based on the simplifying model assumption that the depth horizon of dissolved matter conincides with the aerobic layer. Consequently all organic matter generated by aerobic bacteria in the sediments is of particulate form.

Phil Wallhead:

p7119, Eqn 163. Doesn't the oxygen dependence only apply to aerobic bacteria?

No, in both layers the mortality is enhanced at low oxygen, but while for the aerobic bacteria the enhancement occurs due to reduced dissovled oxygen leading to a thinner aerobic layer, for the anaerobic bacteria it is enhanced by reduced levels of oxidised nitrogen and a thinning of the reduced layer (see Eq. 244). We have clarified this in the manuscript now:

Bacterial mortality is fully regulated by oxygen (see Eq. 244) and proportional to the bacteria biomass by factor r_{mort}^{χ} :

$$\left. \frac{\partial \overset{\chi}{\mathcal{H}}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\mathsf{mort}} = \overset{\chi}{r}_{\mathsf{mort}} \left(1 - \overset{\chi}{l_{\mathbb{O}}} \right) \overset{\chi}{\mathcal{H}'}_{\mathbb{C},\mathbb{N},\mathbb{P}} .$$
 ,

where aerobic bacteria use oxygen in dissolved form while anaerobic bacteria satisfy their oxygen requirements from oxidised nitrogen.

Phil Wallhead:

p7120, Eqn 166. Why do we have the food preference constants in the detectability fraction, unlike in the pelagic (e.g. Eqn 27)? Same comment for Eqn 168.

The reasoning here is that while the pelagic predators may be considered more passive feeders benthic feeders are assumed to search for prey more actively. Consequently the detection capability for the benthic fauna is assumed to vary by food-source as preferred food will attract the predator at relatively lower amounts. We have updated the manuscript to include this concept:

The total prey available to each zoobenthos type χ is composed of the individual prey types ψ as

$$\Pr^{\chi}_{\mathbb{C},\mathbb{N},\mathbb{P}} = \sum_{\psi} \left. f_{\mathrm{pr}} \right|_{\psi}^{\chi} \frac{f_{\mathrm{pr}} \left|_{\psi}^{\chi} \psi_{\mathbb{C}}'}{\left. f_{\mathrm{pr}} \right|_{\psi}^{\chi} \psi_{\mathbb{C}}' + h_{\mathrm{min}}^{\chi}} \psi_{\mathbb{C},\mathbb{N},\mathbb{P}}',$$

where $f_{pr}|_{\psi}^{\hat{Y}}$ are the food preferences and h_{min}^{χ} is a food half-saturation constant limiting the detection capacity of predator

 χ of individual prey types similar to the zooplankton predation (Eq. 27). In contrast to the pelagic form the detection capability for the benthic fauna is assumed to vary by food-source assuming that benthic predators search their food more actively. The prey contents in the half-saturation term are consequently multiplied by the food-preferences.

Phil Wallhead:

p7125, Eqn 181-182. I find this whole derivation a bit dubious. Eqn 182 implies that burial only occurs when the mean penetration depth *D* is changing, but in a system in quasi-equilibrium I would expect a constant burial flux even with a constant *D*. The argument seems to be based on approximating the burial flux as the product of a 'burial velocity', independent of the concentration, and the concentration at the total depth. But this sounds more like an advective flux, whereas the sediment system is earlier assumed to be diffusion-dominated for inorganic states (Eqn 138). I would have rather expected an argument based on a diffusive flux at the total depth. Assuming the exponential decay profile and a constant organic matter diffusivity ν_{odiff} , this diffusive flux would result in a burial rate independent of the rate of change of *D*:

$$\left. \frac{\partial Q}{\partial t} \right|_{bur} = \frac{\nu_{odiff} Q}{D^2 (1 - e^{-d/D})} e^{-d/D}$$

Perhaps there is in fact a good foundation for Eqn 182 but if so it should be better explained here (noting that the Kohlmeier 2004 reference is in German).

The use of the term velocity was misleading here. The reasoning behind this formulation is as follows: bioturbation will inevitably lead to redistribution of matter that will eventually carry matter across the total horizon for biogeochemical processes. As bioturbation is stronger in the uppermost part of the sediments (as expressed by equation 150), the assumption of a flat diffusivity is unsatisfactory. However, it is possible to derive the burial flux from the time derivative of the integrated sediment content between the surface and the depth horizon, using Eq.s 147 and 152. This derivation is straight-forward, but somewhat lengthy, so we have devided to replace it hear by a simple geometric argument assuming that the change of penetration depth maintains its exponential shape stretching the original profile. The flux across any depth interface is then given by the local concentration times the dislocation rate of the profile. We stress again that this is a purely geometrical argument here that doesn't correspond to an advective process.

Unfortunately, the explanation was further obscured by the arbitrary use of *z* and ζ for the depth coordinate (which should have been ζ throughout in this paragraph) and the subscript "diff", which should have been "bturb" as given in Eq. 150.

We have removed these mistakes and replaced the paragraph by the following text in order clarify the derivation of the burial flux:

The diffusive process of bioturbation leads to the downward displacement of refractory material. The resulting flux of refractory organic matter across the total depth horizon of living organisms in the model d_{tot} may be interpreted as burial flux (activated by the ISWbur switch), as material is removed from the biogeochemical active part of the model.

To derive this flux we use a simple geometric argument here: it is assumed that the diffusive process will preserve the vertically exponential distribution of refractory organic matter (Eq. 147), stretching it. Consequently the flux across any horizontal interface can be expressed as the product of the local concentration ${}^{refr}_{C,\mathbb{N},\mathbb{P}}$ and the displacement rate of the exponential profile at the given level. Specifically, we know that the local displacement rate at the level of the penetration depth is precisely the change of penetration depth due to bioturbation

$$\frac{\partial \frac{D}{D}}{\partial t}$$

To derive the local displacement rate of the exponential profile at the total depth we can use the displacement time scale at d_{tot} , that is independent of the local concentration:

$$\frac{1}{\tau_{\mathsf{bur}}(\zeta)} = \frac{1}{\Pr_{\mathcal{C}_{\mathbb{C},\mathbb{N},\mathbb{P}}(\zeta)}^{\mathsf{refr}}} \frac{\partial \stackrel{\mathsf{refr}}{\mathcal{C}_{\mathbb{C},\mathbb{N},\mathbb{P}}(\zeta)}}{\partial t} = \frac{\zeta}{\Pr_{\mathcal{C}_{\mathbb{N},\mathbb{P}}}^2} \frac{\partial \stackrel{\mathsf{refr}}{D}}{\partial t} \bigg|_{\mathsf{bturb}}$$

Scaling the disclacement rate with this scale the flux of matter

at d_{tot} , and hence the burial flux, can be computed as:

$$\frac{\partial \overset{\text{refr}}{Q}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{bur}} = \overset{\text{refr}}{c} \underset{\mathbb{C},\mathbb{N},\mathbb{P}}{\underset{\mathbb{C},\mathbb{N},\mathbb{P}}{\text{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}} \left(d_{\text{tot}} \right) \frac{\tau_{\text{bur}}(\overset{\text{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{D}}{\tau_{\text{bur}}(d_{\text{tot}})} \frac{\partial \overset{\text{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{D}}{\partial t} \bigg|_{\text{bturb}} = \overset{\text{refr}}{c} \underset{\mathbb{C},\mathbb{N},\mathbb{P}}{\underset{\mathbb{C},\mathbb{N},\mathbb{P}}{\text{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}}} \frac{\partial \overset{\text{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{D}}{\partial t} \bigg|_{\text{bturb}} = \frac{\overset{\text{refr}}{c} \underset{\mathbb{C},\mathbb{N},\mathbb{P}}{\underset{\mathbb{C},\mathbb{N},\mathbb{P}}{\text{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}}}{\overset{\text{refr}}{D} \left(1 - e^{-\frac{d_{\text{tot}}}{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}}\right)} e^{-\frac{d_{\text{tot}}}{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}} \frac{\partial \overset{\text{refr}}{D}}{\partial t} \bigg|_{\text{bturb}}}$$

This result can be formally confirmed by a straight-forward, but fairly lengthy derivation of the time derivative of the integrated content of refractory matter between the sediment surface and d_{tot} using Eq. 147 and Eq. 152.

Note that this process removes biomass from the biogeochemically active part of the model, as there are no processes connected to buried organic matter and the model currently does not consider remobilisation. This means that during long term simulations the loss of nutrients needs to be compensated, e.g. by riverine inputs or atmospheric deposition (carbon is restored by air-sea exchange).

Note, that this formulation is absent in previous references (e.g. Kohlmeier).

Phil Wallhead:

p7135, I6. Only the slowly or never degrading part of the sediment matter is eroded?

The particulate matter in the benthos is actually split in slowly degrading and refractory matter so the "slow" labled POM is actually the faster degrading one, as the slow was originally intended with respect to the DOM. In resuspension we take only this more available part labled as slowly degradable into consideration while the fully refractory part is more compact in structure and assumed to have a higher penetration depth. It is therefore not considered in resuspension. In response, we have in any case decided to relable the slowly degradable matter to degradable matter in order to avoid confusion.

Phil Wallhead:

p7136, l3. Not clear how this slope (units mass-length $^{-4}$) is translated into a time scale.

This formulation is indeed not very precise and unclear. We have extended the paragraph which now reads:

For phosphorus, ammonium, silicate and DIC the relaxtion fluxes towards equilibrium are computed by assuming a parabolic vertical distribution of excess biomass with 0 surface concentration and 0 bottom flux and assuming contributions to the generation of the excess proportional to the layer depth. The compensation flux across the seabed is then again computed from the production-diffusion balance in Eq. 138.

Phil Wallhead:

p7151, I1-11. It looks like there is also an persistent underestimation of summer nutrient levels, consistent with the weak secondary blooms mentioned in the text. Perhaps the benthic system is not remineralizing fast enough (cf. silicate), or GOTM is not capturing enough summer mixing events... I notice also an apparent decreasing trend in the surface oxidized nitrogen, perhaps also because of too-weak benthic return fluxes. It's also notable that the interannual variability in the model seems consistently weaker than in the data (Figures 2 and 3). Perhaps some aspect of the forcings is responsible?

While there is clearly some weaknesses in the representation of the summer chlorophyll a compared to the observational data, which may well be caused by the slighter underestimation of oxidised nitrogen, speculations as for the cause of these are difficult in the idealised 1D context. The Oyster Ground site is characterised by strong lateral influences including estuarine, coastal and channel waters that include strong direct impacts on the nutrient concentrations in the area. Particularly in the stratified season in summer these lateral effects are dominating the surface water signal while the deeper part of the depression is essentially isolated from the surface layer (see Weston et al. 2008). Similarly, the interannual variability can be expected to be dominated by relative variations in the prevailing currents of the area, that is receiving inflows from the continental coast, the channel, the English coast and the central North Sea and can not be fully captured in this 1D case study. We have included these considerations in the revised manuscript:

In addition, some deficiencies, in the model simulations are to be expected as the Oyster Ground site is characterised by strong lateral influences including estuarine, coastal and channel waters that include strong direct impacts on the nutrient concentrations in the area that can not be captured in this idealised setting. Particularly in the stratified season in summer these lateral effects are dominating the surface water signal while the deeper part of the depression is essentially isolated from the surface layer (Weston et al., 2008)

1.3 On the technical comments / typos

Phil Wallhead:

"food web" not "food-web"

"North Sea" not "North-Sea"

"case study" not "case-study"

p7065, I1. "Given the importance of these applications, transparent descriptions..."

p7065, l9. "occurred"

p7065, l19. "a scientific tool"

p7065, l22. "Allen et al. (2001) adopted"

p7065, l23. "Holt et al. (2012) and Artioli et al. (2012)"

p7065, l24. "Blackford et al. (2004) applied"

p7065, l25. "Barange et al. (2014) used applications of the model in the major coastal upwelling zones of the planet, and..."

p7066, l1. "(2014) have assessed the skill of the model, demonstrating..."

p7066, l9. "climate change"

p7066, l21. "nitrogen, phosphorus,"

p7066, l24. "The present paper provides a full description of all model components, simple case studies illustrating the model capabilities in an idealised mesocosm type framework and three vertical water-column implementations of opposing character, and a brief illustration of a full-scale three dimensional application."

p7067, l4. "licence" assuming this is UK English. p7067, l17. "feedback"

These have been corrected, thanks.

Phil Wallhead:

p7070, I7-8. Actually the \mathcal{F} is used in many instances to denote rates with units [time $^{-1}$] rather than fluxes with units [concentration time $^{-1}$] (e.g. Eqns 14, 20, 23, ...). Perhaps those \mathcal{F} s should be changed to \mathcal{S} s?

The different letters as we use them are not so much about their units, but about the underlying processes: while S is more for rates related to

physiological processes of a functional type like specific uptake or lysis, \mathcal{F} is used for uptake fluxes that are directed from one functional type to another.

Phil Wallhead:

p7070, l17. "equations" p7070, l26. "exception" p7071, l14. "radiation" p7071, l16. "coefficients" p7071, l20. Latex failure. p7072, l3. "numerical" p7072, l19. "heterotrophic nanoflagellates" p7072, l25. "silicic" p7073, l5. "simplicity; their pathways. . ." p7073, l7. "dissolved"

p7073, l19. "a net result"

These have been corrected, thanks.

Phil Wallhead:

p7074, l15. Shouldn't this be Geider et al., 1998?

Either of the two works as example here, but we had the Geider et al. 1997 paper in mind, specifically table 2.

Phil Wallhead:

p7075, Eqn6. Q_{exc} should be the fraction excreted, but the RHS appears to be 1 minus this fraction.

In fact, we have corrected this.

Phil Wallhead:

p7075, Eqn7. Doesn't this blow up (or give poor numerics) as either limitation factor approaches zero?

In fact this formula has been transcribed erroneously from the code, the corrected equation now reads:

$$\overset{\chi}{\mathcal{S}}_{\mathsf{lys}} = \frac{1}{\min\left(\overset{\chi}{I_{\langle \mathbb{NP} \rangle}}, \overset{\chi}{I_{\mathbb{S}}}\right) + 0.1} \quad \overset{\chi}{r_{\mathsf{lys}}} \, .$$

(See also Blackford et al. 2004, Eq. 7.)

Phil Wallhead:

p7076, I5. Break this sentence in two, e.g.: "This formulation differs from the original formulation of Geider et al. (1997) in its asymptotic limit of the carbon to chlorophyll a synthesis at high PAR. In the original formulation..."

p7076, l16. Remove "consequently".

p7079, Eqn 24. Missing parentheses around pCO2-379.48.

Corrected.

Phil Wallhead:

p7081, Eqns 28-30. The notation may be a bit confusing here. Eqn 28 uses a "specific uptake capacity" S, but it is not specific to the uptaker concentration (as it was for phytoplankton uptake of nutrients), but rather to the concentration of "total available prey" (this could be made clearer by a second equality in Eqn 30). Seems it would have been better to define S_{growth} via Eqn 28 with Pr substituted for Z (and adjust Eqn 29). Maybe too dangerous to redefine anything now. Perhaps the best solution is to replace "specific" in 11 with "total prey-specific" and in 15 with "prey-specific".

We should indeed have stated to what state the specific rate refers. We have clarified the use of specific not only here, but throughout the manuscript, in reponse to a similar, more generic comment by referee M. Baird. As for the motivation of the prey uptake formulation we hope our earlier answer on the specific comment related to p7080-81, Eqs. 27-31 has clarified the reasoning behind.

Phil Wallhead:

p7082, I5. "activity-related"

Corrected.

Phil Wallhead:

p7082, Eqn 33. $\frac{\partial Z}{\partial t}\Big|_{growth}$ is not defined.

This should have been $\frac{\partial Z}{\partial t}\Big|_{upt}$ and has been corrected.

Phil Wallhead:

p7084, Eqn 38. It would be better to write this as a sum of concentrations multiplied by layer thickness, divided by the total water column height.

We have voluntarily used the integral in line with all the rest of the mathematical description that is formulated in continous rather than discrete space. It is not divided by the water column height as the criterium we want to use for hibernation of mesozooplankton (that within limits are able to move vertically) is the vertically integrated prey mass and not an average concentration.

We have in any case corrected the formula, which was missing the final dz.

Phil Wallhead:

p7086, Eqns 45-46. Again I think it would have been better to define the rate Supt as a flux specific to bacterial biomass instead of available DOM.

The formulation of bacteria uptake of substrate is in fact switching between saturated uptake when substrate is abundant (proportional to bacteria biomass) and substrate-limited uptake, which is proportional to the substrate available and consequently substrate specific. See also the answer to the specific comment related to p7086, Eqns 45-46.

Phil Wallhead:

p7087, Eqns 49-50. r_{lab} should be replaced with r_{rel} ? p7087, l16. "occurs"

Corrected.

Phil Wallhead:

p7091, Eqn 64. Might be clearer to divide by $q_{refN:C}$, so that the ratio $q_{refN:C}/q_{refN:C}$ can be seen as a factor accounting for nutritional status (from the point of view of the decomposing bacteria that are not explicitly resolved).

This would in fact be clearer in the equation, but we have chosen to stick to the $\mathbb{C} : \mathbb{N}$ parameter for easy comparison as this is usually used in literature (e.g. the Redfield ratio is usually expressed as $\mathbb{C} : \mathbb{N}$).

Phil Wallhead:

p7098, Eqns 86 and 87. I think there are three typos: "upt" in overhead of Eqn 86, and "lab" in two overheads in Eqn 87, unless I missed something.

That's correct, apologies for the careless editing.

Phil Wallhead:

p7098, l16. Replace "where" with something like: "The dynamics of particulate inorganic carbon (or "calcite") may be decomposed as:"

We have replaced with:

The calcite dynamics are then described by the equation:

Phil Wallhead:

p7100, l1. Insert something like "(plus scavenging of dissolved inorganic iron)"

We have added the phrase:

Dissolved inorganic iron is additionally subject to scavenging.

Phil Wallhead:

p7108, l8. "non-modelled forms of inorganic matter and the back-ground. . ."

Corrected.

Phil Wallhead:

p7110, l10. The *R* for calcite has changed into an *L*.

For consistence with the code lable and the state variable table, it is actually the R^{calc} s in the equations above that should have been L^{calc} s. This has been changed consistently throughout the manuscript now.

Phil Wallhead:

p7111, l23-24. "the silicate and iron cycles are simplified, bypassing the living functional types in a similar manner to the pelagic part of the model"

Corrected.

Phil Wallhead:

p7111, l27. Clash of singular "a particularity" with plural "are" - rephrase.

This has been replaced by

In addition, the benthic model includes dedicated state variables that describe the vertical strucutre of the sediments, given by ...

Phil Wallhead:

p7113, l2. "biogeochemical" p7114, l9. Should be c_b not c I think. p7115, Eqn 151. Surplus "/"

p7117, Eqn 158. Shouldn't the *R*s be *Q*s for the benthos?

p7118, Eqn 159. Shouldn't that be a Q instead of H in the first term on RHS?

p7121, l2. "capable of feeding on itself"

Corrected.

Phil Wallhead:

p7121, Eqns 170-171. The uptake terms should be specific to the ϕ ("upt, ϕ "), or use the *F*s.

We have corrected using the Fs:

$$\frac{\partial \overset{\chi}{\mathbf{Y}_{\mathbb{C}}}}{\partial t} \bigg|_{\mathsf{excr}} = \sum_{\psi}^{\psi \neq \overset{\mathsf{degr} \, \mathsf{med}}{Q}, \overset{\chi}{R}} \overset{\chi}{q}_{\mathsf{excr}} \mathcal{F} \big|_{\psi}^{\overset{\chi}{\mathbf{Y}}} \psi_{\mathbb{C}}' + \sum_{\psi}^{\overset{\mathsf{degr} \, \mathsf{med}}{Q}, \overset{\chi}{R}} \overset{\chi}{q}_{\mathsf{pexcr}} \mathcal{F} \big|_{\psi}^{\overset{\chi}{\mathbf{Y}}} \psi_{\mathbb{C}}'$$

$$\frac{\partial \overset{\chi}{\mathbf{Y}_{\mathbb{N},\mathbb{P}}}}{\partial t} \bigg|_{\mathsf{excr}} = \overset{\chi}{q}_{\mathsf{dil}} \left(\sum_{\psi}^{\psi \neq \overset{\mathsf{degr} \, \mathsf{med}}{Q}, \overset{\chi}{R}} \overset{\chi}{q}_{\mathsf{excr}} \mathcal{F} \big|_{\psi}^{\overset{\chi}{\mathbf{Y}}} \psi_{\mathbb{N},\mathbb{P}}' + \sum_{\psi}^{\overset{\mathsf{degr} \, \mathsf{med}}{Q}, \overset{\chi}{q}_{\mathsf{pexcr}} \mathcal{F} \big|_{\psi}^{\overset{\chi}{\mathbf{Y}}} \psi_{\mathbb{N},\mathbb{P}}' \right)$$

Phil Wallhead:

p7125, l1. "Note that this..." p7125, l3. "does not" p7131, l2. "atmospheric inputs, otherwise denitrification..." p7133, Eqn 209. Shouldn't the "depo" and "sed" be subscripts and the

"cp" overhead

Corrected.

Phil Wallhead:

p7133, l10. Is it an *R* or an *L* for calcite? Be consistent!

It should in fact be *L*, we have made this consistent across the manuscript.

Phil Wallhead:

p7135, l2. "In the case" p7135, l13-14. "towards equilibrium" p7136, l23. "cycle" p7137, l16. "identical between" Corrected.

Phil Wallhead:

p7138, Eqn 229. Should the *G* be an *O*? The "s" is also not defined in the text.

It should indeed, corrected. The oxygen saturation $s_{\mathbb{O}}$ mentioned here is actually the same as the one in Eq. 240 and is given in the supplements, we have added the reference to the supplements also at this point:

The regression formula for s_0 is given in the Supplement.

Phil Wallhead:

p7144, I7. Should be > or < 1?

Corrected.

Phil Wallhead:

p7145, Eqn 258. pcrowd on the LHS and RHS?

These should have read $\stackrel{\chi}{p}_{\mathbb{C}}$ throughout the RHS. In addition the result should have been constrained to a lower limit of 0 by a maximum function:

$$\overset{\chi}{p}_{\mathsf{crowd}} = \max\left(0, \, \overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p}_{\mathbb{C}}\right) \frac{\overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p}_{\mathbb{C}}}{\overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p}_{\mathbb{C}} + \overset{\chi}{h_{\mathsf{sat}}}}$$

Phil Wallhead:

p7149, l10. Better "strong nutrient limitation"? p7149, l11. "microbe dominated" p7149, l14. "an order of magnitude"

Corrected.

Phil Wallhead:

p7155, l22. Shouldn't this read "product of the chlorophyll a content and PAR"?

It should indeed, it's the carbon-specific rate that is proportional to PAR and the chlorophyll a to carbon ratio, so that the actual absolute rate is proportional to irradiation and chlorophyll a. In any case, the corresponding phrase has been removed in response to a comment by Yool et al.

Phil Wallhead:

p7157, l2. "pigment complements"

Corrected.

2 Answers to Referee Mark Baird

Marc Baid:

The ERSEM model is one of the most sophisticated biogeochemical models available for shallow water ecosystems. It contains a broad range of elements (C, N, P, Si, Fe), has dynamic quotas for 4 phytoplankton types, 3 zooplankton types, bacteria mediating remineralisation, a carbon / oxygen chemistry suite, as well as a benthos with three zooplankton. There are models with more sophisticated optical sub-models, sizeresolution of plankton, benthic plants and sediment chemistry (metals etc.), but in general ERSEM contains one of the broadest set of processes of any available model. The representation of bacteria in the microbial loop is, in particular, world-leading. This manuscript describes in detail the ERSEM model with the ambitious goal to be the definitive complete mathematical description for users of this model at its present, mature state. In general the manuscript achieves this goal, although a significant number of errors appear in the text that need attention, and elements of the structure are worth considering. I am a strong supporter of peerreview publication of this type of work and wish to provide the following comments in order to improve the manuscript. Any bluntness in the comments is due to brevity, as I understanding the challenge in achieving an error-free document with this many details. Thank you for your commitment to the thorough scientific presentation of your biogeochemical model.

Thanks again for your effort and time in reviewing our work, we are glad to receive your constructive feed-back and suggestions.

2.1 On the major comments on clarity

Marc Baid:

It is awkward that Eqs. like (3) consider all dP/dt terms to be positive (i.e. dP/dt|pred is positive), such that it must be subtracted from growth in Eq. 3. Of course dP/dt due to predation is negative. This awkwardness is compounded later when the individual terms are calculated. For example Eq. 32 gives excretion being equal to uptake, when in fact the terms are the negative of each other. I would suggest that dP/dt|pred be negative, as well as all other loss terms. This issue comes up many times in the manuscript.

We understand the problem of a loss term being positively correlated to a production term, but we had to make a choice here:

- either we incorporate the sign into the sub-process (as you suggest) to have loss processes anticorrelated to the production term they originate from, stating all processes of the overall balance equations in a simple sum,
- or we distinguish already at the top level between loss and production terms putting the sign in the actual balance equation and assume all sub-processes as positive amounts.

We have voluntarily opted for the latter approach which seemed clearer and more immediate to us to show at a first glimpse what increases and what decreases the respective state. As a side note, this approach is not particular to our work, but has been used in other related works (e.g. Vichi et al. 2007, Fasham 1990, Fennel 1995).

Marc Baid:

2. The symbol 'q' is overused, resulting in confusion. 'q' is used as a quota, a fraction, and a turnover rate. In principle, it would be best to assign a symbol one class of entity to quantify, and then use subscripts and superscripts to be more specific.

We feel that a single letter representing fractions and proportions is restrictive enough to make a logical and conceptual distinction between parameters, but We agree that the letter "q" should not be used as turnover rate, as this is substantially different to the other uses. However, we could not find any such occurences.

Marc Baid:

3. The quotas are state variables? Wouldn't you need a set of equations to describe their advection and diffusion like Eq. 1 that conserves mass? In Section 3.2 of J. Mar. Sys. 50 (2004) 199– 222 I give a description of how conservation of mass is achieved in the advection of quotas. Is this what you do?

The quotas themselves are not state variables. The actual state variables are the components or constituents of the functional groups, e.g. the diatom carbon concentration and the diatom nitrogen concentration, rather than its carbon to nitrogen quota. Hence the actual differential equations are solved on these (conservative) states, while the quotas are a purely diagnostic consequence. We have clarified this in the statement describing the model state variables under Eq (1):

"...where c_p are the pelagic concentrations (per volume) and c_b the benthic contents (per sediment surface area) of each chemical component of the organic model types or the inorganic model components."

Marc Baid:

4. The use of calligraphic symbols for chemical elements does not abide by conventions in chemistry, although it is still clear.

We assume this refers to the subscripts \mathbb{C} , \mathbb{N} , \mathbb{P} , \mathbb{S} , \mathbb{F} . We have chosen to distinguish these from the general font used to evidence them with respect to the "descriptive" subscripts. We believe this facilitates the reading of the equation, even if it breaks with the conventions used in purely chemical literature.

Marc Baid:

5. 'Specific' is used regularly though the text, but we are not told whether it is carbons-pecific etc. In a model with varying stoichiometries I think this is important. Without this I had trouble with the Eqs. on p7081, as noted below.

Generally, when we say specific, it would be specific with respect to all chemimical components of a state. E.g. a specific mortality becomes absolute carbon, nitrogen or phosporus loss by multiplying it with the current carbon, nitrogen or phosporus concentration. We agree however
that there is considerable ambiguity in our use of specific that led to confusion (see also some of the comments below), particularly in the cases you mention, where rates are specific to prey rather than predator concentrations. We have ensured that all uses of specifc rates are clearly defined in the revised manuscript.

Marc Baid:

6. The terms lysis and mortality are used interchangeably at times. Are they the same thing in the model?

Mostly mortality would consist of lysis, but there are some exceptions. E.g. in the case of zooplankton it would also include predation by nonmodelled organisms. For clarity, in the equations we refer now to mortality only, which is intended as general mortality predation excluded.

Marc Baid:

7. Primes are used in the sense of B' = B + small number, to avoid numerical integration issues. I was not confident the prime was used in consistently in the text. In any case, this is a numerical integration issue, whereas this manuscript is mostly concerned with the symbolic presentation of processes formulations. I suggest primes are removed from all equations, and an additional section added to describe any numerical approximations that are recommended for the solution of the equations.

We have carefully checked again that we have used the primes consistently in the descriptions and the model. Even being a numerical issue, we think that specifying the use of full or "available" biomass in the equations is important as there are cases where the use of either of the two is ambiguous, such as half-saturation terms (e.g Eq 29 or Eqs 49,50). Therefore, in order to support the reproducibility of the model from the equations given, we have decided to keep the primes in the equations.

Marc Baid:

8. The usefulness of this document would be greatly enhanced by providing a list of parameters for one of the applications given. This is particularly necessary as many of the parameters are not given units in the text. I see this as an advantage, as the model equations are therefore not presented in a specific units system. But at some point units must be given so that the consistency of the model can be assessed. Indeed, the full parametrisation used in all examples is given in the Supplement, stating the mathematical representation in the equations of the manuscript, the name in the code and the value and units used. Given the volume of these tables and the volume of the manuscript without it and considering the fact that the parametrisation is a customisable element and not strictly part of the model definitions, we felt that the Supplement is the adequate place for this information.

2.2 On the specific major comments

Marc Baid:

1. If Eq. 1 contains a seabed term, then Eq. 2 should have a water column term?

In fact this term should not be there, it is covered by the boundary conditions in form of the fluxes. It remained there by mistake from a previous formulation where we had included these fluxes in the balance equation for the interior, but it shouldn't be there being a boundary condition of the system. Apologies for that. Eq 1 now reads:

$$\frac{\partial c_{\rm p}}{\partial t} + \vec{u} \cdot \frac{\partial c_{\rm p}}{\partial \vec{x}} + \overset{c_{\rm p}}{w_{\rm sed}} \frac{\partial c_{\rm p}}{\partial z} = \nu \frac{\partial^2 c_{\rm p}}{\partial \vec{x}^2} + \left. \frac{\partial c_{\rm p}}{\partial t} \right|_{\rm bgc}$$
(2)

Marc Baid:

2. Eq. 4 – should this have an excretion term?

Nutrient excretion was covered by the net uptake term (Eq 18,21) which may turn negative, e.g. in conditions of no growth (see pg 7078, lines 2-4. This is not clear from the Eq.4, so we have decided to split the term explicitly into uptake and release. The corresponding passage in the manuscript now reads:

Nutrient uptake of nitrogen, phosphorus and iron is regulated by the nutrient demand of the phytoplankton group, limited by the external availibility. Excretion is modelled as the disposal of non-utilisable carbon in photosynthesis while the release of nutrients is limited to the regulation of the internal stoichiometric ratio. This approach is consistent with observations that nutrient excretion plays a minor role in the phytoplankton fluxes (Pujo-Pay et al., 1997) Consequently, demand of nutrients may be positive or negative in sign in relation to the levels of the internal nutrient storages and the balance between photosynthesis and carbon losses, so that:

$$\frac{\partial \overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{upt} = \begin{cases} \min\left(\left.\mathcal{F}_{demand}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}}, \left.\mathcal{F}_{avail}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}}\right) & \text{if} \quad \mathcal{F}_{demand}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}} > 0 \\ 0 & \text{if} \quad \mathcal{F}_{demand}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}} < 0 \\ \frac{\partial \overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{rel} = \begin{cases} 0 & \text{if} \quad \mathcal{F}_{demand}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}} > 0 \\ \mathcal{F}_{demand}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}} 0 & \text{if} \quad \mathcal{F}_{demand}\right|^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}_{\mathcal{N}_{\mathbb{N},\mathbb{P},\mathbb{F}}} < 0 \end{cases} \end{cases}$$

The nutrient demand (with the exception of silicate) is computed from assimilation demand at maximum quota $\overset{\chi}{q}_{\max_{\mathbb{N},\mathbb{P},\mathbb{P},\mathbb{C}}}$ complemented by a regulation term relaxing the internal quota towards the maximum quota and compensating for rest respiration:

$$\begin{aligned} \mathcal{F}_{demand} \Big|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\chi} = & \overset{\chi}{\mathcal{S}}_{gpp} \left(1 - \overset{\chi}{\mathcal{Q}}_{excr} \right) \left(1 - \overset{\chi}{q}_{aresp} \right) \overset{\chi}{q}_{max_{\mathbb{N},\mathbb{P},\mathbb{F}:\mathbb{C}}} \quad \overset{\chi}{P}_{\mathbb{C}} \\ & + r_{nlux} \left(\overset{\chi}{q}_{max_{\mathbb{N},\mathbb{P},\mathbb{F}:\mathbb{C}}} \quad \overset{\chi}{P}_{\mathbb{C}}' - P_{\mathbb{N},\mathbb{P},\mathbb{F}}' \right) - \overset{\chi}{r}_{resp} \quad P_{\mathbb{N},\mathbb{P},\mathbb{F}}' \end{aligned}$$

where r_{nlux} is the rate of nutrient luxury uptake towards the maximum quota.

Note, that these terms may turn negative when rest respira-

tion exceeds the effective assimilation rate $\overset{\chi}{\mathcal{S}}_{gpp}\left(1-\overset{\chi}{\mathcal{Q}}_{excr}\right)\left(1-\overset{\chi}{q}_{aresp}\right)\overset{\chi}{P}_{\mathbb{C}}$

or the internal nutrient content exceeds the maximum quota resulting in nutrient release in dissolved inorganic from. The maximum quota for nitrogen and phosphorus may exceed the optimal quota allowing for luxury storage while it is identical to the optimum quota for iron and silicate.

The uptake is capped at the maximum achievable uptake depending on the nutrient affinities $r_{aff_{\mathbb{P},\mathbb{F},n,a}}^{\chi}$ and the external dis-

solved nutrient concentrations:

$$\mathcal{F}_{\text{avail}} \begin{vmatrix} \overset{\chi}{\mathcal{P}}_{\mathbb{P},\mathbb{F}} \\ N_{\mathbb{P},\mathbb{F}} \end{vmatrix} = \overset{\chi}{r}_{\text{aff}_{\mathbb{P},\mathbb{F}}} N'_{\mathbb{P},\mathbb{F}} \overset{\chi}{\mathcal{P}}_{\mathbb{C}}, \qquad (3)$$

$$\mathcal{F}_{\text{avail}} \begin{vmatrix} \overset{\chi}{\mathcal{P}}_{\mathbb{N}} \\ N_{\mathbb{N}} \end{vmatrix} = \begin{pmatrix} \overset{\chi}{r}_{\text{aff}_{n}} & N'_{\mathbb{N}} + \overset{\chi}{r}_{\text{aff}_{a}} & N'_{\mathbb{N}} \end{pmatrix} \overset{\chi}{\mathcal{P}}_{\mathbb{C}},$$

where the nitrogen need is satisfied by uptake in oxidised and reduced form in relation to the respective affinities¹ and external availability.

And for silicate:

$$\frac{\partial \stackrel{\text{dia}}{\partial P_{\mathbb{S}}}}{\partial t} \bigg|_{\text{upt}} = \max \begin{pmatrix} \stackrel{\text{dia}}{q_{\text{ref}_{\mathbb{S}:\mathbb{C}}}} & \stackrel{\text{dia}}{\mathcal{S}_{\text{growth}}}, & 0 \end{pmatrix},$$
$$\frac{\partial \stackrel{\text{dia}}{\partial P_{\mathbb{S}}}}{\partial t} \bigg|_{\text{rel}} = \max \begin{pmatrix} \stackrel{\text{dia}}{P_{\mathbb{S}}} & \stackrel{\text{dia}}{q_{\text{ref}_{\mathbb{S}:\mathbb{C}}}} & \stackrel{\text{dia}}{P_{\mathbb{C}}}, & 0 \end{pmatrix},$$
(4)

Similarly the uptake and release of nutrients and bacteria was covered by a single term, which has now been been split in two explicit terms as well:

$$\frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{upt} = \begin{cases} r_{rel}^{B} \begin{pmatrix} B \\ q_{\mathbb{P}:\mathbb{C}} - P \\ q_{\max_{\mathbb{P}:\mathbb{C}}} \end{pmatrix} B_{\mathbb{C}} \frac{N'_{\mathbb{P}}}{N'_{\mathbb{P}} + h_{\mathbb{P}}} & \text{if } q_{\mathbb{P}:\mathbb{C}} < q_{\max_{\mathbb{P}:\mathbb{C}}} \\ 0 & \text{if } q_{\mathbb{P}:\mathbb{C}} \geq q_{\max_{\mathbb{P}:\mathbb{C}}} \\ \frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{rel} = \begin{cases} 0 & \text{if } q_{\mathbb{P}:\mathbb{C}} < q_{\max_{\mathbb{P}:\mathbb{C}}} \\ r_{rel}^{B} \begin{pmatrix} B \\ q_{\mathbb{P}:\mathbb{C}} - q_{\max_{\mathbb{P}:\mathbb{C}}} \end{pmatrix} B'_{\mathbb{C}} & \text{if } q_{\mathbb{P}:\mathbb{C}} \geq q_{\max_{\mathbb{P}:\mathbb{C}}} \end{cases} \end{cases}$$

Marc Baid:

3. Eq. 7 will produce an undefined number when either of the limiting functions is zero.

¹Note that the dimensions of these are [volume¹ * mass⁻¹ * time⁻¹] as opposed to [time⁻¹] as for most other rates.

This is a mistake in the transcription, the formulation in the code in fact augments the denominator by 0.1. The corrected equation reads:

$$\overset{\chi}{\mathcal{S}}_{\mathsf{lys}} = rac{1}{\min\left(\overset{\chi}{l}_{\langle \mathbb{NP}
angle}, \overset{\chi}{l}_{\mathbb{S}}
ight) + 0.1} \quad \overset{\chi}{r}_{\mathsf{lys}} \, .$$

Marc Baid:

4. Eq. 24 – I think there should be a bracket around (p-379.48)

Thanks, this has been corrected in the manuscript.

$$\gamma_{\mathsf{enh}\mathbb{C}} = 1.0 + (\mathsf{p}_{\mathsf{CO}_2} - 379.48) imes 0.0005$$
 .

Marc Baid:

5. I think Eq. 28 should have Prc on the nominator?

No, not at this stage of prey-specific uptake. The prey biomass comes into play later, when the absolute uptake is computed (Eq. 30). This should be clearer now that we have clarified the meaning of the various occurences of specific rates (see the response to major comment number 5).

Marc Baid:

6. Eq. 27-30. To illustrate an inconsistency, imagine you have one phytoplankton species P = 1 mg C m-3, fmin = 1. fpr becomes 1, and the grazing rate is proportional to $1 \times 1 / (1+1) = 21$. Now split the phytoplankton into two identical populations, indistinguishable to the zooplankton, then fpr becomes 0.5 for both, and the grazing rate is proportional to $0.5 \times 0.5/(0.5+1) + 0.5 \times 0.5/(0.5+1) = 0.3333$. I am not sure about the definition of fpr, but the definition of fmin is problematic. This same issue is exists for benthic feeders. Here (Eq. 168) a detection capacity is assumed. The only justification I could imagine for a detection capacity is that the concentration is

less than one individual. If so, then there would be a calculation that could be made to determine the value. But I don't think this is what you are trying to represent. If it is relative availability, then you could use an affinity for prey in the same manner as you consider NH4 and NO3 uptake.

If the two prey types are indistinguishable to the zooplankton, i.e. they are percieved as the same thing by the predator, then the fmin, i.e. the detection concentrations for the single perceived prey type, should be split between the two actual prey types equally. Specifically, in your example, if the single prey type has fmin=1, than the two prey types perceived as one should have fmin=0.5, which then yields 0.5 as prey availability in both cases.

The detection capacity is essentially an attempt to include sub-scale effects, in that different prey types are likely to be distributed in the water volumn in separate patches. At that point, if one prey type is very rare it is unlikely to be detected with respect to other prey types that are abundant. We have amended the manuscript to explain this concept better:

This formulation is similar to the approach used in Fasham et al. (1990), but introduces additional Michaelis-Menten terms for inidividual prey types. The purpose here is to include subscale effects of pooling as prey of different types can be assumed to be distributed in separate patches in the comparatively large cell volume. Consequently, individual prey patches below a certain size are less likely to be grazed upon compared

to the larger patches, which is expressed by the h_{\min}^{χ} parameter.

Marc Baid:

7. Eq. 38 might be incomplete. The LHS implies a depth-average concentration, which would require the integral through the water column to be divided by the depth, while the RHS implies the depth integral (although the dummy variable, dz, is not given)

This is a misunderstanding, the "av" subscript here stands for available prey as stated in the phrase on top of the equation. It is given by the vertical integral of prey in each horizontal position. Nevertheless, the integral formula was missing the integrand and has been corrected:

Marc Baid:

8. Eq. 45,46. I don't see how these equations work. If Sup is the bacteria-specific uptake rate, then Eq. 46 should be dB/dt = S B, where Sup depends on the available organic matter, not the bacterial population? In Eq. 45, should it be Rlab?

There was a minor mistake in the super- and subscripts of these equations: the "lab"s should have been "dis", so refer to the labile dissolved organic matter. This possibly has caused confusion here and has been corrected. In any case, the uptake rate of equation 45 is specific with respect to the substrate available and not to the bacteria biomass (similar to the predation uptake being specific to prey, see the comment to your point 5). This means that under the condition of the first case of the minimum function (representing the case that sufficient substrate to saturate uptake by bacteria is available), specific uptake will increase the bigger the bacteria biomass. The second term represents uptake that is limited by scarcity of substrate with respect to the bacteria biomass in a simplified manner as a fixed substrate specific rate, compared to the half-saturation formulation of the predators. The formulation essentially is a switch between uptake proportional to bacteria biomass when enough substrate is available or proportional to substrate if substrate is scarce, regulated by the bacteria over substrate ratio. This explanation was added to the manuscript, which now reads:

Bacterial uptake of DOM is given by a substrate mass specific turn-over rate r_{lab}^{B} for labile dissolved organic matter when substrate is scarce and by a maximum bacteria mass specific potential uptake regulated by temperature and limited by nutrient and oxygen conditions when substrate is abundant and the uptake per bacteria is saturated , regulated by the ratio of bacteria over substrate biomass:

$$\begin{split} & \overset{B}{\mathcal{S}}_{upt} = \min\left(\begin{matrix} \overset{B}{r_{lab}}, & \overset{B}{g} & \overset{B}{max} & \overset{B}{l_{T}} & \overset{B}{l_{0}} \min\left(\overset{B}{l_{\mathbb{P}}}, \overset{B}{l_{N}} \right) \frac{B_{\mathbb{C}}}{\overset{lab}{R_{\mathbb{C}}'}} \right), \\ & \frac{\partial B_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \middle|_{upt} = \overset{B}{\mathcal{S}}_{upt} & \overset{lab}{R'_{\mathbb{C},\mathbb{N},\mathbb{P}}}, \end{split}$$

Marc Baid:

9. I am not sure of the meaning of the bold brackets in Eqs. 57 and 58, but they seem to imply multiplication of local derivatives, which I don't think is the intention.

The squared brackets here and in other places represent terms that hold only for individual functional groups, e.g. the silicate components in the phytoplankton equations that are only present in diatoms. We have added the following phrase to the nomenclature section:

In equations that hold for multiple functional groups or components squared brackets are used for terms that are only valid for a single functional group or component.

However, the terms in Eq 57 sepcifically shouldn't have had brackets. We have taken them out.

Marc Baid:

10. P7091. Is r_decomp = r_remin by definition in the equations? If so, it would be better to have just one parameter.

"r_remin" is not used in the manuscript. If the comment refers to the remineralisation rates from dissolved organic matter to inorganic matter ($r_{\text{rem}\mathbb{N},\mathbb{P}}$), the decomposition of particulate matter to dissolved matter in the standard bacteria model is in principle independent of the remineralisation of dissolved matter by bacteria, which is why we have preferred to use two parameters.

Note: Point 11 seems to have been removed by the referee?

Marc Baid:

12. P7105 – If alkalinity is correlated to temperature, which is nonconservative, then alkalinity will be non-conservative. Why not initialise the model with alkalinity based on T and S, and then advect total alkalinity (not just the bgc perturbations), with bgc processes as local sink/sources.

Indeed this option is included in the model by switching the regressions off (ISWTALK=5). Then whatever initial condition provided will be advected and diffused conservatively if the transport operator of the physical driver is conservative. This is in fact the option used in the global ERSEM simulation in Kwiatkowski et al. 2014. However, we have chosen to allow a hybrid formulation of alkalinity as not all processes contributing to the carbonate system are included in the model, so conservation is not necessisarily a desirable feature in this case. At the same time relatively robust regressions for alkalinity from salinity or alternatively temperature and salinity exist at least for some areas of the world ocean (see e.g. Artioli et al. 2012, Lee et al. 2006), that in combination with the biological changes give a good approximation for the total alklinity, as demonstrated in the Artioli et al. paper. In these areas this semiprognostic approach gives a much better representation of the carbonate system compared to the fully prognostic description used in Kwiatkowski that performed comparatively poor. In any case, we have rewritten the final part of the carbonte system section in order to clarify the different options:

Two different modes to compute total alkalinity are provided with the model:

- A diagnostic mode, that computes alkalinity from salinity or salinity and temperature. This mode is non conservative and the field of alkalinity is recomputed at each time step without physical tranport. It does not include changes to alkalinity by the biogeochemical processes of the model.
- A prognostic model, that includes biogeochemical changes to alkalinity. It is fully conservative and adds a state variable for alkalinity that is subject to physical transport.

As a third semi-diagnostic option, these two modes can be combined as a sum by setting the prognostic alkalinity state to 0, so that the diagnostic mode provides the backgound field and the prognostic mode gives a trace of the contribution of biogeochemical processes to the total alkalinity.

The recommended option is the semi-diagnostic option for coastal applications and shelf seas, where reliable and robust regressions exist or the fully prognostic mode, where no single reliable regression is available, e.g. in global simulations. (For further detail the reader is referred to Artioli et al., 2012)

The changes of alkalinity due to biological processes are given by sources and sinks of phosphate, oxidised nitrogen and ammonium as well as calcification and dissolution of calcite:

$$\frac{\partial A_{\text{bio}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial N_{\mathbb{N}}}{\partial t}\Big|_{\text{bgc}} + 2 \frac{\partial L_{\mathbb{C}}}{\partial t}\Big|_{\text{diss}} - \frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{bgc}} - \frac{\partial N_{\mathbb{N}}}{\partial t}\Big|_{\text{bgc}} - 2 \frac{\partial L_{\mathbb{C}}}{\partial t}\Big|_{\text{calc}}$$

In three dimensional simulations, these changes are accompanied by the effect of riverine inputs (see Artioli et al., 2012).

Marc Baid:

13. The equation of the vertical attenuation of light (Eq. 128) calculates light at a depth z. But the model considers discrete layers, in which case any single depth (top, centre, or bottom of the layer) does not represent the mean available light in the layer. The correct depth-averaged light within a layer is given by (Etop-Ebot)/(Kd dz) where Kd is the vertical attenuation of light coefficient, and dz is the thickness of the layer. A similar problem is described on the ROMS forum: https://www.myroms.org/forum/viewtopic.php?f=33&t=1314.

Indeed, this issue relates to the fact that the "average" light in an individual cell should not be the light at the cell centre, but the integral of the exponentially decaying light over the cell thickness, divided by the cell thickness, which is how it is implemented in the aquarium and gotm drivers provided with the model release code and also in the various coupled systems using the POLCOMS and NEMO ocean models cited in the paper. We have amended the corresponing point in the section on dependencies on the physical environment:

 Primary production relies additionally on the photosynthetically active radiation (PAR) as energy input which should be computed from shortwave radiation at the sea surface I_{surf} , taking into account the attenuation coefficients given in Section 3.9. Note, that the model requires the average light in each discrete model cell, which is not given by the light at the cell centre, but by the vertical integral of the light curve divided by the cell depth.

Marc Baid:

14. Eqn 245 has a parameter h with units of (mass/length)^3. If you replace h with h^3, the units of h will be concentration, and the value will be a meaningful concentration. Same for Eq. 246.

We had considered the option of setting this parameter to the units of simple concentration, but have opted for leaving it cubic at this point for easier comparison with previous parametrisations (Blackford et al., 2004).

Marc Baid:

15. Eqn 247 – is this really a 2. If so explain.

That value has been chosen to limit the impact of pH on nitrification rate at high pH to a factor of 2, to avoid unreasonable extrapolation of Huesmann et al. 2002 Anyway, this limit is purely a safety-valve for pathological cases because such doubling of nitrification rate will occur only when pH>9.637, i.e. a value that is usually higher than the values simulated by the model in natural environment.

Marc Baid:

16. You could replace equation 254-255 with x./(abs(x)+hcalc) where x = omega – 1, which would be positive for calcification and negative for dissolution.

That would be a possibility, but would still require the "non active" limitations to be set to zero and the dissolution ones to be reset positive in case of a negative result. Overall, this seems less transparent to us, so we prefer the original formulation.

Marc Baid:

17. P7145 – So the calcification is unaffected by temperature above say10 C? Rather than use the rain ratio, would it be easier to have an explicit calcifier.

We don't fully understand the first half of the comment: the effect of temperature on calcification is described by a saturating curve (Eq 256), with half saturation constant equal to $2^{\circ}C$. This implies that at $10^{\circ}C$ calcification is 83% of the maximum value and at $30^{\circ}C$ is about 94%.

Although the implementation of an explicit calcifiers would improve the ability of the model to simulate some aspect of calcification (e.g. the dependency of calcification from the physiological state of the calcifier), including a specific group of calcifier is problematic given the diversity of calcifying organisms in the marine environment and will therefore lead to the exclusion of the contribution of calcifiers that are not included in this new group. Hence, in order to include all possible sources of calcification, and given the limited knowledge on the mechanistic representation of the process involved, we decided to use this implicit parametric formulation, that is simlar to the ones used in other biogeochemical models (e.g. PISCES - Gehlen 2007, MEDUSA - Yool 2013).

2.3 On the minor comments

Marc Baid:

1. L10 p7083. I know what you mean, but 'enhanced inefficiency' is an oxymoron? Perhaps 'reduced efficiency' would be simpler.

Thanks, we have changed this in the manuscript to:

It is capable of scavenging on medium size organic matter whose assimilation is less efficient and therefore subject to enhanced excretion $q_{\text{Rexcr}}^{\text{MESO}}$:

Marc Baid:

2. L9, p7068 replace 'with respect to' with 'compared to'.

Corrected.

Marc Baid:

3. P9 'according to the internal quota and storage capacity' – are these different quantities?

Yes, the internal quota would be the actual internal quota and the storage capacity its maximum threshold (or better the difference of maximum and reference internal quota). This should become clearer in the section on primary producers.

Marc Baid:

4. Eq. 2 direction of z is important in this definition.

The direction of the z coordinate is given in the Nomenclature section just beneath, but to make this clearer at this point of the manuscript, we have inserted the phrase:

 \vec{x} represents the vector of spatial coordinates of which z is the vertical coordinate being 0 at sea surface and increasing downwards.

Marc Baid:

5. P7070, l12 'equations'.

We assume this comment is referring to line 17 on the same page and have corrected it.

Marc Baid:

6. P7071, I15 small 'P' production, radiation misspelt.

Corrected.

Marc Baid:

7. P7071, I20 vecu_wind is not defined.

This was a latex typo and has been corrected to \vec{u}_{wind} . *Marc Baid:* 8. P7072, l3 'numerical' misspelt.

Corrected.

Marc Baid:

9. P7073, l19 'as the net result'

This has been corrected to "as a net result" on suggestion of referee P. Wallhead.

Marc Baid:

10. P7073, l21 'predation by zooplankton'

Corrected.

Marc Baid:

11. P7074 l4 'for diatoms is the'

We have corrected to:

"and where the silicate component ($\ensuremath{\mathbb{S}}$) is only active for diatoms."

Marc Baid:

- 12. P7074, I10-I14 quotae? 'in unlimiting conditions at the reference'
- 13. P7078 l16 replace tendency with rate, and misspelling of luxury.

Corrected.

Marc Baid:

14. P7080 I16 – I thought 'h' was going to be for half-saturation constants? Might be worth saying that a low f means better detectability (i.e. f is actually a measure of indetectability!) Thanks, we have followed the suggestion to lable the half-saturation constant with h. Labeled clearly as half-saturation constant now, we believe that the relation of a low half-saturation meaning high detection capacity should be clear.

Marc Baid:

15. P7082 – internal stoichiometric quota.

If this refers to line 10, we couldn't find any mistake with the original phrase.

Marc Baid:

16. Eq. 57 – the meaning of 'adj' is not given.

Apologies, this shouldn't have read 'exu' as in exudation, which is defined below. We have corrected this.

Marc Baid:

17. P7086, l15 – what is the meaning of 'at rest'

"at rest" here refers to the pure maintenance metabolism of the microbes without any decomposition of substrate. We have added the phrase:

(representing the maintenance cost of the metabolism in absense of uptake activity)

Marc Baid:

18. P7090 l4, 'excretion by zooplankton', l6 'respectively'

Corrected.

Marc Baid:

19. In some places (Eqs. 144,145, 152) zeta is used as the dummy variable for distance in the vertical, where z is used elsewhere. Might be clearer to stick with z.

We have chosen to use a separate depth coordinate for the sediments, as for the benthos the level 0 is at the sediment interface, while for the pelagic part it is at the sea surface, so strictly they are separate coordinates.

Marc Baid:

20. P7098. L8 replace 'quota' with 'proportion' or something other than quota.

We have replaced with "ratio".

Marc Baid:

21. P7117 Eq. 158 – the use of the vertical line delimited by depths is unusual.

We agree that the vertical line is a fairly ambiguously used symbol in mathematical notation, but at the same time think that our use here is sufficiently clear ("substrate concentrations available in the respective

layer", "where the layer limits d_{low} , d_{up} are 0, $\stackrel{\text{oxy}}{D}$ for aerobic bacteria and $\stackrel{\text{oxy}}{D}$, d_{tot} for anaerobic bacteria") " and we don't think our use is particularly uncommon (See e.g. https://en.wikipedia.org/wiki/Vertical_bar: "Sometimes a vertical bar following a function, with sub- and super-script limits 'a' and 'b' is used when evaluating definite integrals to mean 'f(x) from a to b', or 'f(b)-f(a)'.")

Marc Baid:

22. P7138 l5 'through'

Corrected.

Marc Baid:

23. P7141 replace 'M-M constants' with 'half-saturation' constants.

24. P7143 I9 - 'nitrification'

Corrected.

Marc Baid:

25. P7144 | 6 Do you mean > 0?

This should indeed read > 1, it has been corrected. *Marc Baid:*

26. P7155 I13-14 – check units of PAR and Ns.

The relevant phrase as been removed as a response to a comment by A. Yool et al. on this section.

3 Answers to Andrew Yool, Tom Anderson and Katya Popova

Andrew Yool, Tom Anderson and Katya Popova:

In the first instance, we are very pleased to see ERSEM get a thorough and updated description, and the authors are to be commended. As a long-standing and much-used staple of many marine biogeochemistry studies, particularly in the shelf seas region, it is crucial that ERSEM is transparent and accessible to interested researchers. Especially since recent work (e.g. Kwiatkowski et al., 2014) has shown ERSEM now running at the largest possible scales. However, while welcoming this manuscript, there are a number of weaknesses in it that we feel do not allow ERSEM to be shown in its best light. In our opinion, addressing these would make the resulting manuscript a much more valuable resource, both for existing ERSEM users and as an advert to potential new users of ERSEM. We have divided our comments into general, overarching points and shorter remarks on specific facets of the manuscript.

Thank you again for the attention you have given to our work, we have considered your points carefully and have tried to address them in our aswers that you find below.

As a general remark, we believe that some of the criticism raised is based on a misconception of our purpose of this paper having a conceptually different paper in mind that would "show case" the model in its entire broadness with a considerable weight on the variety of full scale applications. This however wouldn't be possible in reasonable space (as you recognise yourself in point 4), if not at the cost of an incomplete mathematical description which would repeat the short-coming of earlier works on this model. In addition, there is a variety of examples in the scientific literature that illustrate the spectrum of ERSEM applications, so adding these here would only repeat previous efforts, therefore we have limited ourselves in this occasion to refer to these works in the introductory and concluding remarks.

On the contrary our main objectives for this paper were:

- providing a full, transparent mathematical description and a full illustration of the model software.
- provide test cases that demonstrate the main model capabilities, but at the same time allow for a full replication of results within reasonable effort and at a low level of requirements in terms of computational resources.

We realise that this approach may be slightly different to at least some previous papers in GMD on similar types of models, but we believe it is fully supportive of the GMD standards for a model description paper. Specifically it:

- fully supports reproducibility, either of all model equations in a different framework, either of the test cases presented,
- provides examples of model output with comparison to observational data.

We believe that this focus on transparency and reproducibility renders the work interesting and relevant to both, expert modellers familiar to models of similar type, and modellers of related fields as well as other scientists that are interested in the backgrounds and details of our model.

We have rephrased the beginning of the last paragraph of the introduction in order to reflect these intentions:

Our main objective with this paper is to provide a full description of all model components, accompanied by simple case studies with low resource requirements that illustrate the model capabilities and enable the interested reader to implement our model and reproduce the test cases shown. To this purpose we present the examples of a mesocosm type framework and three vertical water-column implementations of opposing character complemented with basic validation metrics against in-situ observations. All material required to replicate these test cases, such as parameterisation and input files, are provided in the Supplement. In addition, a brief illustration of a full scale three dimensional implementation is given to show the model in a large scale application.

The next section gives...

3.1 On the general points

Andrew Yool, Tom Anderson and Katya Popova:

 While the model equations are doubtless mathematically correct, they are expressed throughout in an overly nested and quite repetitive style that makes following and interpreting them unnecessarily difficult. We would suggest that the authors examine descriptions of comparable models (e.g. PISCES was very recently published; Aumont et al., 2015) and adopt some of the style conventions there.

The way we have presented the equations follows the strategy to first present the balance equation for each functional class giving an overview of the processes that change it, and then specify the individual processes in more detail. We appreciate that the volume of mathematical descriptions may at first be a bit overwhelming to readers who are not familiar with the model, but at the same time, we think that this is the best way in which a description of a model of this detail can be presented, when completeness of the description is our main goal. This approach allows unfamiliar users to get an idea of what is changing a state by a quick look at the head of each section, with the possibility to get more into detail, where desired. The same approach has also been followed in other works (e.g. Vichi et al. 2007) of comparable model detail. Specifically, we think that the more "all in one" approach, which works well e.g. for the mentioned PISCES model description, is unsuitable here as the balance equation for the individual states would become excessively long, spreading over several lines, rendering them essentially unreadable. For this reason, we are inclined to stick to our general approach of mathematical representation, also considering, that none of the two referees expressed a similar concern and one of them even finding the current form "surprisingly readable". Nevertheless, we have reviewed our description and reordered in several places equations where they appeared excessively nested or hard to follow (see e.g. some of the comments raised by Referee P. Wallhead and their response).

Andrew Yool, Tom Anderson and Katya Popova:

2. More broadly, while the model equations are scrupulously documented, their origins are not explained. As such, it is difficult for readers to chase up particular functions to understand the rationale for framing them or their underlying assumptions and limitations. Where possible, we suggest that the authors either make reference to their sources and / or identify where they have used "standard" functions (e.g. type-II or type-III responses).

We agree that the origin of the model formulation is at times weakly motivated and documented and have amended the formulations to improve this point adding the reasoning for a particular formulation, including references where adequate (see some of the reponses to the tow referees).

Andrew Yool, Tom Anderson and Katya Popova:

3. Oddly, the model description includes a number of additional optional functionalities for particular processes, but it offers no information on how these perform (functionally and computationally), how they impact model performance, or under which circumstances they should be preferred. We would suggest that an obvious inclusion on these occasions would be to perform a simple sensitivity analysis that illuminates on these points. Alternatively, if these options have formed part of a preceding publication, a pointer to this would help.

We agree that the various options of the model formulations are not clear enough. We have decided to add a section on optional model choices to summarise these along with information on their impact, advantages and disadvantages. However, we believe that a sensitivity analysis, even if brief, for each of these options would exceed the volume of the present work (see point 4), whose main purpose is a a full description of the model formulations. We have ensured in any case that references to relevant previous works are in place.

Andrew Yool, Tom Anderson and Katya Popova:

4. The paper is exceptionally long, even by GMD standards, and we appreciate that our suggestions are unlikely to shorten it. One possible avenue might be to separate the manuscript into two shorter manuscripts in which the pelagic and benthic submodels are (semi-)separately described and explored. At present, the manuscript does not do the benthic submodel justice.

This underlines a fundamental problem in accomadating a significant number of your comments. Given the considerable size of the manuscript in the submitted form and the addition of the background information on the various model formulations we can not accomodate a lot of the suggestions you've made without splitting the work into pieces. This would result in a different work, that is against our main purpose with this manuscript which is to provide a description of the model as a whole. On the contrary, we have opted to focus on a full mathematical description in this work accompanied with reproducible examples. Summarising a model of this volume in a single publication will always be a challenge as it is impossible to enter into the details of the individual processes within a reasonable limit of length, but we believe there is merit in presenting the concise description in itself as a reference to interested readers. Furthermore, we have refrained from splitting the benthic from the pelagic model description as the two systems are deeply interconnected therefore both systems should be thought of as a single framework and not as two separate pieces.

With respect to the sediment model, we have amended the section of the benthic model in various parts, which we believe gives now an adequate description of this part of the model.

Overall, we believe that the paper in its current form, including the amendments we suggest for the revised manuscript, is certainly longer than average, but still of acceptable length for GMD.

Andrew Yool, Tom Anderson and Katya Popova:

5. The extensive use of idealised 0D and 1D configurations followed by just two paragraphs on a 3D configuration does something of an injustice to ERSEM's long record in 3D work. While the former configurations have particular uses, as the authors note, they are a poor representation of what ERSEM is capable of. We would suggest that that manuscript would be much improved if the focus was on the 3D model (either in shelf seas or global mode) with passing mention made of these useful, cut-down modes.

Andrew Yool, Tom Anderson and Katya Popova:

6. On a related point, the demonstration of ERSEM's range and utility is very weak. The ways chosen to illustrate this are limited and do not provide any context for the model-observation comparisons (i.e. is ERSEM doing well / badly relative to other models?). This is compounded by some weak figures and analysis, but is principally hampered by the focus on idealised cases rather than ERSEM's work in 3D (which, as already noted, is given seriously short shrift in this draft of the manuscript). Again, we would strongly suggest that the authors examine recent model descriptions in GMD, of which the PISCES model provides (in our opinion) a good example.

Our decision to focus on "simpler" test cases here is following two main motivations in order to support transparency and reproducibility:

- This class of test cases eases the approach to the model to unfamiliar readers as the effect of model mechanisms is more directly tractable and clearer than in a full 3D applications where the interactions with the physical driver are much more complex.
- The 0D and 1D test cases are easier and faster to set-up and have much lower demands on data volumes of in- and output data and much lower requirements in computational power to run the simulations allowing the reader to reproduce our examples on any standard work station or laptop. This enables us to provide the full input data and configuration required to reproduce the test cases, and it enables the interested reader to reproduce all our test cases on a standard work station without the need of access to a high perfomance computing system.

This approach offers the interested reader the actual possibility of taking the paper, downloading the code and reproducing the examples given at full extent.

In addition, as you rightly state, the model has a long history of simulations in full 3D. But instead of repeating these we have decided to focus on the simpler reproducible applications. The full spectrum of model applications and validation studies it has been subject to is extensively referenced in the introductury and concluding remarks providing providing the background of more detailed work at full scale.

Finally, model intercomparison is surely a useful and interesting exercise (and ERSEM already participated in one of these exercises, see

Kwiatkowski et al., 2014), however it is not the aim of this paper that is focussed on describing ERSEM and its ability to reproduce observed patterns in some illustrative test cases (see also point 8).

Andrew Yool, Tom Anderson and Katya Popova:

7. ERSEM's treatment of alkalinity appears to have several confusing elements. Calcifiers are included, but alkalinity is effectively implicit ... while also being open to modification - it's not at all clear how the model can "remember" this modification in the absence of an explicit TA tracer. It is also unclear what this does to carbonate chemistry and air-sea CO2 exchange. On a related point, if TA is a function of T S, what happens to it at depth where these relationships completely breakdown because of the biological pump? More broadly, either ERSEM or the manuscript (or both?) are not self-consistent when it comes to alkalinity - even simple nutrient-restoring models manage this more straightforwardly.

The description of the alkalinity options in the carbonate system submodule unfortunately hasn't been very clear. We have clarified the options for the alkalinity computation in an amended version of the final part of the carbonate system section:

Two different modes to compute total alkalinity are provided with the model:

- A diagnostic mode, that computes alkalinity from salinity or salinity and temperature. This mode is non conservative and the field of alkalinity is recomputed at each time step without physical tranport. It does not include changes to alkalinity by the biogeochemical processes of the model.
- A prognostic model, that includes biogeochemical changes to alkalinity. It is fully conservative and adds a state variable for alkalinity that is subject to physical transport.

As a third semi-diagnostic option, these two modes can be combined as a sum by setting the prognostic alkalinity state to 0, so that the diagnostic mode provides the backgound field and the prognostic mode gives a trace of the contribution of biogeochemical processes to the total alkalinity. The recommended option is the semi-diagnostic option for coastal applications and shelf seas, where reliable and robust regressions exist or the fully prognostic mode, where no single reliable regression is available, e.g. in global simulations. (For further detail the reader is referred to Artioli et al., 2012)

The changes of alkalinity due to biological processes are given by sources and sinks of phosphate, oxidised nitrogen and ammonium as well as calcification and dissolution of calcite:

$$\frac{\partial A_{\text{bio}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial N_{\mathbb{N}}}{\partial t}\Big|_{\text{bgc}} + 2 \frac{\partial L_{\mathbb{C}}}{\partial t}\Big|_{\text{diss}} - \frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{bgc}} - \frac{\partial N_{\mathbb{N}}}{\partial t}\Big|_{\text{bgc}} - 2 \frac{\partial L_{\mathbb{C}}}{\partial t}\Big|_{\text{calc}}$$

In three dimensional simulations, these changes are accompanied by the effect of riverine inputs (see Artioli et al., 2012).

Andrew Yool, Tom Anderson and Katya Popova:

8. The concluding statement "The ERSEM 15.06 model is the only model currently available that provides the structure for simulating in one coherent system the biogeochemical cycles of carbon, the major macronutrients and iron, the carbonate system and calcification, the microbial food-web and the benthic biogeochemistry" is overreaching in the extreme. That this description is not backed up in this manuscript by any strong evidence that it does a good job on any of these components makes it difficult to sustain. The manuscript needs to demonstrate ERSEM's skill (e.g. comparison with a range of other models) to justify as strong a statement as this.

It is not our intention with this phrase to underline that ERSEM would be better with respect to any other models in all these aspects. Given that we don't provide a model inter-comparison in this paper (which would go beyond the scope of this paper), we have omitted any comment at this point on the actual quality of the model elements mentioned compared to other models. We have simply stated that the model in the current form *"provides the structure"* to include these processes in simulations and that is to our knowledge unique. Given that we also provide a full description of each of these elements, it is transparent to the reader/user how and to what detail these processes are included or not. Based on these considerations, we believe this is a fair statement. In any case, we have slightly changed the phrase to: The ERSEM 15.06 model is to our knowledge the only model currently available that provides the structure for simulating in one coherent system the biogeochemical cycles of carbon, the major macronutrients and iron (using variable stochiometric relationships), the carbonate system and calcification, the microbial food web and the benthic biogeochemistry.

3.2 On the specific points

Andrew Yool, Tom Anderson and Katya Popova:

• Why is this version "15.06" of ERSEM?; why not version 15?; like many models, ERSEM is documented sporadically so does it really need a ".06" designation in its version number?; this especially seems odd given that previous manuscripts do not routinely report a specific model revision, and also because this manuscript will presumably be the go-to description for the model for years to come; in the language of modern marketing, Apple promotes iOS 9, not iOS 9.06 ...

The version number refers to the year.month of the release. There are undoubtedly different approaches to versioning computer software, most of them are based on either a running number, like iOS, or on the time of the release, like some windows releases or the ubuntu operating system. We have decided to go for the release number based on the release time in order to avoid the difficulty of attributing an adequate running number given the dispersive development previous to this release. The decision to include year and month leaves us the opportunity to release more than once in a year, which may or may not be necessary, but in this way at least we are not restricted by the version number.

We have added the following phrase to the code availability section:

The versioning convention used with this software refers to the year and month of the release.

Andrew Yool, Tom Anderson and Katya Popova:

• An explanation of the differences between BFM and ERSEM might be helpful; they are introduced as cousins but one is shelf seas while the other is (at least ostensibly) open ocean Actually also the BFM branch of the ERSEM model has been applied on the shelf and in the global ocean as alluded to in the introduciton on pg. 7065, lines 8-13, references to Leeuwen et al. 2012 and van der Molen 2014. As the main concepts of the two models are very similar, but the differences lie in smaller details of the model equations, we believe that a listing of the differences in between the two models would be more confusing to the reader than it would help and would lengthen the manuscript considerably. In addition, we would be obliged to compare an up-to-date description of 2015 with the last publication of the BFM dated 2007, which would probably not give a fair representation of the current state of the BFM. Again, a model comparison is not our purpose here, but on the base of this work any interested reader has full access to the description of our model in order to compare.

Andrew Yool, Tom Anderson and Katya Popova:

 Lots of examples of diverse use are given in the introduction, but it's used in a very narrow way in this manuscript; arguably, the 1D uses are rather passé when we know that it's more routinely used in 3D and even at the global scale (of which, the manuscript is rather coy about its performance)

There is a variety of expamples of 0D and 1D uses of the ERSEM model along the 3D works in recent scientific literature and the manuscript gives references to these works. We believe that scrupulous, intensive and well documented model develpoment in idealised 0D and 1D implementations should be at the base of any full scale model implementation, because by simplifying the context they allow to isolate the different model components and to better understand the interactions among these. Up to this day there is a long record of publications using the ERSEM model in idealised 0D or 1D simulations (including recent ones) and as far as we are concerned, there will be a lot more in the future.

Andrew Yool, Tom Anderson and Katya Popova:

 A "model of intermediate complexity" is an odd way to hear ERSEM described; relative to most other plankton models, it's more a "kitchen sink" model in which complexity has been successively extended to include functional groups for which there is arguably still only limited knowledge about; perhaps some examples of other models would make this intermediate status clearer? What we intended here is that the model is certainly on the complex side of biogeochemical models, but compared to some models of the marine food-web, the complexity of the ecosystem representation is rather reduced.

In any case, we have removed the statement concerning the complexity of the model as it is not further explored in this work.

Andrew Yool, Tom Anderson and Katya Popova:

 What does "a particularity of ERSEM" actually mean?; this is not unique to ERSEM by a long chalk

Of all the main models currently in wider use, to our knowledge the majority of models still uses fixed stochiometric or limited stochiometric dynamics of individual constituents. So while we don't insinuate this is an exclusive charateristic of ERSEM, it is still a particular element compared to the bulk of models available. Nevertheless, we have rephrased to:

Importantly, ERSEM uses a fully dynamic stoichiometry in essentially all its types (with the exception of mesozooplankton, benthic bacteria and zoobenthos which use fixed stoichiometric ratios).

Andrew Yool, Tom Anderson and Katya Popova:

• Figure 1 does not do a good job of describing something as complex as ERSEM; it would be far better to separate out the pelagic and benthic components and do a better job separately for each; for instance, the diagram makes it look like all phytoplankton use all nutrients, that all zooplankton have access to all phytoplankton, and that there's only a single size class of detritus (which the text later makes clear is not the case); also, the diagram has no need of including the carbonate system in this way - one assumes pH and omega; the arrows on the diagram, in particular, for this part are unhelpful since they imply that alkalinity is consumed by not just the phytoplankton (and possibly the "microbes" and zooplankton; which P and Z, incidentally, is left to the imagination of the reader) but also the DIC system, which in turn is consumed by pCO2

Just as the paper is aiming to give an all-in-one description, the rationale for this figure is to give an overview of the model in its entity, which we believe is a crucial requirement for a manuscript such as this. Consequently much detail is omitted from this diagram, which aims to show the interactions between model components, not just fluxes of biomass or compounds. This is why the links with the carbonate system are appropriate, and we believe pertinent to include. We have however improved the figure in order to make our intentions clearer.



Figure 1: ERSEM schematic showing how model components interact with or influence each other. Blue connectors represent inorganic carbon fluxes, red represents nutrient fluxes, yellow represents oxygen, black represents predator-prey interactions and green represents fluxes of non-living organics. Dashed arrows indicate the influence of carbonate system variables.

Multiple size classes of particulate organic matter (and labilities of dissolved organic matter) were already implied by the previous diagram, but have been made more explicit. Very similar versions of this figure have been published in many other publications to date as an introductory overview of the model.

We agree that additional diagrams help to illustrate some of the more detailed aspects of the model in other points of the manuscript (e.g. the connections between prey and predators mentioned in a later comment and diagrams of the two bacteria sub-models) and we have provided these in the revised manuscript.

Andrew Yool, Tom Anderson and Katya Popova:

• Stating "small scale and high resolution applications" would benefit from having scales attributed to them; among other things, the continuity assumption is only ever an approximation

The continuity assumption is in fact always an approximation. The point we are making here is that one needs to keep in mind that this approximation is only justifyable when one is looking at the dynamics from scales coarse enough so that the abrupt discrete changes vanish. A precise limit is hard to define and depends on the precision required, but as a rule of thumb one should use scales that are at least an order of magnitude larger than the body and patch size of the modelled organisms. We have added the following phrase to the manuscript:

As a rule of thumb, in order to guarantee the validity of the equations, the modelled scales should at least be an order of magnitude bigger than the organims modelled and smaller patches.

Andrew Yool, Tom Anderson and Katya Popova:

• Table 3, which describes the predator-prey relationships in the model, would surely have been better off as a diagram; Figure 1's job should have been this

We agree, we have added these figures to the revised manuscript.

Andrew Yool, Tom Anderson and Katya Popova:

From the get-go the equations, while doubtless mathematically correct, are fairly impenetrable to read; it would be a lot of work to understand and follow them enough to reproduce them in another model; and why is the format of a vertical line followed by a shorthand description used?; wouldn't underbraces, or just well-chosen names, be better?

The general principle we have followed in presenting the equations, as described in the answer to the similar general comment above (1.), is to give an overview of what processes affect a single orangism in form of the general balance equation, followed by the specification of the individual terms. Taking also into consideration the feed-back of the two nominated referees, we don't have the impression that the general layout of the equations is a major problem in principle. However, we admit that on occasions the specification of individual terms was slightly convulsive and has not helped readibility. Consequently, we have changed these where they've occured to us. We believe that these changes have improved the readibility of the overall manuscript even further.

As for the notation style of vertical lines specifying types of source-sink terms, the choice between our notations and other forms as underbraces is surely subjective and we have favoured the vertical lines (which has also been used in other works, e.g. Vichi et al., 2007).

Andrew Yool, Tom Anderson and Katya Popova:

• In section 2.3, how sensitive is the model to the size of this number?; while it's small, it's a value that the model could reach relatively easily; also, does this mean that the ocean has an enormous standing stock of biological material when integrated everywhere?

Sensitivity studies we have performed when introducing this threshold have shown that the results in spun-up simulations remain unaltered in between runs using this negativity control and runs that do not use the concentration buffer. The model indeed reaches values of 0.01 mg m-3 carbon at times, but these occasions have entirely negligible impact on the model dynamics and overall flux budgets. The formulation and magnitude of these litmits is similar to the overwintering limits in Fennel (1995). As for the biomass budgets over entire domains, one should use the available biomasses to compute the overall budgets in order to exclude these background concentrations. We have added a corresponding comment to the revised manuscript:

...These small resilient buffers additionally support the spawning of new biomass as soon as favourable conditions occur, similar to the low overwintering biomass limits in Fennel (1995). Note that when calculating the overall budgets of a domain, these background concentrations should be subtracted in order to give adequtate results.

Andrew Yool, Tom Anderson and Katya Popova:

• We presume that "hetero nanoflagellates" are "heterotrophic nanoflagellates"?

Thanks, we have corrected this.

Andrew Yool, Tom Anderson and Katya Popova:

 The equations contain a large number of diverse functional forms, but these are neither sourced to particular work, nor are the functional responses of them illustrated diagrammatically - this might help in the more complex cases; for instance, how is the rather complex nitrification equation derived?; is there empirical support for such a multi-factorial form, or is it a composite function based on separate studies for each factor?

We agree and have added a significant amount of background on the origin of the model formulations to the revised manuscript, as stated in response to general comment "2.". Also we have added some diagrammatical representations of parts of the model (within limits to keep the paper at a sensible length, see also response to the comment on figure 1). More specifically on the description of nitrification, we have amended the manuscript as follows:

...where $\overset{B}{r_{nitr}}$ is the maximum ammonium mass specific nitrification rate at reference temperature. In the absense of explicit nitrifiers, nitrification is modelled as an implicit process depending on multiple environmental factors, based on temperature, oxygen and availibility ammonium taking into account the poor competitiveness of nitrifying microbes with respect to other pelagic consumers of ammonium (Ward, 2008). The various regulation and limitation factors...

Andrew Yool, Tom Anderson and Katya Popova:

 Is there any exploration in the manuscript of the different bacterial degradation schemes?; if not, why not?; the text makes a point of describing both at length The DOCDYN sub-model is simply an updated version of the standard ERSEM formulation meant to represent the bacteria-mediated production of recalcitrant DOC. The enhancements offered with this new feature in simulations is already documented in the literature (Polimene et al., 2006, 2007). As such we think that going further in exploring the differences between the two formulations is outside the scope of this paper. The tendency within the group of developers is to use the DOCDYN formulation as default bacteria model. However, for the sake of completeness we have left the possibility to choose the "old" version also considering that, in some cases, it could be convenient to run the model without the semi-refractory DOC (R3 variable in the code) reducing the computational cost. In order to make the differences of the two sub-models more transparent we intend to include diagrams showing the different versions in the revised manuscript.

Andrew Yool, Tom Anderson and Katya Popova:

 Where does this calcification form originate?; it is not sourced; also, extra functionality is described for CaCO3 dissolution but again appears unexplored; ordinarily one would expect a sensitivity analysis section in the manuscript, not least to help users of ERSEM decide which of the optional functions (here and elsewhere) they should use; of course, it may be obvious from the sources of the functional responses, but - as noted - these are not made clear

We have amended the introduction of the calfication section in order to clarify reasoning and background of this sub-module. It now reads:

The model in its current form does not include calcifiers as a dedicated

functional group given the limited knowledge of the physiological constraint of calcification. Therefore, the process of calcification is not directly modelled, but is treated implicitly by considering part of the nanophytoplankton to act as calcifiers. Calcification processes are inferred from the system dynamics based on the assumption of a given ratio between particulate inorganic carbon over particulate organic carbon in sedimenting material, usually referred to as rain-ratio. Here this ratio is used as a proxy for the calcite production matching the local increase of POC originating from nanophytoplankton. Since the rain ratio has been defined for the sinking fluxes and calcite is the more resistant mineral, we limit the description to calcite in this part of the model, neglecting aragonite. This approach is similar to the implementations in other biogeochemical models, e.g. PISCES (Gehlen et al, 2007) or MEDUSA (Yool et al., 2013).

Andrew Yool, Tom Anderson and Katya Popova:

• Nice light modelling, but, again, what's the difference in the schemes presented?; is either functionally superior, and does it come at extra cost?

The two models can be tuned to give essentially the same results, but the new formulation includes the major advantage of being formulated on the base of inherent optical properties, which with respect to the apparent optical properties of the earlier formulation are more directly and much more often measured. This gives the possibility to:

- base parameter choices on collected data available,
- validate the optical sub-model against data sets of inherent optical properties,
- constrain the non-modelled optical parts on observed quantities that are closer to the model formulation (e.g. ADYTRACER option),
- assimilate optical data directly rather than the derived product ocean coulour.

The computational cost of the two models is comparable.

We have added the following phrase to the manuscript at the end of the section:

The two models can be calibrated to give comparable results, but the latter formulation based on inherent properties has the advantage to be based on quantaties that are frequently measured, which helps in constraining the parameterisation, validation and enables the direct assimilation of optical data.

Andrew Yool, Tom Anderson and Katya Popova:

• The second benthic scheme is a bucket; would it be better to present this as tier 1, with the more advanced one as its successor (which is doubtless how the model actually evolved)

We have followed this order as the second scheme is strictly speaking not a full benthic sub-model, but more of an extended boundary condition or benthic closure as no internal process of the sediments is included. Therefore its description in fact resides in section 5 on horizontal interfaces rather than in section 4 on the benthic model. In this context we admit that the introductory section of section 4 is a bid misleading and have rephrased accordingly, see the reponse to the following comment.

Andrew Yool, Tom Anderson and Katya Popova:

 On benthic schemes, again, is there any sensitivity analysis on the choice?; also, the "complex" scheme is simplified from a model that is 20 years old - why not include the full scheme it's derived from as an option?; one would expect it to be more computationally tractable now than before

The original full scheme is for most applications of unnecessary detail and numerically significantly more vulnerable than the currently implemented form, which is why it has been abandoned. On the choice of the benthic model, we have rephrased the introductory paragraph of the benthic system as follows:

The benthic model in ERSEM is predicated on muddy sediments of the continental shelf, including zoobenthos, bacteria, different forms of organic matter and implicit vertical distribution of material within the sea-bed. It explicitly describes the main functions of the sediment such as benthic predation, decomposition and recycling of organic matter, bioirrigation and bioturbation. As an alternative to using a full benthic model, the benthic-pelagic interface can be described by a simple benthic closure given in Sec. 5.1.5. This scheme adsorbs depositing particulate matter and phytoplankton and returns dissolved inorganic nutrients and carbon to the water column at a given time scale reducing the sediments to a simple buffer layer of organic matter recycling, that however does not involve any explicit benthic processes. It is computationally considerably lighter compared to the full model, but the computational effort in both cases is neglectible compared to the pelagic component. While the full benthic model is more adequate for shelf seas application that are dominated by the sediment type it represents with a close connection to

the productive upper ocean, the simplified closure scheme is more suitable in deep domains under oligotrophic conditions, where the sediment processes are of lesser importance.

Andrew Yool, Tom Anderson and Katya Popova:

• In passing, it is difficult to ascertain the total number of tracers (and parameters) in the model; a table could help

The full list of tracers in the model is in fact provided in tables 1 to 6. These tables have been split into various categories in order to fit each table on a single GMD discussion format page, but we aim to merge these into a single table for pelagic and benthic state variables each, which should make the total number of state variables transparent. Tables including all parameters are given in the supplements.

Andrew Yool, Tom Anderson and Katya Popova:

• The information in Section 6 seems oddly placed; should this not have appeared when these terms were first introduced?

The reason they appear in an individual section is that they are overarching formulations used in several parts of the model, e.g. the temperature response factor, or that their detailed description would have interrupted the logical flow of the process description if they would have been left in place, e.g. the internal nutrient limitation factors of phytoplankton. We believe that moving these where they were first introduced would deteriorate the readibility of the manuscript.

Andrew Yool, Tom Anderson and Katya Popova:

• Section 6.2's stoichiometric adjustments are presented as if they are a simple fudge rather than being derived from an existing formulation; is this correct?

These terms are indeed stochiometric correction fluxes in order to close the mass balances, we have clarifedy this point in the manuscript:

For states $\stackrel{\chi}{\varphi}$ with fixed stoichiometric quota $q_{\mathbb{N},\mathbb{P}:\mathbb{C}}^{\chi}$ (mesozooplankton, benthic bacteria and predators) the process rates are complemented by exudation fluxes that regulate imbalances on order to preserve the fixed reference quotas as follows: ...

Andrew Yool, Tom Anderson and Katya Popova:

• ERSEM-Aquarium seems to be a perfect system that could be used to examine the model's sensitivity to the extra functionality that's loaded onto it; but that hasn't been done here

As stated in an earlier point, we are unable to address the suggestions raised that would extend the length of the work considerably, given that we are inclined to stick to our approach of provding a single paper with the full description of the model. To underline our issue here, we are asked to

- consider the excessive length of the paper.
- change the balance of 0D, 1D and 3D applications in favour of 3D applications.
- include more 0D applications with sensitivity studies.

which is simply not possible maintaining the same concept of the paper.

Having to choose, we have decided to show as a 0D simulation an example that illustrates the pathways of the model in contrasting environments to illustrate the overall model dynamics in different conditions rather than an individual sensitivity study.

Andrew Yool, Tom Anderson and Katya Popova:

 The manuscript's imbalance towards idealised frameworks (0D, 1D) is difficult to understand given that ERSEM is largely used in 3D simulations

The motivation for our balance is given by our aim to provide lightweight and easily reproducible examples along with a complete transparent description as described more in detail in the general comments above, while the full-scale applications are best dealt with within dedicated publications that do justice to the physical processes and their interactions with the biogeochemistry. For this paper that deals specifically with the ingredients of the biogeochemical model we believe that the expamples we give provide the better focus. In addition, we are referring to some recent examples that use the ERSEM model in various parts of the manuscript.

Andrew Yool, Tom Anderson and Katya Popova:
Section 8 is an anomaly; ostensibly about the "Development and Testing Framework", it wraps up on a discussion of diatoms and chlorophyll which should really appear during the model description

The purpose of this paragraph illustrates on the base of a practical example of how the sofware infrastructure can be used to test individual components of the model and perform sensitivity analysis. The discussion of the photosynthesis description of the model occurs in this place in order to explain the context of the example plots, but the purpose of the paragraph remains the illustration of the possibilities offered by the software package in isolating the individual process formulation. We have modified passages across the entire section in order to maintain the focus and make its purpose clearer.

In addition to the 0- and 1-D ERSEM implementations a framework is provided with the model that allows developers and users of the code to analyse and plot the result of calls to individual ERSEM procedures from Python. This facility is supported through Fortran-C interoperability, that arrived with the Fortran 2003 standard (ISO/IEC 1539-1:2004(E)), and the Python Ctypes package. ERSEM test harnesses consist of the ERSEM library and a set of C wrappers, which are jointly compiled as a shared library. A Python interface to the shared library permits access to Fortran data structures and procedures from Python. This allows developers and users of the code to quickly interrogate the validity and behaviour of individual procedures, without first reimplementing them in a second language, and without running the full model. Here we illustrate this feature by examining the photosynthesis model implemented in ERSEM.

The photosynthesis model used in ERSEM is based on Geider et al. (1997), and is described in Sect. 3.1. In the model, photosynthetic cells are able to regulate their chlorophyll *a* to carbon ratio in response to changes in irradiance, temperature and silicate (in the case of diatoms) by modifying the proportion of photosynthate that is directed towards chlorophyll biosynthesis ($\stackrel{\chi}{\rho}$; see Eq. 9). Balanced growth is achieved when cells are fully acclimated, in which case:

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} \chi \\ \dot{P}_{\mathcal{C}} \\ \mathcal{P}_{\mathbb{C}} \end{pmatrix} = 0 \tag{5}$$

Chlorophyll *a* biosynthesis is assumed to be up-regulated in response to a reduction in irradiance and down regulated in response to an increase in irradiance. Through this process, cells are able to balance the rate of energy supply through light absorption, and energy demands for growth. The maximum, light saturated photosynthesis rate g(T) is assumed to be independent of changes in irradiance, which is consistent with observations which indicate Rubisco content is relatively invariant with respect to changes in irradiance (Sukenik et al. 1987), and the hypothesis that these cells are adapted to survive and reproduce in dynamic light environments (Talmy et al. 2014).

Using the ERSEM testing framework, it is possible to investigate this process in isolation. Model cells can be artificially acclimated to a given set of environmental conditions by finding a value for $q_{\mathcal{C}:\mathbb{C}}^{\chi^-}$ which satisfies Eq. (263). Figure 8 shows a plot of $q_{C,C}^{\chi}$ vs. I_{PAR} for fully photo-acclimated diatoms in ERSEM. Cells were acclimated to a given irradiance by holding cellular carbon fixed and varying the cellular chlorophyll a content within the range $\overset{\chi}{q}_{\min_{\mathcal{C}:\mathcal{C}}} \leq \overset{\chi}{q} \leq \overset{\chi}{q}_{\varphi\max}$ in order to achieve balanced growth. Using the testing framework, the model can be compared with observations in order to sanity check the validity of the implementation, or parameterised against observations using curve fitting procedures. In Figure 8, observations for the diatom T. Pseudonana have been overlaid. No attempt was made to fit the curve to this particular set of observations, although the fit appears reasonable. The parameter set is the same as used in the simulations of Sect. 7 and is given in the Supplement.

Diatoms are a physiologically and morphologically diverse group, which are characterised by their requirement for silicate, which they use to construct their cell wall. It is perhaps unsurprising that model fits to photosynthesis-irradiance curves for different diatom species result in a range of parameter values, including differences in the maximum light saturated carbon specific photosynthesis rate as a function of temperature, and the initial slope of the photosynthesis-irradiance curve (e.g. Geider et al., 1997). Ultimately, many of these differences arise due to differences in organism morphology and physiology, with, for example, different pigment complements or levels of investment in biosynthesis, being reflected in derived parameter values. These within group variations pose a perennial problem to the development of marine ecosystem and biogeochemical models. The diatom group in ERSEM is designed to be representative of diatoms as a whole, and to reflect the important biogeochemical role these organisms perform in nature.

ERSEM includes four phytoplankton functional groups: diatoms, which are characterised by their requirement for silicate, and three further groups which are characterised according to their size. These are the pico-, nano-, and microphytoplankton. The choice to characterise groups according to their size reflects the importance of size as a physiological trait (Litchman et al., 2007, 2010), which influences an organism's competitive ability through its effect on nutrient acquisition, carbon and nutrient storage, the intracellular transport of solutes, photosynthesis rates through pigment packaging effects, and susceptibility to predation (e.g. Chisholm, 1992; Finkel et al. 2010).

Using ERSEM's testing framework it is possible to demonstrate how this classification impacts the competitive ability of the four photosynthetic groups represented in the model. Figure 9 shows photosynthesis-irradiance curves for ERSEM's four phytoplankton groups under the condition of balanced growth. As with the diatoms, the use of a single parameter set for each size-based group ignores within group variations that are observed in nature. It is important to take such abstractions into consideration when interpreting model outputs.

This example illustrates how ERSEM's testing framework can be used to study and check the implementation of different processes within the code. Importantly, this is achieved without having to rewrite sections of the code in a second language with visualisation capabilities, which is an inherently error prone procedure. This capability is designed to complement the 0-D and 1-D drivers that simulate more complex time-varying environments, in which it is often difficult to study processes in isolation.

Andrew Yool, Tom Anderson and Katya Popova:

• Section 8's concluding paragraph on not having to write visualisation for the model in a second language is unnecessary; most users would almost certainly run the model and visualise the output alongside in a separate program anyway

This is a misunderstanding, this statement is not referring to a second programming language in order to perform the visualisation after running the full model. On the contrary the purpose of this part is to demonstrate, that the test harness enables the testing of isolated pieces of the code running only a specifc part of it without the need to export it or even rewrite the mathematical formulation in a separate environment. Importantly, this is achieved by directly operating on the same instance of the code that is used for the full simulation, without having to extract and rewrite the part of the code related to the investigated process. It is simply compiled against the test harness library.

This should be clearer now that we have rephrased the section (see previous comment).

Andrew Yool, Tom Anderson and Katya Popova:

 Table 2 - this has got to be among the most arcane naming convention we've seen

We are sorry that you don't appreciate our naming convention. It is an attempt to use a consistent convention throughout, starting from a basis that relates functional types to variables in the model without using numbers for legibility and were possible relating to the code names inherited from the early ERSEM versions.

Andrew Yool, Tom Anderson and Katya Popova:

• Table 3 (and other locations in the text) - "preys" is grammatically incorrect; "prey" is both plural and singular, like "sheep"

Thanks, corrected.

Andrew Yool, Tom Anderson and Katya Popova:

Table 4 - "particulate" spelt wrong

Corrected.

Andrew Yool, Tom Anderson and Katya Popova:

 Figure 1 - inadequate; would benefit from being split into pelagic and benthic components, and from a focus on the core nutrient cycles rather than including peripheral (in a diagrammatic sense) processes; arrow heads are also missing in places, and sometimes convey implausible pathways (e.g. TA -> DIC -> pCO2)

See previous comment on the same topic.

Andrew Yool, Tom Anderson and Katya Popova:

 Figure 2 - the use of line thickness does not make this diagram clear; it's also missing what would be interesting detail re: differing phytoplankton and zooplankton fluxes between functional types; the diagram also makes it look like different model structures were used rather than just different pathways being favoured; that these different foodwebs are derived from idealised simulations makes the inclusion of this diagram questionable

We are not sure why the use of line thickness woud be not clear. The choice to omit details concerning the functional types of phytoplankton and zooplankton was taken to keep this diagram readable and clear. Also, the general behaviour of the modelled phytoplankton community structure is later on illustrated in the summary plot on the 1D simulations (figure 6).

Concerning the model structures, we assume this refers to the benthic componenents and they are in fact different. As is clearly stated in the text on this test case and referring to this figure, on pg. 7149 lines 1-4 the oligotrophic case uses the simple benthic closure while the eutrophic case uses the full benthic model.

Andrew Yool, Tom Anderson and Katya Popova:

 Figure 3 - are the modelled cycles really out of phase in places?; that's not good; also, these target diagrams would be much more useful if they compared the model to another model (or different versions of the same model; like, for instance, versions using different options); as it stands, all the reader can see is that the model performs differently well for different properties (which, to be fair, is all that showed in our MEDUSA-1 paper, but in MEDUSA-2 we also included model intercomparisons); that the model shows that the relative fit for different properties varies between sites (Figures 3-5) makes it difficult to judge how ERSEM is actually performing.

We are interested here in a full description of the ERSEM model and already push the manuscript to its size limit. The inclusion of a fair comparison to a different model would require an adequate description of this model and planned common joint experiments like the one published in Kwiatkowski et al., 2014, in order to achieve a proper and fair comparison. Comparing different version of the model would be surely ineresting, however we believe that this would push the manuscript beyond its limits. That the model behaves quantitatively differently in different environments should not be a big surprise. In our experience, any model would perform differently between fundamentally different sites, the important point here is that it doesn't completely fail in one with respect to the other. As for the chlorophyll-a being out of phase, we have alluded to possible reasons for episodic deficiencies in the text, these occur mainly in periods when data is scarce and is barely sufficient to individuate the seasonal cycle, while for the last, more data rich years, the bloom timing appears to be well captured for a 1D model of a shelf site, where lateral advection is not included. We have added a paragraph explaining the issue and limitations of modelling a shelf site in 1D:

In addition, some deficiencies, in the model simulations are to be expected as the Oyster Ground site is characterised by strong lateral influences including estuarine, coastal and channel waters that include strong direct impacts on the nutrient concentrations in the area that can not be captured in this idealised setting. Particularly in the stratified season in summer these lateral effects are dominating the surface water signal while the deeper part of the depression is essentially isolated from the surface layer (Weston et al., 2008)

Andrew Yool, Tom Anderson and Katya Popova:

• Figure 4 - seems to show the model including a bloom that doesn't occur in the real world at all

We do agree that the simulation of chlorophyll a presents limits (especially at L4). Our intention was to make this clear by the objective comparison with data we presented and by discussing the issue in the text. In particular, as you correctly point-out, some chlorophyll peaks seem to be out of place. However, it should to considered that the L4 station is a highly variable site, strongly affected by riverine inputs (Smyth et al., 2010) which are only partially (through the assimilation of T&S observed profiles) taken into account in our one dimensional framework.

All these issues make the simulation of chlorophyll a at L4 particularly challenging. However, even with all these caveats, the simulated spring bloom (chlorophyll) is still comparable with the climatological values (in terms of both phenology and concentration) for the L4 site. From figure 4 it emerges that the spring bloom is simulated in April which is consistent with Fig 12 of Smyth et al 2010

Andrew Yool, Tom Anderson and Katya Popova:

Figure 5 - this figure has a number of issues; these include: 1. Including the model spin-up period in the plot when it should be perfectly possible not to do this; 2. Showing the model for a period when there's no data; 3. Not having data on a plot when the data is widely known to exist (this looks suspicious); 4. Showing the same data twice for no good reason

We agree to the first two points. As for the data, we have taken the Turner chlorophyll-a data from the source we are referring to in the manuscript and are not aware of any omission. In any case, in order to adress your concern, we have replaced this with the HPLC data available, which doesn't have the gaps and extended the simulation period up to July 2012. In the new Hovmoeller plot of chlorophyll-a we have now exluded the scatter plot and show only the interpolated in-situ data. (We had included the scatter plot in order to illustrate to the reader the level of availability of data.) Both, the Hovmoeller plot and the statistics now exclude a spin-up period of four years.

Andrew Yool, Tom Anderson and Katya Popova:

 Figure 6 - any observations here?; for instance, Hirata et al. (2011) and Ward (2015) present absolute and fractional chlorophyll data that would provide a good comparison; as it happens, it looks like ERSEM is going a good job here



Figure 2: Simulation results vs. in situ data at BATS – left: chlorophyll *a* concentrations (Top – model, bottom – interpolated HPLC data); right: target diagram with bias (abscissa), MAE' (ordinate) and spearman correlation (colour code) for oxidised nitrogen (NO3), phosphate (PO4), silicate (Sil), dissolved inorganic carbon (DIC), dissolved oxygen (O_2), chlorophyll *a* (Chl) and particulate organic carbon (POC).

We are in fact referring to the Hirata et al. paper in the text discussing the figure and specifically to figure 2a-c therein which shows the close match in comunity structure (pg. 7154 line 25 to 7155 line 4).

Andrew Yool, Tom Anderson and Katya Popova:

• Figure 7 - while eyeballing model vs. observations is considered bad form these days, would it really hurt here to show the spatial map of observed chlorophyll?; we know it exists because the model has been compared to it

We believe that it is not possible to produce a meaningful comprehensive map comparable to the model based on the data used for the comparison. As stated in the text (7154 lines 22-23) and in the figure caption, we compared the full hindcast with in situ data from the ICES database, i.e. with bottle data. For this reason data are sparse in time and space, therefore a synpotic map cannot be produced without significant interpolation bias. We could produce a comparable map if we used satellite derived Chlorophyll, however this way we should limit the comparison to a much shorter period. Finally, the aim of section 7.3 and figure 7 is not to provide a comprehensive validation of the 3D implementation of ERSEM in the North Western European Shelf, this has already been done several times (e.g. Lewis et al., 2006, Allen et al., 2007, Allen and Somerfield 2009, Shutler et al., 2011, Artioli et al., 2012, Holt et al., 2012 to name a few) but to illustrate the potential use of ERSEM in a 3D implementation.

Andrew Yool, Tom Anderson and Katya Popova:

 Figure 8 – is this comparing the model to a dataset that was used to parameterise it?; that seems to undercut the rationale for this figure

In the first instance, we are quoting pg. 7156 line 17:

"No attempt was made to fit the curve to this particular set of observations."

In addition, this figure appears in the section of the testing framework whose purpose is to check the correct implementation of isolated pieces of the model. So we don't think it undercuts the purpose, quite the contrary, it shows that the model behaves as was intended.

Andrew Yool, Tom Anderson and Katya Popova:

• Figure 9 - is there any observational data to add to this plot?; and why is this plot not in colour?; it is difficult to discern the different lines easily

Again, the purpose of this plot is not a model validation, but the possibility to isolate parts of the code and use them on their own for sensitivty studies, in this case an illustration of the effect of different parameter values for the modelled P-I-curve. For this purpose the data is not required. We have included this plot in colour now.

References

- Aksnes, D. L. and Egge, J. K.: A theoretical model for nutrient uptake in phytoplankton, Mar. Ecol.-Prog. Ser., 70, 65–72, doi:10.3354/meps070065, 1991.
- Allen, J., Somerfield, P., and Gilbert, F.: Quantifying uncertainty in high-resolution coupled hydrodynamic-ecosystem models, in: Contributions from Advances in Marine Ecosystem Modelling Research, 27–29 June, 2005, Plymouth, UK AMEMR, 64, 3–14, available at: http://www.sciencedirect.com/science/article/pii/ S0924796306001035 (last access: 14 August 2015), 2007.



Figure 3: Phytoplankton growth over PAR for the four phytoplankton types.

- Allen, J. I. and Somerfield, P. J.: A multivariate approach to model skill assessment, J. Marine Syst., 76, 83–94, doi:10.1016/j.jmarsys.2008.05.009, 2009.
- Anderson, T. R., Hessen, D. O., Mitra, A., Mayor, D. J., and Yool, A.: Sensitivity of secondary production and export flux to choice of trophic transfer formulation, J. Marine Syst., 125, 41–53, doi:10.1016/j.jmarsys.2012.09.008, 2013.
- Artioli, Y., Blackford, J. C., Butenschön, M., Holt, J. T., Wakelin, S. L., Thomas, H., Borges, A. V., and Allen, J. I.: The carbonate system in the North Sea: sensitivity and model validation, J. Marine Syst., 102–104, 1–13, doi:10.1016/j.jmarsys.2012.04.006, 2012.
- Aumont, O., Ethé, C., Tagliabue, A., Bopp, L. and Gehlen, M.: PISCESv2: an ocean biogeochemical model for carbon and ecosystem studies, Geosci. Model Dev., 8, 2465–2513, doi:110.5194/gmd-8-2465-2015, 2015.
- Baretta, J. W., Ebenhöh, W., and Ruardij, P.: The European regional seas ecosystem model, a complex marine ecosystem model, Neth. J. Sea Res., 33, 233–246, doi:10.1016/0077-7579(95)90047-0, 1995.
- Baretta-Bekker, J. G., Baretta, J. W., and Ebenhöh, W.: Microbial dynamics in the marine ecosystem model ERSEM II with decoupled carbon assimilation and nutrient uptake, J. Sea Res., 38, 195–211, doi:10.1016/S1385-1101(97)00052-X, 1997.
- Broecker, W. S. and Peng, T. H.: Tracers in the sea, Eldigio Press, New York, USA, 1982.
- Brzezinski, M. A.: The Si:C:N ratio of marine diatoms: interspecific variability and the effect of some environmental variables, J. Phycol., 36, 87–96, doi:10.1111/j.0022-3646.1985.00347.x, 1985.
- Broekhuizen, N., Heath, M. R., Hay, S. J., and Gurney, W. S. C.: Modelling the dynamics of the North Sea's Mesozooplankton, Neth. J. Sea Res., 33, 381–406, doi:10.1016/0077-7579(95)90054-3, 1995.
- Burchard, H., Deleersnijder, E., and Meister, A.,: A high-order conservative Patankar-type discretisation for stiff systems of production-destruction equations, Appl. Numer. Math., 47, 1–30, doi:10.1016/S0168-9274(03)00101-6, 2003.

- Chesson, J.: The estimation and analysis of preference and its relatioship to foraging models, Ecology, 64, 1297–1304, doi:10.2307/1937838, 1983.
- Chisholm, S.: Phytoplankton size, in: Primary Productivity and Biogeochemical Cycles in the Sea, edited by: Falkowski, P. and Woodhead, A., 213–237, Plenum Press, New York, 1992.
- Dugdale, R. C., Wilkerson, F. P., and Minas, H. J.: The role of a silicate pump in driving new production, Deep-Sea Res. Pt. I, 42, 697–719, doi:10.1016/0967-0637(95)00015-X, 1995.
- Falkowski, P. G. and Raven, J. A.: Aquatic photosynthesis, Princeton University Press, Princeton, USA, 2007.
- Fasham, M. J. R., Ducklow, H. W., and McKelvie, S. M.: A nitrogen-based model of plankton dynamics in the oceanic mixed layer, J. Mar. Res., 48, 591–639, 1990.
- Fennel, W.: A model of the yearly cycle of nutrients and plankton in the Baltic Sea, J. Mar. Sys., 6, 313–329, doi:10.1016/0924-7963(94)00031-6, 1995.
- Finkel, Z. V., Beardall, J., Flynn, K. J., Quigg, A., Rees, T. A. V., and Raven, J. A.: Phytoplankton in a changing world: cell size and elemental stoichiometry, J. Plankton Res., 32, 119–137, doi:10.1093/plankt/fbp098, 2010.
- Franks, P. J., S.: Planktonic ecosystem models: perplexing parameterizations and a failure to fail, J. Plankton Res., 31, 1299–1306, doi:10.1093/plankt/fbp069, 2009.
- Gehlen, M., Gangstø, R., Schneider, B., Bopp, L., Aumont, O., and Ethe, C.: The fate of pelagic CaCO₃ production in a high CO₂ ocean: a model study, Biogeosciences, 4, 505–519, doi:10.5194/bg-4-505-2007, 2007.
- Geider, R. J., MacIntyre, H. L., and Kana, T. M.: A dynamic model of phytoplankton growth and acclimation: responses of the balanced growth rate and chlorophyll *a*:carbon ratio to light, nutrient limitation and temperature, Limnol. Oceanogr., 148, 679–694, doi:10.4319/lo.1998.43.4.0679, 1998. Geider 1998

- Geider, R. J., MacIntyre, H. L., and Kana, T. M.: A dynamic regulatory model of phytoplanktonic acclimation to light, nutrients, and temperature, Mar. Ecol-Prog. Ser., 43, 187–200, doi:10.3354/meps148187, 1997.
- Heath, M., Roberston, W., Mardaljevic, J., and Gurney, W. S. G.: Modelling the population dynamics of Calanus in the Fair Isle current of northern Scotland, J. Sea Res., 38, 381–412, doi:10.1016/S1385-1101(97)00047-6, 1997.
- Holt, J., Butenschön, M., Wakelin, S. L., Artioli, Y., and Allen, J. I.: Oceanic controls on the primary production of the northwest European continental shelf: model experiments under recent past conditions and a potential future scenario, Biogeosciences, 9, 97–117, doi:10.5194/bg-9-97-2012, 2012.
- Huesmann, M., H., Skillman, A. D., and Crecelius, E. A.: The inhibition of marine nitrification by ocean disposal of carbon dioxide, Mar. Pollut. Bull., 44, 142–148, 2002.
- Jassby, A. D. and Platt, T.: Mathematical formulation of relationship between photosynthesis and light for phytoplankton, Limnol. Oceanogr., 21, 540–547, doi:10.4319/lo.1976.21.4.0540, 1976.
- Kleypas, J. A., Buddemeier, R., W., Archer, D., Gattuso, J.-P., Langdon, C., and Opdyke, B., N. : Geochemical consequences of increased atmospheric carbon dioxide on coral reefs, Science, 284, 118–120, doi:10.1126/science.284.5411.118, 1999.
- Kohlmeier, C.: Modellierung des Spiekerooger Rückseitenwatts mit einem gekoppelten Euler-Lagrange-Modell auf der Basis von ERSEM, PhD thesis, Carl von Ossietzky Universität, Oldenburg, 2004.
- Kwiatkowski, L., Yool, A., Allen, J. I., Anderson, T. R., Barciela, R., Buitenhuis, E. T., Butenschön, M., Enright, C., Halloran, P. R., Le Quéré, C., de Mora, L., Racault, M.-F., Sinha, B., Totterdell, I. J., and Cox, P. M.: iMarNet: an ocean biogeochemistry model intercomparison project within a common physical ocean modelling framework, Biogeosciences, 11, 7291–7304, doi:10.5194/bg-11-7291-2014, 2014.
- Lee, K., Tong, L. T., Millero, F. J., Sabine, C. L., Dickson, A. G., Goyet, C., Park, G.-H., Wanninkhof, R., Feely, R. A., and Key, R. M.: Global relationships of total alkalinity with salinity and temperature in sur-

face waters of the world's oceans, Geophys. Res. Lett., 33, L19605, doi:10.1029/2006GL027207, 2006.

- Litchman, E., Klausmeier, C. A., Schofield, O. M., and Falkowski, P. G.: The role of functional traits and trade-offs in structuring phytoplankton communities: scaling from cellular to ecosystem level, Ecol. Lett., 10, 1170–1181, doi:10.1111/j.1461-0248.2007.01117.x, 2007.
- Litchman, E., Pinto, P. d. T., Klausmeier, C. A., Thomas, M. K., and Yoshiyama, K.: Linking traits to species diversity and community structure in phytoplankton, Hydrobiologia, 653, 15–28, doi:10.1007/s10750-010-0341-5, 2010.
- Moore, C. M., Mills, M. M., Arrigo, K. R., Berman-Frank, I., Bopp, L., Boyd, P. W., Galbraith, E. D., Geider, R. J., Guieu, C., Jaccard, S. L., Jickells, T. D., La Roche, J., Lenton, T. M., Mahowald, N. M., Maranon, E., Marinov, I., Moore, J. K., Nakatsuka, T., Oschlies, A., Saito, M. A., Thingstad, T. F., Tsuda, A., and Ulloa, O.: Processes and patterns of oceanic nutrient limitation, Nat. Geosci., 6, 701–710, doi:10.1038/ngeo1765, 2013.
- Patankar, S. V.: Numerical Heat Transfer and Fluid Flow, McGraw-Hill, New York, USA, 1980.
- Platt, T., Harrison, W. G., Irwin, B., Horne, E. P., and Gallegos, C. L.: Photosynthesis and photoadaptation of marine phytoplankton in the arctic, Deep-Sea Res., 29, 1159–1170, doi:10.1016/0198-0149(82)90087-5, 1982.
- Polimene, L., Allen, J. I., and Zavatarelli, M.: Model of interactions between dissolved organic carbon and bacteria in marine systems, Aquat. Microb. Ecol., 43, 127–138, doi:10.3354/ame043127, 2006.
- Polimene, L., Pinardi, N., Zavatarelli, M., Allen, J. I., Giani, M., and Vichi, M.: A numerical simulation study of dissolved organic carbon accumulation in the northern Adriatic Sea, J. Geophys. Res.-Oceans, 112, C03S20, doi:10.1029/2006JC003529, 2007.
- Pujo-Pay, M. and Conan, P. and Raimbault, P.:Excretion of dissolved organic nitrogen by phytoplankton assessed by wet oxidation and ¹⁵N tracer procedures, Mar. Ecol.-Prog. Ser., 153, 99–111, doi:10.3354/meps153099, 1997.

- Smyth, T. J., Fishwick, J. R., AL-Moosawi, L., Cummings, D. G., Harris, C., Kitidis, V., Rees, A., Martinez-Vicente, V., and Woodward, E. M. S.: A broad spatio-temporal view of the Western English Channel observatory, J. Plankton Res., 32, 585–601, doi:10.1093/plankt/fbp128, 2010.
- Sukenik, A., Bennett, J., and Falkowski, P.: Light-saturated photosynthesis Limitation by electron transport or carbon fixation?, BBA-Bioenergetics, 891, 205–215, doi:10.1016/0005-2728(87)90216-7, 1987.
- Talmy, D., Blackford, J., Hardman-Mountford, N. J., Polimene, L., Follows, M. J., and Geider, R. J.: Flexible C:N ratio enhances metabolism of large phytoplankton when resource supply is intermittent, Biogeosciences, 11, 4881–4895, doi:10.5194/bg-11-4881-2014, 2014.
- Weiss, R. F.: The solubility of nitrogen, oxygen and argon in water and seawater, Deep-Sea Res., 17, 721–735, doi:10.1016/0011-7471(70)90037-9, 1970.
- Vichi, M., Pinardi, N., and Masina, S.: A generalized model of pelagic biogeochemistry for the global ocean ecosystem. Part I: Theory, J. Marine Syst., 64, 89–109, 2007.
- Yool, A., Popova, E. E., and Anderson, T. R.: MEDUSA-2.0: an intermediate complexity biogeochemical model of the marine carbon cycle for climate change and ocean acidification studies, Geosci. Model Dev., 6, 1767–1811, doi:10.5194/gmd-6-1767-2013, 2013.

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ERSEM 15.06: a generic model for marine biogeochemistry and the ecosystem dynamics of the lower trophic levels

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Abstract

The ERSEM model is one of the most established ecosystem models for the lower trophic levels of the marine food web in the scientific literature. Since its original development in the early nineties it has evolved significantly from a coastal ecosystem model for the North-Sea North Sea to a generic tool for ecosystem simulations from shelf seas to the global ocean. The current model release contains all essential elements for the pelagic and benthic part of the marine ecosystem, including the microbial food-webfood web, the carbonate system and calcification. Its distribution is accompanied by a testing framework enabling the analysis of individual parts of the model. Here we provide a detailed mathematical description of all ERSEM components along with case-studies case studies of mesocosm type simulations, water column implementations and a brief example of a full-scale application for the North-West European shelf. Validation against in situ data demonstrates the capability of the model to represent the marine ecosystem in contrasting environments.

1 Introduction

Over the last two decades a number of marine ecosystem models describing ocean biogeochemistry and the lower trophic levels of the food-web food web have emerged in a variety of contexts ranging from simulations of batch cultures or mesocosms over estuarine and coastal systems to the global ocean (e.g. Fasham et al., 1990; Flynn, 2010; Geider et al., 1997; Wild-Allen et al., 2010; Zavatarelli and Pinardi, 2003; Aumont et al., 2003; Follows et al., 2007; Yool et al., 2013; Stock et al., 2014). Some of them have matured with the years into sound scientific tools in operational forecasting systems and are used to inform policy and management decisions regarding essential issues of modern human society, such as climate change, ecosystem health, food provision and other ecosystem goods and services (e.g. Lenhart et al., 2010; Glibert et al., 2014; van der Molen et al., 2014; Doney et al., 2012; Bopp et al., 2013; Chust et al., 2014; Barange et al., 2014). Given the importance of these applications, transparent descriptions of the scientific contents of these

models are necessary in order to allow full knowledge and assessment of their strength and weaknesses, as well as maintenance and updating according to scientific insight and progress.

Here we provide full description of one of these models. а ERSEM (European Regional Seas Ecosystem Model), developed in the early nineties (Baretta et al., 1995; Baretta, 1997)¹ out of a European collaborative effort, building on previous developments (Radford and Joint, 1980; Baretta et al., 1988). Subsequent development of the model has occurred occurred in separate streams leading to individual versions of the model, the main ones being the ERSEM version described in Allen et al. (2001); Blackford and Burkill (2002); Blackford et al. (2004) and the version of Vichi et al. (2004, 2007); Leeuwen et al. (2012); van der Molen et al. (2014); http://www.nioz.nl/northsea model, also referred to as the Biogeochemical Flux Model. The present release is based on the former development stream (Blackford et al., 2004). It has since the beginnings of ERSEM gradually evolved into what is now the principal model for shelf-seas applications within the UK and beyond. It is part of the operational suite of the UK Met Office, and the biogeochemical component for the North-West European shelf seas within the European Copernicus Marine Service.

While it was originally created as a scientific tool for the North Sea ecosystem (hence the name), it has since evolved considerably in its scientific content, broadening the scope of the model to coastal systems across the globe as well as the open ocean. Allen et al. (2001) have adopted the model for simulations across the entire North-West European shelf sea, further extended in Holt et al. (2012); Artioli et al. (2012) Holt et al. (2012) and Artioli et al. (2012) to include the North East Atlantic. Blackford et al. (2004) have applied the model across six different ecosystem types across the globe, Barange et al. (2014) have used applications of the model in the major coastal upwelling zones of the planet, and Kwiatkowski et al. (2014) have assessed the skill of the model, demonstrating its com-

¹The two given references are the introductions to two special issues published on the original model versions ERSEM I and II, representing the entire volumes. More specific reference to single papers within these volumes are given in the relevant process descriptions.

petitiveness with respect to other established global ocean models. The model has been subject to validation on various levels ranging from basic statistical metrics of point-to-point matches to observational data (Shutler et al., 2011; de Mora et al., 2013) to multi-variate analysis (Allen et al., 2007; Allen and Somerfield, 2009) and pattern recognition (Saux Picart et al., 2012).

The model has been applied in a wide number of contexts that include short-term forecasting (Edwards et al., 2012), ocean acidification (Blackford and Gilbert, 2007), climate-change climate change (Holt et al., 2012), coupled climate-acidification projections (Artioli et al., 2013), process studies (Polimene et al., 2012, 2014), biogeochemical cycling (Wakelin et al., 2012), habitat (Villarino et al., 2015) and end-to-end modelling (Barange et al., 2014). The wide range of applications and uses of the model coupled with developments since earlier manuscripts documenting the model (Baretta-Bekker, 1995; Baretta, 1997; Blackford et al., 2004) make a thorough and integral publication of its scientific ingredients overdue.

Being an evolution of former models within the ERSEM family that emerged in parallel to other, separate development streams of the original model, the core elements of the current model version closely resemble earlier versions even if presented in much more detail compared to previous works. We present a model for ocean biogeochemistry, the planktonic and benthic parts of the marine ecosystem that includes explicitly the cycles of the major chemical elements of the ocean (carbon, nitrogen, phosphorus, silicate and iron); it includes the microbial food-webfood web, a sub-module for the carbonate system, calcification and a full benthic model.

The present paper provides Our main objective with this paper is to provide a full description of all model componentsand simple case-studies illustrating, accompanied by simple case studies with low resource requirements that illustrate the model capabilities in an idealised and enable the interested reader to implement our model and reproduce the test cases shown. To this purpose we present the examples of a mesocosm type framework and in-three vertical water-column implementations of opposing character supplemented by complemented with basic validation metrics against in-situ observations.

All material required to replicate these test cases, such as parameterisation and input files, are provided in the Supplement. In addition, a brief illustration of a full scale three dimensional application. implementation is given to show the model in a large scale application.

The next section gives an overview of the model and its philosophy while the two following sections contain the descriptions of the pelagic and benthic components, describe the air-sea and seabed interfaces and detail some generic terms that are used throughout the model. The model description is complemented by two sections that present different implementations of the model and illustrate the testing framework. We complete the work with a section on optional choices of model configuration and a section on the technical specifications of the software package, license licence and instructions of where and how to access the model code.

2 The ERSEM model

ERSEM is, since its origins, an ecosystem model of intermediate complexity for marine biogeochemistry, pelagic plankton and benthic fauna. Its functional types (Baretta et al., 1995; Vichi et al., 2007) are based on their macroscopic role in the ecosystem rather than species or taxa and its state variables are the major chemical components of each type (carbon, chlorophyll a, nitrogen, phosphate, silicate and optionally iron). It is composed of a set of modules that compute the rates of change of its state variables given the environmental conditions of the surrounding water body, physiological processes and preditorprey interactions. In the simplest case the environmental drivers can be provided offline, or through a simple 0-dimensional box model. However, for more realistic representations, including the important processes of horizontal and vertical mixing (or advection) and biogeochecmial feed-backsfeedback, a direct (or online) coupling to a physical driver, such as a 3-D hydrodynamic model, is required.

The organisms in the model are categorised along with the main classes of ecosystem function into primary producers, consumers and bacterial decomposers, particulate and dissolved organic matter (POM, DOM) in the pelagic and consumers, bacterial decomposers, particulate and dissolved organic matter in the benthos. Most of these classes are further subdivided into sub-types to allow for an enhanced plasticity of the system in adapting the ecosystem response to the environmental conditions in comparison to the classical NPZD type models. A particularity of ERSEM is the Importantly, ERSEM uses a fully dynamic stoichiometry in essentially all its types (with the exception of mesozooplankton, benthic bacteria and zoobenthos which use fixed stoichiometric ratios). The model dynamics of a living functional type are generally based on a standard oragnism that is affected by the assimilation of carbon and nutrients into organic compounds by primary production or uptake, and the generic loss processes of respiration, excretion, exudation and mortality (release, predation and non predatory mortality (Fig. 1, see also Vichi et al., 2007 - "2. Towards a generic formalism for pelagic biogeochemistry"). These are accompanied by nutrient uptake In this framework we refer to excretion as inefficencies of the uptake processes, while the release terms represent regulatory processes of the current nutritional state. More specifically, uptake, which may occur in inorganic or organic formaccording to, is given by the external availability and, actual requirement and uptake capacity of the relevant functional type balanced by nutrient loss leading to stochiometric variations in its chemical components that are balanced by losses according to the internal quota and storage capacity. This stoichiometric flexibility allows for a diverse response in between the functional types in adapting to the environmental conditions with respect compared to fixed guota models (e.g. through varying resistance against low nutrient conditions and luxury storages supporting a more realistic evolution of the community structure). Figure 2 illustrates the pathways of these fluxes within the food-web food web of the model.

ERSEM is not designed to directly model cell physiology. Its equations are a synthesis of physiological processes and their macroscopic consequences on larger water bodies in which the distributions of the plankton biomass, organic and inorganic material can be approximated as smooth continuous fields. This is important to keep in mind in small scale and high-resolution applications where this basic assumption of the continuum hypothesis may break down, in which case the system of partial differential balance equations no longer

holds. As a rule of thumb, in order to guarantee the validity of the equations, the modelled scales should at least be an order of magnitude bigger than the organims modelled and smaller patches.

Mathematically, the set of prognostic equations describing the dynamics of marine biogeochemical states is generally given by:

$$\frac{\partial c_{\mathbf{p}}}{\partial t} + \boldsymbol{u} \cdot \frac{\partial c_{\mathbf{p}}}{\partial \boldsymbol{x}} + \overset{c_{\mathbf{p}}}{w_{\text{sed}}} \frac{\partial c_{\mathbf{p}}}{\partial z} = \nu \frac{\partial^2 c_{\mathbf{p}}}{\partial \boldsymbol{x}^2} + \frac{\partial c_{\mathbf{p}}}{\partial t} \Big|_{\text{bgc}} + \frac{\partial c_{\mathbf{p}}}{\partial t} \Big|_{\text{seabed}}$$
(1)
$$\frac{\partial c_{\mathbf{b}}}{\partial t} = \frac{\partial c_{\mathbf{b}}}{\partial t} \Big|_{\text{bgc}},$$
(2)

where c_{p} are the pelagic concentrations (per volume) and c_{b} the benthic contents (per sediment surface area) of each chemical component of the organic model types or the organic or inorganic model components. $\overset{\rm sed}{w_{\rm Cp}}$ is the velocity of gravitational sinking of particles in the water column. x represents the vector of spatial coordinates of which z is the vertical coordinate being 0 at sea surface and increasing downwards.

The set of equations is closed by the horizontal boundary conditions of the system generally given by the air–sea fluxes $\mathcal{F}|_{sea}^{air}$ and the fluxes across the seafloor $\mathcal{F}|_{ben}^{pel}$ and lateral boundary conditions if present in the given configuration.

ERSEM computes the biogeochemical rates of change in pelagic $\left(\frac{\partial c_p}{\partial t}\Big|_{boc}\right)$ and benthic $\left(\frac{\partial C_{b}}{\partial t}\Big|_{bac}\frac{\partial c_{b}}{\partial t}\Big|_{bac}\right)$ systems, the gas transfer across sea-surface $(\mathcal{F}|_{sea}^{air}$ for oxygen and car-

bon) and the fluxes across the seabed ($\mathcal{F}|_{ben}^{pel}$). The actual numerical integration of these rates along with the advection-diffusion processes that solves Eqs. (1) and (2) needs to be addressed appropriately through an external driver as e.g. discussed in (Butenschön et al., 2012).

2.1 Nomenclature and units

Pelagic state variables in ERSEM are concentrations and are referred to as cp. When indicating a specific class or type, they are denoted by upper case letters (P: phytoplankton, Z: zooplankton, B: bacteria, R: organic matter, O: gases, N: nutrients), with the chemical component in the subscript in blackboard style (\mathbb{C} : carbon, \mathbb{N} : nitrogen, \mathbb{P} : phosphorus, \mathbb{S} : silicon, \mathbb{F} : iron with the exception of the chlorophyll *a* components which are distinguished by using C, as chlorophyll a is not a chemical element but a compound), and the specific type in the super-script, e.g. $P_{\mathbb{C}}^{\text{dia}}$ for diatom carbon. Correspondingly, benthic states use c_{b} for generic contents and the specific states (H: bacteria Y: zoobenthos, Q: organic matter, G: gases, K: nutrients, D: states of vertical distribution). Primes (') mark available concentrations or contents to loss processes (see Sect. 2.3). Where equations are valid for more than one specific functional type χ, ψ, Ψ are used as place holders for functional types and the chemical components may be given as a comma separated list, implying that an equation is valid for all these components, e.g. $\overset{\chi}{P}_{\mathbb{C},\mathbb{N},\mathbb{P}}$ represents the carbon, phosphorus and

nitrogen content of each phytoplankton type. The physical environment is given in roman letters, e.g. T for temperature.

Parameters are represented by lower case letters with r for specific rates, q for quotas or fractions, l for limitation or regulating factors, h for half-saturation constants and p for most others. Food preferences of predators on their prey are given as $f_{pr}|_P^Z$ being the preference of predator Z on food P.

Fluxes between state variables are given as $\mathcal{F}|_A^B$ for the flux from A to B. Specific rates are notated using \mathcal{S} . Dynamic internal quotas of two components A and B are given by the notation $q_{A:B}$, e.g. $\overset{\text{dia}}{q}_{\mathbb{N}:\mathbb{C}}$ being the internal nitrogen to carbon quota of diatoms $\overset{\text{dia}}{\frac{P_{\mathbb{N}}}{dia}}$. Derived quotas or fractions are given by a caligraphic Q.

The coordinate system used describes the horizontal coordinates in x and y, while the vertical coordinate is given by z, 0 at the sea surface increasing downwards. The corre-

sponding velocity fields are given by u, v and w. We are referring to Cartesian coordinates in this publication for simplicity.

The sediment depth coordinate is given by ζ , which is 0 at the sediment surface increasing downwards.

All equations equations are given as scalar equations for a single pixel of the model domain.

Rates of change of the biogeochemical state variables due to individual sub $rac{\partial \phi}{\partial t}$ processes or groupings of these are given as where the followsubprocess' ing abbreviations are used for the subprocesses: bgc=biogeochemical fluxes, bur = burying, calc = calcification, decomp = decomposition, denit = denitrification, lys = lysis, mort = mortality, dis = dissolution, excr = excretion, net = comprehensive net fluxes, nitr = nitrification, pred = predation, rel = release, remin = remineralisation, resp = respiration, scav = scavenging, sed = sedimenation, upt = uptake.

In equations that hold for multiple functional groups or components squared brackets are used for terms that are only valid for a single functional group or component.

Units in the model for all organic and inorganic nutrient concentrations are in mmol m⁻³ with the exception exception of iron being in μ mol m⁻³. All forms of organic carbon are in mg m⁻³ while all species of inorganic carbon are in mmol m⁻³ with the exception of the internal computations of the carbonate system where they are converted to μ mol kg⁻³ μ mol kg⁻¹. Corresponding benthic contents are two-dimensional and consequently given in mmol m⁻², mg m⁻² and μ mol m⁻². The penetration depth and depth horizons in the sediments are given in m. Temperatures are generally considered in °C, salinity in psu, sea-water density in $\frac{kg m^{-3}}{kg m^{-3}}$ and pressure is given in Pa, with the exception of the internal calculations of the carbonate system where temperature is converted to absolute temperature in K and pressure to bar. Partial pressure of carbon dioxide is used in ppm.

2.2 Dependencies on the physical environment

Several processes in the model depend directly on the physical environment that the model states are exposed to:

- Metabolic processes depend on the sea-water temperature.
- Primary Production production relies additionally on the photosynthetically active radiation (PAR) as energy input which is should be computed from shortwave radtion radiation at the sea surface Isurf-, taking into account the attenuation coefficients given in Sect. 3.9. Note, that the model requires the average light in each discrete model cell, which is not given by the light at the cell centre, but by the vertical integral of the light curve divided by the cell depth.
- Empirical regressions for alkalinity, saturation states and chemical equilibrium coefficient coefficients of the carbonate system reactions require temperature T, salinity S, pressure p and density ρ of the sea-water.
- Air-sea fluxes of carbon dioxide and oxygen depend on temperature T and the absolute wind speed $vecu_{wind}$ uwind near the sea-surface.
- Deposition of organic matter on the sea floor and resuspension depend on the shear stress at the sea floor τ_{bed} .
- The optional light attenuation model based on inherent optical properties requires the geographical coordinates of each model pixel and the current simulation date and time in order to compute the zenith angle.

2.3 States and negativity control

In order to avoid the occurrence of negative concentrations or contents in the integration process and reduce the vulnerability to numerical numerical noise all state variables include a lower buffer $\epsilon_{p,b}$, based on a carbon concentration of $0.01 \,\mathrm{mg}\,\mathrm{m}^{-3}$ modified adequately for the various state variables variables using reference stoichiometric quotas and unit conversions. This buffer is not accessible to the loss processes of the biogeochemical dynamics. Consequently all process processes that diminish the biomass of each state are based on the available concentrations or contents given by $c'_{p,b} = c_{p,b} - \epsilon_{p,b}$. These small resilient buffers additionally support the spawning of new biomass as soon as favourable conditions occur, similar to the low overwintering biomass limits in Fennel (1995).

Note that when calculating the overall budgets of a domain, these background concentrations should be subtracted in order to give adequtate results.

The pelagic system 3

In its current form the pelagic part of ERSEM comprises 4 functional types for primary producers, originally defined as diatoms, nanoflagellates, picophytoplankton and dinoflagellates. This classification was historically coined for the North Sea but has since been widened to a broader interpretation almost exclusively based on the single trait size (with the exception of the requirement of silicate by diatoms and an implicit calcification potential of nanoflagellates) leading to the classes of picophytoplankton, nanophytoplankon, microphytoplankton and diatoms. Similarly the zooplankton pool is divided into hetero heterotrophic nanoflagellates, microzooplankton and mesozooplankton. Particulate organic matter is treated in three size classes (small, medium and large) in relation to its origin. Dissolved organic matter is distinguished according to its decomposition time scales into a labile dissolved inorganic state, semi-labile and semi-refractory carbon (see Sect. 3.3.1).

The inorganic state variables of the pelagic model are dissolved oxidised nitrogen, ammonium, phosphate, silicid silicic acids, dissolved inorganic iron, dissolved inorganic carbon, dissolved oxygen and calcite. In addition the model holds a state variable for alkalinity subject to fluctuations generated from the modelled biogeochemical processes (see Sect. 3.8 and Artioli et al., 2012). The complete list of pelagic state variables is given in Tables 1 and 2Table 3.

The recently implemented iron cycle (following largely the implementation of Vichi et al., 2007) and the silicate cycle are abbreviated for simplicity, their pathways by-pass the predator predators and decomposers by turning grazing of phytoplankton iron or silicate directly into detritus and remineralising iron implicitly from detritus into the dissolved dissolved inorganic form, while silicate is not remineralised in the water column. Chlorophyll a takes a special role in between the chemical components of the model: being a compound of other elements it is not strictly conserved by the model equations but rather derived from assimilation of carbon and subsequent decomposition of organic compounds. The addition of chlorophyll a states to the model allows for dynamic chlorophyll a to carbon relationships in the photosynthesis description and a more accurate comparsion to observations of biomass or chlorophyll a.

The growth dynamics in the model are generally based on mass-specific production and loss equations that are expressed in the currency of each chemical component, regulated and limited by the availability of the respective resources.

3.1 **Primary producers**

The phytoplankton dynamics are modelled for each phytoplankton type as a net result of source and loss processes (Varela et al., 1995)given by . The carbon and chlorophyll a component is given by uptake in the form of gross primary production and the losses through excretion, respiration, lysis and predation of zooplankton for the carbon and chlorophyll a component predation by zooplankton and mortality in the form of lysis, while the nutrient content is balanced by uptake, lysis and predation : release, predation and

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 $\partial \tilde{P}_{\mathbb{C},\mathcal{C}}$

 ∂t

predmort



 $\frac{\partial \hat{P}_{\mathbb{C},\mathcal{C}}}{\partial t}$

llvspred

 $= \frac{\partial \overset{\chi}{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \bigg| - \frac{\partial \overset{\chi}{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \bigg| - \frac{\partial \overset{\chi}{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \bigg|$

mortality in the form of lysis :

 $\frac{\partial \overset{\lambda}{P}_{\mathbb{C},\mathcal{C}}}{\partial t}\Big|$

with χ in (pico, nano, micro, dia) and where only for diatoms (pico, nano, micro, dia) and where the silicate component (S) is active only active for diatoms.

Specific gross primary production is The formulation of photosynthesis combines the form originally presented in Baretta-Bekker et al. (1997) for the balance of carbon assimilation, excretion and respiration with the negative exponential light harvesting model based on Jassby and Platt (1976), Platt et al. (1982) and Geider et al. (1997) in order to describe the total specific carbon fixation. In this formulation the gross carbon assimilation is assumed to be not depending on nitrogen and phosphorus. Total gross primary production (GPP) is assumed to be composed of a fraction which is assimilated (cellular GPP) through photosynthesis and a fraction which is not utilisable, e.g. due to nutrient limitation, and excreted. A similar approach can be found in Falkowski and Raven (2007). The idea behind this assumption is that nutrient (or specifically nitrogen and phosphorus) limitation affects more the assimilation of newly fixed carbon into cellular biomass (assimilation) than the photosynthesis itself.

Phytoplankton mass-specific gross primary production is then computed as

$$\overset{\chi}{\mathcal{S}_{\mathsf{gpp}}} = \overset{\chi}{g}_{\mathsf{max}} \overset{\chi}{l_{\mathsf{T}}} \overset{\chi}{l_{\mathbb{S}}} \overset{\chi}{l_{\mathbb{F}}} \left(1 - e^{-\frac{\chi}{\mathsf{P}_{\mathsf{I}} E_{\mathsf{PAR}}}{\chi} \frac{\chi}{\mathsf{Q}_{\mathbb{C}}\mathbb{C}}}{\operatorname{g}_{\mathsf{max}}} \right) e^{-\frac{\chi}{\mathsf{P}_{\mathsf{I}} E_{\mathsf{PAR}}}{\chi} \frac{\chi}{\mathsf{Q}_{\mathbb{C}}\mathbb{C}}}{\operatorname{g}_{\mathsf{max}}} ,$$
(5)

based on the formulation by Geider et al. (1997) modified for photoinhibition according to Blackford et al. (2004). The symbols in this equation represent the chlorophyll a to carbon quotae quota of each functional type $q_{\mathcal{C}:\mathcal{C}}^{\chi} = P_{\mathcal{C}}^{\chi}/P_{\mathcal{C}}^{\chi}$, the metabolic response to temperature \tilde{l}_{T} (see Eq. 235) and the silicate and iron limitation factors $\tilde{l}_{S,F} \epsilon [0,1]$ (see Eqs. 239) and 240). The g_{max}^{χ} are the maximum potential photosynthetic rate parameters in unlimited unlimiting conditions at reference temperature. Note, that these are different to the maximum potential growth rates usually retrieved in physiological experiments (e.g. in the work of Geider et al., 1997) or measured at sea, in that they are exclusive upper bounds of the specific growth rate function. In fact, the products of the exponential terms in Eq. (5) have

a maximum of $\left(1.0 - \frac{\chi}{\beta_{\text{Pl}}} \right) \left(\frac{\chi}{\alpha_{\text{Pl}} + \beta_{\text{Pl}}}\right) \left(\frac{\chi}{\alpha_{\text{Pl}} + \beta_{\text{Pl}}}\right)^{\chi} < 1$. In addition, we refer to gross primary production here as total carbon fixation, a fraction of which is directly excreted to the dissolved organic carbon pool. Other parameters are the initial slope $\overset{X}{lpha}_{Pl}$ and the photoinhibition parameter $\stackrel{\chi}{\beta}_{PI}$ of the light saturation curve (Platt et al., 1982).

A fraction of the specific gross production is directly excreted to the dissolved organic carbon (DOC) pool as a fixed fraction q_{excr}^{χ} augmented according to the combined nitrogen

and phosphorus limitation up to the total gross production:

$$\overset{\chi}{\mathcal{Q}}_{\mathsf{excr}} = \left[1 - \left(\left(1 - \overset{\chi}{l_{\langle \mathbb{NP} \rangle}} \right) \left(1 - \overset{\chi}{q_{\mathsf{excr}}} \right) + \overset{\chi}{q_{\mathsf{excr}}} \right) \right]$$

$$\overset{\chi}{\mathcal{Q}}_{\mathsf{excr}} = \overset{\chi}{q}_{\mathsf{excr}} + \left(1 - \overset{\chi}{l}_{\langle \mathbb{NP} \rangle}\right) \left(1 - \overset{\chi}{q}_{\mathsf{excr}}\right),$$
(6)

where $\overset{\chi}{l}_{\langle \mathbb{NP} \rangle}$ is the combined nitrogen-phosphorus limitation factor defined in Eq. (238), based on the internal nutrient to carbon quotas according to Droop (1974).

The second generic sink term is given by lysis which occurs proportional to the current biomass by the constant specific rate $\frac{\chi}{r_{\text{lys}}}$ augmented by nutrient stress according to:

$$\overset{\chi}{\mathcal{S}}_{\text{tys}\,\underline{\text{mort}}} = \frac{1}{\min\left(\overset{\chi}{l}_{\langle \mathbb{NP} \rangle}, \overset{\chi}{l}_{\mathbb{S}}\right) \pm 0.1} \overset{\chi}{r}_{\text{tys}\,\underline{\text{mort}}} .$$
(7)

The carbon and chlorophyll a dynamics of each phytoplankton type in Eq. (3) are then specified by the following terms:

Carbon is assimilated according to

$$\frac{\partial \tilde{P}_{\mathbb{C}}}{\partial t} \bigg|_{\text{gpp}} = \overset{\chi}{\mathcal{S}}_{\text{gpp}} \overset{\chi}{P}_{\mathbb{C}}.$$
(8)

Chlorophyll The synthesis rate of chlorophyll a is synthesised at the acclimated quota given by:

$$\frac{\partial \overset{\chi}{P_{\mathcal{C}}}}{\partial t}\bigg|_{gpp} = \overset{\chi}{l}_{\langle \mathbb{NP} \rangle} \overset{\chi}{\varphi} \overset{\chi}{\mathcal{S}}_{gpp} \overset{\chi}{P}_{\mathbb{C}},$$
(9)

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where $\overset{\chi}{\varphi}$ is the ratio of chlorophyll a synthesis to carbon fixation under nutrient replete conditions. It is given by:

$$\overset{\chi}{\varphi} = \begin{pmatrix} \chi \\ q_{\varphi \max} - q_{\min_{\mathcal{C}:\mathbb{C}}} \end{pmatrix} \frac{\overset{\chi}{\mathcal{S}_{gpp}}}{\overset{\chi}{\alpha_{Pl} E_{PAR}} \overset{\chi}{q_{\mathcal{C}:\mathbb{C}}}} + q_{\min_{\mathcal{C}:\mathbb{C}}},$$
(10)

where $\overset{\chi}{q}_{arphi \max}$ are the maximum achievable chlorophyll a to carbon quota for each type, $q_{\min_{C:C}}$ is the minimum chlorophyll *a* to carbon quota.

This formulation differs from the original formulation of Geider et al. (1997) in its asymptotic limit of the carbon to chlorophyll a synthesis at high PAR, which in , In the original formulation the ratio is unbound, while in this formulation it is bound by the inverse minimum chlorophyll a to carbon ratio $q_{\min_{C:C}}$ in order to avoid excessive quotas not observed in nature.

The synthesis rate of chlorophyll *a* is then given by:

$$\frac{\partial P_{\mathcal{C}}}{\partial t} \bigg|_{\mathsf{gpp}} = \overset{\chi}{l}_{\langle \mathbb{NP} \rangle} \overset{\chi}{\varphi} \overset{\chi}{\mathcal{S}}_{\mathsf{gpp}} \overset{\chi}{P}_{\mathbb{C}}.$$

As opposed to the previous formulation of Blackford et al. (2004), the relative synthesis of chlorophyll a is directly limited by the internal nutrient quota in order to compensate for the enhanced demand required to maintain the cell structure leading to a reduced investment into the light harvesting capacity.

The excretion of phytoplankton in terms of carbon and chlorophyll a is consequently given by:

$$\frac{\partial \tilde{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \bigg|_{\text{excr}} = \frac{\chi}{\mathcal{Q}_{\text{excr}}} \left. \frac{\partial \tilde{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \right|_{\text{gpp}}.$$
(11)

Respiration of phytoplankton is split into respiration at rest, that is proportional to the current biomass by the constant specific rate $\overset{\chi}{r_{\mathsf{resp}}}$ complemented with an activity related term that is a fraction $\overset{\chi}{q}_{\rm aresp}$ of the assimilated amount of biomass per time unit after excretion:

$$\frac{\partial \overset{\chi}{P}_{\mathbb{C},\mathcal{C}}}{\partial t}\bigg|_{\text{resp}} = \overset{\chi}{r}_{\text{resp}} \overset{\chi}{P'}_{\mathbb{C},\mathcal{C}} + \overset{\chi}{q}_{\text{aresp}} \left(\frac{\partial \overset{\chi}{P}_{\mathbb{C},\mathcal{C}}}{\partial t}\bigg|_{\text{gpp}} - \frac{\partial \overset{\chi}{P}_{\mathbb{C},\mathcal{C}}}{\partial t}\bigg|_{\text{excr}} \right).$$
(12)

The losses of phytoplankton by lysis are given by

$$\frac{\partial \hat{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \bigg|_{\text{tys mort}} = \overset{\chi}{\mathcal{S}}_{\text{tys mort}} \overset{\chi}{P'}_{\mathbb{C},\mathcal{C}}$$
(13)

while the individual terms of loss through predation of predator Ψ in

$$\frac{\partial \hat{P}_{\mathbb{C},\mathcal{C}}}{\partial t} \bigg|_{\text{pred}} = \sum_{\Psi} \mathcal{F} \big|_{P}^{\Psi} \begin{array}{c} \hat{P}'_{\mathbb{C},\mathcal{C}} \,. \end{array}$$
(14)

are specified in the sections of the respective predators in Eqs. (30) and (172).

Nutrient demand uptake of nitrogen, phosphorus and iron is regulated by the nutrient demand of the phytoplankton group, limited by the external availability. Excretion is modelled as the disposal of non-utilisable carbon in photsynthesis while the release of nutrients is

limited to the regulation of the internal stoichiometric ratio. This approach is consistent with observations that nutrient excretion plays a minor role in the phytoplankton fluxes (Puyo-Pay et al., 1997). Consequently, demand of nutrients may be positive or negative in sign in relation to the levels of the internal nutrient storages and the balance between photosynthesis and carbon losses, so that:

$$\frac{\partial \overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{upt} = \begin{cases} \min\left(\mathcal{F}_{demand} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}}, \mathcal{F}_{avail} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}}\right) & \text{if } \mathcal{F}_{demand} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}} > 0 \\ 0 & \text{if } \mathcal{F}_{demand} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}} < 0 \\ \end{cases}$$
$$\frac{\partial \overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{rel} = \begin{cases} 0 & \text{if } \mathcal{F}_{demand} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}} > 0 \\ \mathcal{F}_{demand} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}} > 0 \\ \mathcal{F}_{demand} \middle|_{N_{N,\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{N,\mathbb{P},\mathbb{F}}} < 0 \end{cases} .$$
(15)

Nutrient demand (with the exception of silicate) is computed from assimilation demand at maximum quota $q_{\max_{\mathbb{N},\mathbb{P},\mathbb{P}:\mathbb{C}}}$ complemented by a regulation term relaxing the internal quota towards the maximum quota and compensating for rest respiration:

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$$\mathcal{F}_{\text{demand}} \Big|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\chi} = \stackrel{\chi}{\mathcal{S}}_{\text{gpp}} \left(1 - \stackrel{\chi}{\mathcal{Q}}_{\text{excr}} \right) \left(1 - \stackrel{\chi}{q}_{\text{aresp}} \right) \stackrel{\chi}{q}_{\text{max}_{\mathbb{N},\mathbb{P},\mathbb{F}:\mathbb{C}}} \stackrel{\chi}{P}_{\mathbb{C}} + r_{\text{nlux}} \left(\stackrel{\chi}{q}_{\text{max}_{\mathbb{N},\mathbb{P},\mathbb{F}:\mathbb{C}}} \stackrel{\chi}{P}_{\mathbb{C}}' - P'_{\mathbb{N},\mathbb{P},\mathbb{F}}' \right) - \stackrel{\chi}{r}_{\text{resp}} \stackrel{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}'$$
(16)

where r_{nlux} is the tendency of nutrient luxuary rate of nutrient luxury uptake towards the maximum quota.

Note, that these terms may turn negative when rest respiration exceeds the effective assimilation rate $\overset{\chi}{\mathcal{S}_{\mathsf{gpp}}}\left(1-\overset{\chi}{\mathcal{Q}_{\mathsf{excr}}}\right)\left(1-\overset{\chi}{q_{\mathsf{aresp}}}\right)\overset{\chi}{P_{\mathbb{C}}}$ or the internal nutrient content exceeds

the maximum quota resulting in nutrient excretion in dissolved inorganic from. The maximum quota for nitrogen and phosphorus may exceed the optimal quota allowing for luxury storage while it is identical to the optimum quota for iron and silicate.

 $\frac{\partial \tilde{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} |_{upt} \underbrace{\text{The uptake is capped at the maximum achievable uptake depending on the}}_{Upt} \underbrace{\text{The uptake is capped at the maximum achievable uptake depending on the}}_{\mathcal{N}}$

nutrient affinities $\overset{\chi}{r}_{\mathrm{aff}_{\mathbb{P},\mathbb{F},n,a}}$ and the external dissolved nutrient concentrations:

$$\mathcal{F}_{\text{avail}}\Big|_{N_{\mathbb{P},\mathbb{F}}}^{\overset{X}{P}_{\mathbb{P},\mathbb{F}}} = \overset{\chi}{r}_{\text{aff}_{\mathbb{P},\mathbb{F}}} N'_{\mathbb{P},\mathbb{F}} \stackrel{\chi}{P}_{\mathbb{C}},$$
(17)

$$\mathcal{F}_{\text{avail}}\Big|_{N_{\mathbb{N}}}^{\chi} = \begin{pmatrix} \chi & \text{ox} & \text{amm} \\ r_{\text{aff}_n} & N'_{\mathbb{N}} + r_{\text{aff}_a} & N'_{\mathbb{N}} \end{pmatrix} P_{\mathbb{C}}^{\chi}, \tag{18}$$

where the nitrogen need is satisfied by uptake in oxidised and reduced form in relation to the respective affinities² and external availability.

The resulting net uptake of nitrogen, phosphorus and iron is then

$$\left. \frac{\partial \overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \right|_{\mathrm{upt}} = \min\left(\left. \mathcal{F}_{\mathrm{demand}} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}, \left. \mathcal{F}_{\mathrm{avail}} \right|_{N_{\mathbb{N},\mathbb{P},\mathbb{F}}}^{\overset{\chi}{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}} \right)$$

This purely linear formulation of maximum uptake proportional to the affinity is in contrast to the more widely used saturation assumption of Michaelis-Menten type (Aksnes and Egge, 1991). It is justified here as ERSEM treats phytoplankton in pools of functional groups, rather than individual species with defined saturation characteristics (Franks, 2009).

²Note that the dimensions of these are [volume¹ * mass⁻¹ * time⁻¹] as opposed to [time⁻¹] as for most other rates.

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Lysis and predation losses are computed analogous to the carbon component:

$$\frac{\partial \tilde{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{\text{tys mort}} = \tilde{S}_{\text{tys mort}} \tilde{P'}_{\mathbb{N},\mathbb{P},\mathbb{F}}, \qquad (19)$$

$$\frac{\partial \tilde{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial P} \bigg|_{\mathbb{N},\mathbb{P},\mathbb{F}} = \sum_{i=1}^{N} \frac{\chi_{i}}{\partial P} \sum_{i=1}^{N} \frac{\chi$$

$$\frac{\partial \hat{P}_{\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{\text{pred}} = \sum_{\Psi} \mathcal{F}|_{P}^{\Psi} \stackrel{\chi}{P'}_{\mathbb{N},\mathbb{P},\mathbb{F}}.$$
(20)

The silicate component of diatoms is variability of the internal silicate quota of diatoms reported in literature is small and there's little evidence of luxury uptake capacity for this element (Brzezinski, 1985; Moore et al., 2013). The silicate dynamics of diatoms are therefore modelled by a simple relaxation towards the optimal quota given by the equations:

-12.

$$\frac{\frac{\partial P_{\mathbb{S}}}{\partial t}}{\frac{\partial P_{\mathbb{S}}}{\partial t}} \bigg|_{\text{upt}} = \max\left(0, \overset{\text{dia}}{q}_{\text{ ref}_{\mathbb{S}:\mathbb{C}}} \overset{\text{dia}}{\mathcal{S}}_{\text{growth}}\right) - \max\left(0, \overset{\text{dia}}{P_{\mathbb{S}}'} - \overset{\text{dia}}{q}_{\text{ ref}_{\mathbb{S}:\mathbb{C}}} \overset{\text{dia}}{P_{\mathbb{C}}'}\right),$$

$$\frac{\frac{\partial d_{\text{I}a}}{\partial P_{\text{S}}}}{\partial t} \bigg|_{\text{upt}} = \max \begin{pmatrix} \text{dia} & \text{dia} \\ q_{\text{ref}_{\text{S}:\mathbb{C}}} & \mathcal{S}_{\text{growth}}, 0 \end{pmatrix},$$
(21)

$$\frac{\frac{\partial P_{\mathbb{S}}}{\partial t}}{\frac{\partial P_{\mathbb{S}}}{\partial t}} = \max \begin{pmatrix} dia & dia \\ P_{\mathbb{S}}' - q_{\operatorname{ref}_{\mathbb{S}:\mathbb{C}}} & P_{\mathbb{C}}', 0 \end{pmatrix},$$
(22)

$$\frac{\partial P_{\mathbb{S}}}{\partial t} = \mathcal{S}_{\text{hys mort}} \quad P'_{\mathbb{S}}, \quad (23)$$

$$\frac{\partial P_{\mathbb{S}}}{\partial t} \bigg|_{\text{pred}} = \sum_{\Psi} \mathcal{F}|_{\substack{\Psi \\ P}}^{\Psi} P'_{\mathbb{S}}, \qquad (24)$$

where $q_{\text{ref}_{S,\mathbb{C}}}^{\text{dia}}$ is the reference silicate to carbon quota of diatoms. A formulation to model the impact of an increased atmospheric p_{CO_2} on phytoplankton carbon uptake that was introduced in Artioli et al. (2014) is available via the CENH preprocessing option. In this case gross carbon uptake (Eq. 8) and activity respiration (the second


term in Eq. 12) are enhanced by the factor $\gamma_{enh\mathbb{C}}$ defined as:

 $\gamma_{\mathrm{enh}\mathbb{C}} = 1.0 + \mathrm{p_{CO_2}} - 379.48 \times 0.0005 \,. \label{eq:general}$

 $\gamma_{\mathsf{enh}\mathbb{C}} = 1.0 + (\mathsf{p}_{\mathsf{CO}_2} - 379.48) \times 0.0005$,

where p_{CO_2} has the units ppm.

3.2 Predators

Discussion F Predator descriptions dynamics are largely based on the of Baretta-Bekker et al. (1995) and Broekhuizen et al. (1995) Baretta-Bekker et al. (1995); Broekhui Heath et al. (1997) described by the equations:



(27)

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(25)

Note, that the iron and silicate cycles are simplified in a way that the iron/silicate content of phytoplankton subject to predation is directly turned into particulate organic matter (see Eqs. 69 and 70).

The pelagic predators considered in ERSEM are composed of three size classes of zooplankton categorised as heterotrophic flagellates, microzooplankton and mesozooplankton.



According to size, these are capable of predating on different prey types including cannibalism as given in Table 4illustrated in Fig. 3.

The total prey available to each zooplankton type χ is composed of the preys individual prey types ψ using type II Michaelis-Menten type uptake capacities (Gentleman et al., 2003) as (Chesson, 1983; Gentleman et al., 2003) as

$$\overset{\chi}{\mathsf{Pr}}_{\mathbb{C},\mathbb{N},\mathbb{P}} = \sum_{\psi} f_{\mathsf{pr}} |_{\psi}^{\chi} \frac{\psi_{\mathbb{C}}'}{\psi_{\mathbb{C}}' + \underline{f} \underbrace{h}_{\mathsf{min}}} \psi'_{\mathbb{C},\mathbb{N},\mathbb{P}},$$
(28)

where $f_{\rm pr}|_{\psi}^{\chi}$ are the food preferences and $\frac{f_{\rm min}}{f_{\rm min}} \frac{\chi}{h_{\rm min}}$ is a food half-saturation constant reflecting the detection capacity of predator χ of individual prey types.

The prey mass specific uptake capacity for each zooplankton type χ is then given by:

$$\overset{\chi}{\mathcal{S}}_{\text{growth}} = \overset{\chi}{g}_{\text{max}} \quad \overset{\chi}{l_{\text{T}}} \frac{\overset{\chi}{Z_{\mathbb{C}}}}{\overset{\chi}{\text{Pr}_{\mathbb{C}}} + \overset{\chi}{h_{\text{up}}}}, \tag{29}$$

where $\overset{\chi}{g}_{\text{max}}$ is the maximum uptake capacity of each type at the reference temperature, $\overset{\chi}{l_{\text{T}}}$ is the metabolic temperature response (Eq. 235), $\overset{\chi}{h}_{\text{up}}$ is a predation efficiency constant limiting the chances of encountering prey. Introducing the prey mass specific fluxes from prey ψ to predator χ

$$\mathcal{F}|_{\psi}^{\chi} = \overset{\chi}{\mathcal{S}}_{\text{growth}} f_{\text{pr}}|_{\psi}^{\chi} \frac{\psi_{\mathbb{C}}'}{\psi_{\mathbb{C}}' + \underline{f} \overset{\chi}{\underline{h}}_{\text{min}}}$$
(30)

the zooplankton uptake can then be written as:

$$\frac{\partial \tilde{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{upt}} = \sum_{\psi} \mathcal{F} \big|_{\psi}^{\tilde{Z}} \psi_{\mathbb{C},\mathbb{N},\mathbb{P}}^{\chi}.$$
(31)

This formulation is similar to the approach used in Fasham et al. (1990), but introduces additional Michaelis-Menten terms for inidividual prey types. The purpose here is to include sub-scale effects of pooling as prey of different types can be assumed to be distributed in separate patches in the comparatively large cell volume. Consequently, individual prey patches below a certain size are less likely to be grazed upon compared to the larger

patches, which is expressed by the h_{\min}^{χ} parameter.

Note, that in contrast to previous parametrisations, we now normalise the sum of the food preferences for each predator \hat{Z} to

$$\sum_{\psi} f_{\rm pr} |_{\psi}^{\chi} = 1, \qquad (32)$$

as non-normalised preferences lead to a hidden manipulation of the predation efficiency and at low prey concentrations of the maximum uptake capacity \mathring{g}_{max} .

Zooplankton ingestion of prey The ingestion and assimilation of food by the predators is subject to inefficiencies , leading to excretion:

$$\left. \frac{\partial \overset{\chi}{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\mathrm{excr}} = \left(1 - \overset{\chi}{q}_{\mathrm{eff}} \right) \overset{\chi}{q}_{\mathrm{excr}} \left. \frac{\partial \overset{\chi}{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\mathrm{upt}},$$

where q_{eff} is the carbon uptake efficiency and q_{excr} the excreted fraction of inefficiency lossesthat, given the wide diversity of uptake mechanisms within the zooplankton pools, is for simplicity taken as a fixed proportion of the gross uptake $1-q_{\text{eff}}^{\chi}$. These losses are attributed to the excretion of faeces as a constant fraction (q_{excr}) and activity costs in form of enhanced respiration $(1 - \hat{q}_{excr})$.

Zooplankton respiration is composed of an activity related term given by the remainder of the inefficiency losses and a rest respiration term that is The excretion term in Eq. 26 is

then given by:

$$\frac{\partial \tilde{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{excr}} = \left(1 - \tilde{q}_{\text{eff}}\right) \tilde{q}_{\text{excr}} \frac{\partial \tilde{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{upt}}.$$
(33)

Respiration losses are composed of the activity costs and a basal respiration term required for maintenance and hence proportional to the current biomass by the constant factor r_{resp}^{χ} multiplied with the metabolic temperature response (Eq. 235):

$$\frac{\partial Z_{\mathbb{C}}^{\chi}}{\partial t}\bigg|_{\text{resp}} = \left(1 - q_{\text{eff}}^{\chi}\right) \left(1 - q_{\text{excr}}^{\chi}\right) \left.\frac{\partial Z_{\mathbb{C}}^{\chi}}{\partial t}\bigg|_{\text{growth upt}} + r_{\text{resp}}^{\chi} \left.l_{\text{T}}^{\chi} \left.Z_{\mathbb{C}}^{\chi}\right.$$
(34)

This simple formulation of assimilation losses is closely related to the phytoplankton losses described in the previous section following the concept of the standard organism (Baretta et al., 1995) pending a better undestanding of the underlying physiological mechanisms (Anderson et al., 2013).

Nitrogen and phosphorus are released regulating the internal stoichiometric quota:

$$\frac{\partial \overset{\chi}{Z}_{\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{rel}} = \min\left(0, \overset{\chi}{Z'}_{\mathbb{N},\mathbb{P}} - \overset{\chi}{q}_{\mathbb{N},\mathbb{P}:\mathbb{C}} \overset{\chi}{Z'}_{\mathbb{C}}\right) \overset{\chi}{r}_{\text{rel}\mathbb{N},\mathbb{P}},$$
(35)

where $\overset{\chi}{r}_{\rm rel\mathbb{P},\mathbb{N}}$ are the relaxation rates of release into dissolved inorganic form (see Eqs. 106 and 109).

Mortality is proportional to biomass based on a basal rate p_{mort}^{χ} enhanced up to $p_{mort\mathbb{O}}^{\chi} + p_{mort}^{\chi}$ under oxygen limitation $l_{\mathbb{O}}^{\chi}$ (Eq. 245) as:

$$\frac{\partial \hat{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{mort}} = \left(\left(1 - \hat{l}_{\mathbb{O}}^{\chi} \right) \hat{p}_{\text{mort}\mathbb{O}} + \hat{p}_{\text{mort}} \right) \hat{Z}'_{\mathbb{C},\mathbb{N},\mathbb{P}}.$$
(36)

Biomass lost to other predators Ψ is computed as:

$$\frac{\partial \tilde{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{pred}} = \sum_{\Psi} \mathcal{F}|_{\tilde{Z}}^{\Psi} \quad \tilde{Z}'_{\mathbb{C},\mathbb{N},\mathbb{P}}.$$
(37)

Mesozooplankton

The top-level predator mesozooplankton takes a special role in the predator group in three respects:

It is

24

- Its internal nutrient to carbon quota is assumed fixed (Gismervik , 1997; Walve and Larsson, 1999),
- it is capable of scavenging on medium size organic matterwhose uptake inefficiency is subject to the enhanced uptake inefficiency particulate organic matter.
- at low prey it can enter a hibernation state (optional) at which its maintenance metabolism is reduced (Blackford et al., 2004).

The resulting overall balance of the meszooplankton dynamics is in principle identical to the other zooplankton types (Eq.s 26, 27) with the exception of an additional release term for carbon in order to maintain the fixed internal stoichiometric quota:



The differences to the heterotrophic flagellates and microzooplankton are given by the release terms for stochiometric adjustments for carbon, nitrogen and phosphate (Eqs. 264 and 265) that replace nutrient release terms of the other two types (Eq. 35) and enhanced excretion for the scavenging on particulate matter $q_{\text{Rexcr}}^{\text{MESO}}$:

$$\left. \frac{\frac{\partial \overset{\mathsf{MESO}}{Z}_{\mathbb{C}}}{\partial t}}{\partial t} \right|_{\mathsf{excr}} = \left(1 - \overset{\mathsf{MESO}}{q_{\mathsf{eff}}} \right) \overset{\mathsf{MESO}}{q_{\mathsf{excr}}} \sum_{\psi}^{\psi \neq \overset{\mathsf{med}}{R}} \mathcal{F}|_{\psi}^{\overset{\mathsf{MESO}}{Z}} \psi'_{\mathbb{C},\mathbb{N},\mathbb{P}} + \overset{\mathsf{MESO}}{q_{\mathsf{Rexcr}}} \mathcal{F}|_{\overset{\mathsf{MESO}}{R}}^{\overset{\mathsf{MESO}}{Z}} \overset{\mathsf{med}}{R'}_{\mathbb{C},\mathbb{N},\mathbb{P}} \right)$$

with respect to the uptake of living prey:

(40)

(41)

The second particularity is that it involves an optional hibernation state, that can be



The hibernation formulation (optionally activated by the switch $Z4_OW_SW$) for overwintering . In this case is triggered when the vertically integrated prey availability to mesozooplankton is computed according to :-

$$\Pr_{av} = \int_{seafloor}^{0} \Pr_{\mathbb{C}}^{MESO}$$

triggering the hibernation state when it

$$\Pr_{av}^{ow} = \int\limits_{seafloor}^{0} \Pr_{\mathbb{C}}^{MESO} dz$$

falls below the threshold $\stackrel{\text{ow}}{p}_{\text{min}}$.

In hibernation (overwintering) state the only active processes for mesozooplankton are respiration and mortality . The basal rates of respiration and mortality and using reduced

the basal rates (r_{owresp} and r_{owmort}) are modified with respect to the active state:

$$\frac{\partial \stackrel{\text{MESO}}{Z_{\mathbb{C}}}}{\partial t} \bigg|_{\text{resp}} = r_{\text{owresp}} \stackrel{\text{MESO}}{Z'_{\mathbb{C}}}$$

$$\frac{\partial \stackrel{\text{MESO}}{Z_{\mathbb{C}}}}{\partial t} \bigg|_{\text{mort}} = r_{\text{owmort}} \stackrel{\text{MESO}}{Z'_{\mathbb{C}}}$$
(42)

Finally, mesozooplankton have a fixed nutrient to carbon quota and therefore the process rates are adjusted replacing the nutrient release terms with exudation according to Eqs. (264) and (265) by balancing superfluous carbon uptake as large particulate matter excretion and superfluous nutrients as phosphate or ammonium excretion based on the net fluxes of carbon and nutrients. This results in the following equations for mesozooplankton dynamics:



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3.3 Heterotrophic bacteria

The biogeochemical dynamics of heterotrophic bacteria are given by the equations:

$\partial B_{\mathbb{C}}$	$\partial B_{\mathbb{C}}$	$\partial B_{\mathbb{C}}$	$\partial B_{\mathbb{C}}$	$\partial B_{\mathbb{C}}$	
$\overline{\partial t} \Big _{bgc}$	$= \frac{\partial t}{\partial t}\Big _{upt}$	$\overline{\partial t} \Big _{resp}$	$\partial t \Big _{mort}$	$\overline{\partial t}\Big _{\text{pred}}$	
$\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial I}$	$=\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial B_{\mathbb{N},\mathbb{P}}}$	$-\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial B_{\mathbb{N},\mathbb{P}}}$	$-\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial I}$	$-\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial B_{\mathbb{N},\mathbb{P}}}$	
$\partial t \mid_{bga}$	$_{\rm c}$ ∂t $ _{ m up}$	ot ∂t rel	∂t	mort ∂t	pred

Two alternative sub-modules for decomposition of organic material by bacteria are available in the ERSEM model involving different levels of decomposition of organic matter in the microbial food-web:

3.3.1 Original version

In this version (Baretta-Bekker et al., 1997; Allen et al., 2002; Blackford et al., 2004) (Allen et al., 2004) (A

(44)
(45)

The biogeochemical dynamics of heterotrophic bacteria are here given by the equations:

 $\frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{bgc}} = \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{upt}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{resp}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{mort}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{pred}},$

 $\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\mathrm{bgc}} = \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\mathrm{upt}} - \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\mathrm{rel}} - \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\mathrm{pred}} - \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\mathrm{mort}}.$

Bacterial uptake of DOM is given by the a substrate mass specific turn-over rate r_{lab}^{B}
for labile dissolved organic matter when substrate is scarce and by a maximum bacteria
mass specific potential uptake regulated by temperature and limited by nutrient and oxygen
conditions , capped at a maximum turn-over rate r_{lab}^B for the labile dissolved organic matter

by bacteria:

 ∂t

$$\frac{B}{S_{\text{upt}}} = \min\left(\frac{B}{g_{\text{max}}} \frac{B}{l_{\text{T}}} \frac{B}{l_{\mathbb{O}}} \min\left(\frac{B}{l_{\mathbb{P}}}, l_{\mathbb{N}} \right) \frac{B_{\mathbb{C}}}{\frac{\text{dis}}{R_{\mathbb{C}}}}, r_{\text{lab}}} \right),$$
$$\frac{\partial B_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{upt}} = \frac{B}{S_{\text{upt}}} \frac{\text{lab}}{R'_{\mathbb{C},\mathbb{N},\mathbb{P}}},$$

when substrate is abundant and the uptake per bacteria is saturated , regulated by the ratio of bacteria over substrate biomass:

$$\frac{B}{S_{upt}} = \min\left(\frac{B}{r_{lab}}, \frac{B}{g_{max}}, \frac{B}{l_{T}}, \frac{B}{l_{O}}, \frac{B}{l_{P}}, \frac{B}{l_{N}}, \frac{B}{l_{C}}, \frac{B}{l_{D}}, \frac{B}{l_{C}}, \frac{B}{R'_{C}}, \frac{B}{R'_{C}}$$

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where
$$\overset{B}{g}_{max}$$
 is the maximum bacteria mass specific uptake of bacteria.
Mortality is given as a constant fraction of bacteria biomass:

$$\frac{\partial B_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\bigg|_{\text{mort}} = {}^{B}_{r \text{mort}} B'_{\mathbb{C},\mathbb{N},\mathbb{P}},$$
(48)

where $\stackrel{B}{r_{mort}}$ is a constant mass specific mortality rate for bacteria.

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(49)

where r_{resp}^{B} is the mass specific basal respiration rate at rest (representing the maintenance cost of the metabolism in absense of uptake activity) and q_{high}^{B} , low are the bacterial effi-

Bacteria respiration is computed according to activity respiration as an investment of

activity in growth dependent on the oxygen state and a basal part:

ciencies at high and low oxygen levels.

 $\frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{resp}} = \left(1 - \overset{B}{q}_{\mathrm{high}\mathbb{O}} \overset{B}{l_{\mathbb{O}}} - \overset{B}{q}_{\mathrm{low}\mathbb{O}} \left(1 - \overset{B}{l_{\mathbb{O}}}\right)\right) \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\mathrm{upt}} + \overset{B}{r}_{\mathrm{resp}} \overset{B}{l_{\mathrm{T}}} B'_{\mathbb{C}},$

Poor nutritional quality of the substrate may result in deprivation of nitrogen or phosphorus resulting in <u>nutrient uptake in</u> competition with phytoplankton for external dissolved nutrient sources, otherwise bacteria releases superfluous nutrients to the environment. The internal stoichiometric quota of phosphorus is consequently balanced according to:

$$\frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{\mathrm{rel}} = \begin{cases} r_{\mathrm{lab}}^{B} \begin{pmatrix} B \\ q_{\mathbb{P}:\mathbb{C}} - q_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \end{pmatrix} B'_{\mathbb{C}} & \text{if } B_{\mathbb{P}:\mathbb{C}} \geqslant B_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \\ B \\ r_{\mathrm{lab}} \begin{pmatrix} B \\ q_{\mathbb{P}:\mathbb{C}} - q_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \end{pmatrix} B_{\mathbb{C}} \frac{N'_{\mathbb{P}}}{N'_{\mathbb{P}} + h_{\mathbb{P}}} & \text{if } B_{\mathbb{P}:\mathbb{C}} < B_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \\ \frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{\mathrm{upt}} = \begin{cases} r_{\mathrm{rel}}^{B} \begin{pmatrix} B \\ q_{\mathbb{P}:\mathbb{C}} - q_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \end{pmatrix} B_{\mathbb{C}} \frac{N'_{\mathbb{P}}}{N'_{\mathbb{P}} + h_{\mathbb{P}}} & \text{if } B_{\mathbb{P}:\mathbb{C}} < B_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \\ 0 & \text{if } B_{\mathbb{P}:\mathbb{C}} \ge q_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \end{cases} \\ \frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{\mathrm{rel}} = \begin{cases} 0 & \text{if } B_{\mathbb{P}:\mathbb{C}} < B_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \\ B_{\mathrm{rel}}^{B} \begin{pmatrix} B \\ q_{\mathbb{P}:\mathbb{C}} - q_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \end{pmatrix} B'_{\mathbb{C}} & \text{if } B_{\mathbb{P}:\mathbb{C}} \ge q_{\mathrm{max}_{\mathbb{P}:\mathbb{C}}} \end{cases} \end{cases} \end{cases} \end{cases} \end{cases}$$

with $q_{\max_{\mathbb{P}:\mathbb{C}}}$ being the optimal phosphorus to carbon quota of bacteria and r_{rel}^B being the mass specific release rate.

33

50)

For nitrogen the internal stoichiometric quota is balanced using ammonium:

$$\frac{\partial B_{\mathbb{N}}}{\partial t}\Big|_{\mathrm{rel}} = \begin{cases} \frac{B}{r_{\mathrm{lab}}} \begin{pmatrix} B \\ q_{\mathbb{N}:\mathbb{C}} - P \\ q_{\mathrm{max}_{\mathbb{N}:\mathbb{C}}} \end{pmatrix} B'_{\mathbb{C}} & \text{if } q_{\mathbb{N}:\mathbb{C}} \geqslant q_{\mathrm{max}_{\mathbb{N}:\mathbb{C}}} \\ \frac{B}{r_{\mathrm{lab}}} \begin{pmatrix} B \\ q_{\mathbb{N}:\mathbb{C}} - P \\ q_{\mathrm{max}_{\mathbb{N}:\mathbb{C}}} \end{pmatrix} B_{\mathbb{C}} \frac{N'_{\mathbb{N}}}{a_{\mathrm{mm}} B} & \text{if } q_{\mathbb{N}:\mathbb{C}} < q_{\mathrm{max}_{\mathbb{N}:\mathbb{C}}} \end{cases}$$

$$\frac{\partial B_{\mathbb{N}}}{\partial t}\Big|_{\mathsf{upt}} = \begin{cases} B \\ r_{\mathsf{rel}} \begin{pmatrix} B \\ q_{\mathbb{N}:\mathbb{C}} - q_{\mathsf{max}_{\mathbb{N}:\mathbb{C}}} \end{pmatrix} B_{\mathbb{C}} \frac{a_{\mathsf{mm}}}{a_{\mathsf{mm}}} & \text{if } q_{\mathbb{N}:\mathbb{C}} < q_{\mathsf{max}_{\mathbb{N}:\mathbb{C}}} \\ 0 & \text{if } q_{\mathbb{N}:\mathbb{C}} \ge q_{\mathsf{max}_{\mathbb{N}:\mathbb{C}}} \end{cases}$$

$$\frac{\partial B_{\mathbb{N}}}{\partial t}\Big|_{\mathsf{rel}} = \begin{cases} 0 & \text{if } \begin{array}{c} B \\ q_{\mathbb{N}:\mathbb{C}} < P \\ r_{\mathsf{rel}} \left(\begin{array}{c} B \\ q_{\mathbb{N}:\mathbb{C}} - \begin{array}{c} q \\ q_{\mathsf{max}_{\mathbb{N}:\mathbb{C}}} \end{array} \right) B'_{\mathbb{C}} & \text{if } \begin{array}{c} B \\ q_{\mathbb{N}:\mathbb{C}} \ge \begin{array}{c} q \\ q_{\mathsf{max}_{\mathbb{N}:\mathbb{C}}} \end{array} \end{cases}$$
(51)

Predation on bacteria occurs only by heterotrophic flagellates and is given by:

$$\frac{\partial B_{\mathbb{C},\mathbb{P},\mathbb{F},\mathbb{N}}}{\partial t}\bigg|_{\text{pred}} = \mathcal{F}|_B^{\mathsf{HET}} B'_{\mathbb{C},\mathbb{P},\mathbb{F},\mathbb{N}}.$$
(52)

The bacteria mediated fluxes of organic matter for the two different formulations of bacteria are illustrated in Fig. 4.

3.3.2 Dynamic decomposition version

In this version, activated with the DOCDYN preprocessing definition, the decomposition of particulate organic matter is directly mediated by bacteria and the partition between labile dissolved organic matter and dissolved matter with longer degradation time scales (including the additional state of semi-refractory carbon) occurrs occurs in relation to the nutritional

status of bacteria as opposed to the fixed, parametric decomposition and partition of particles in the standard model. (see also the following sections on the fluxes of particulate and dissolved organic matter (Sect.s 3.5,3.4). The formulation includes the bacteria mediated production of recalcitrant dissolved organic carbon (DOC) DOC (Hansell, 2013) and therefore provides the conceptual framework for an implementation of the microbial carbon pump (Jiao et al., 2014, 2010). However, the fractions of recalcitrant DOM DOC with long turnover time ($\gg 1$ year) are not considered in the current formulation. The sub-model is an extended version of the formulation in Polimene et al. (2006, 2007)with bacteria feeding.

The balance equations for bacteria here are mostly identical to the previous formulation (Eq.s 44 and 44) with the addition of the release of recalcitrant carbon:

$$\frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{upt}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{rel}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{pred}} - \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}},$$

$$\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\text{upt}} - \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\text{rel}} - \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\text{pred}} - \frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\text{mort}},$$
(53)

and an alternative formulation of uptake as in this formulation bacteria feed on all forms of particulate and dissolved organic matter:

where the The parameters q_{ψ} are non-dimensional turn-over rates relative to $\overset{\text{lab}}{R}$ turn-over, leading to the equations:

$$\begin{split} \overset{B}{\mathcal{S}_{\mathsf{upt}}} &= \min \left(\overset{B}{g}_{\mathsf{max}} \ \overset{B}{l_{\mathsf{T}}} \ \overset{B}{l_{\mathbb{O}}} \overset{B}{\overline{R}_{\mathbb{C}}}, r^{B}_{\mathsf{dis}} \right. \\ \hline \frac{\partial B_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \Big|_{\mathsf{upt}} &= \overset{B}{\mathcal{S}_{\mathsf{upt}}} \widetilde{R}_{\mathbb{C},\mathbb{P},\mathbb{N}}, \end{split}$$

following equations for substrate specific and absolute uptake:

$$\overset{B}{\mathcal{S}_{upt}} = \min \begin{pmatrix} B & B & B \\ g_{max} & l_T & l_{\mathbb{O}} & \overline{R_{\mathbb{C}}}, r_{dis} \\ \overline{R_{\mathbb{C}}}, r_{dis} \end{pmatrix}$$
(56)

$$\frac{\partial B_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\bigg|_{upt} = \overset{B}{\mathcal{S}}_{upt}\widetilde{R}_{\mathbb{C},\mathbb{P},\mathbb{N}}.$$
(57)

In this case the bacteria losses towards organic carbon differ with respect to the standard model in two ways: the growth carbon uptake is not nutrient limited as the internal stoichiometric quota of bacteria is balanced directly through the regulating fluxes releasing carbon into semi-labile organic matter, semi-refractory matter is produced as release of capsular material proportionally to the activity respiration. The release of recalcitrant carbon in the form of capsular semi-refractory material is assumed proportional by a factor of q_{srefr} , leading to the alternative equations:

$$\begin{split} \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{bgc}} &= \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{upt}} - \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{rel}} - \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{resp}} - \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{mort}} - \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{pred}} \\ \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{rel}} &= r_{\text{dis}}^{B} \max \left(0, \max \left(1 - \frac{q_{\mathbb{P}:\mathbb{C}}}{q_{\max_{\mathbb{P}:\mathbb{C}}}}, 1 - \frac{q_{\mathbb{N}:\mathbb{C}}}{q_{\max_{\mathbb{N}:\mathbb{C}}}} \right) \right) B_{\mathbb{C}} \\ &+ q_{\text{srefr}} \left(1 - \frac{B}{q_{\text{high}\mathbb{D}}} \left|_{\mathbb{D}}^{B} - \frac{B}{q_{\log_{\mathbb{D}}}} \left(1 - l_{\mathbb{D}}^{B} \right) \right) \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{growth}}. \end{split}$$

to the activity respiration representing the metabolic cost of the uptake activity:

$$\frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{rel}} = r_{\text{dis}}^{B} \max\left(0, \max\left(1 - \frac{q_{\mathbb{P}:\mathbb{C}}}{q_{\max_{\mathbb{P}:\mathbb{C}}}}, 1 - \frac{q_{\mathbb{N}:\mathbb{C}}}{q_{\max_{\mathbb{N}:\mathbb{C}}}}\right)\right) B_{\mathbb{C}} + q_{\text{srefr}}\left(1 - \frac{B}{q_{\text{high}\mathbb{O}}} \left| l_{\mathbb{O}}^{B} - \frac{B}{q_{\text{low}\mathbb{O}}} \left(1 - l_{\mathbb{O}}^{B}\right)\right) \frac{\partial B_{\mathbb{C}}}{\partial t} \bigg|_{\text{growth}}.$$
(58)

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3.4 Particulate organic matter

The particulate matter (\hat{R} : χ = small, medium or large) fluxes resulting from the above processes are composed of excretion and mortality inputs and decomposition and scavenging losses (for medium size particulate matter only) complemented by inputs resulting from mesozooplankton regulation of the internal stoichiometric ratio for large particulate matter. As the consumer types for simplicity do not include an internal component for iron or silicate, the corresponding component fluxes resulting from predation are directed to particulate.



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ulate matter as indirect excretion.

ī

$$\frac{\partial \tilde{R}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{bgc}} = \frac{\partial \tilde{R}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{excr}} + \frac{\partial \tilde{R}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{mort}} - \frac{\partial \tilde{R}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{decomp}} \\
\left[- \frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{scav}} \left|_{\text{scav}} \right] + \frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{rel}} \right|, \qquad (59)$$

$$\frac{\partial \tilde{R}_{\mathbb{F}}}{\partial t} \left|_{\text{bgc}} = \frac{\partial \tilde{R}_{\mathbb{F}}}{\partial t} \right|_{\text{excr}} + \frac{\partial \tilde{R}_{\mathbb{F}}}{\partial t} \left|_{\text{mort}} - \frac{\partial \tilde{R}_{\mathbb{F}}}{\partial t} \right|_{\text{decomp}} \left[-\frac{\partial R_{\mathbb{F}}}{\partial t} \right|_{\text{scav}} \right]. \qquad (60)$$

$$\frac{\partial R_{\mathbb{S}}}{\partial t} \left|_{\text{bgc}} = \frac{\partial R_{\mathbb{S}}}{\partial t} \right|_{\text{excr}} + \frac{\partial R_{\mathbb{S}}}{\partial t} \right|_{\text{mort}} . \qquad (61)$$

Only the excretion of by zooplankton (Eq. 33) results in particulate matter by a fraction of $1 - \overset{\Psi}{q}_{dloss}$, while mortality of phytoplankton (Eqs. 13 and 19) and zooplankton (Eqs. 36 and 43) both have a particulate component $(\overset{\psi}{q_{\text{plys}}}\overset{\psi}{\mathcal{Q}_{\text{pmort}}} \text{ or } 1 - \overset{\psi}{q_{\text{closs}}} \xrightarrow{\text{respective}(q_{\text{closs}})}):$

$$\frac{\partial \hat{R}_{\mathbb{C}}}{\partial t} \bigg|_{\text{excr}} = \sum_{\Psi} \left(1 - \overset{\Psi}{q}_{\text{dloss}} \right) \left. \frac{\partial Z_{\mathbb{C}}}{\partial t} \right|_{\text{excr}}$$
(62)

$$\frac{\partial \hat{R}_{\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{excr}} = \sum_{\Psi} \left(1 - \frac{|\text{ab}}{p} \frac{\Psi}{\text{cyto}_{\mathbb{N},\mathbb{P}}} \frac{\Psi}{q}_{\text{dloss}} \right) \frac{\partial \hat{Z}_{\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{excr}}$$

$$\frac{\partial \hat{R}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S}}}{\partial t} \bigg|_{\text{mort}} = \sum_{\Psi} \left. \frac{\Psi}{q}_{\text{plys}} \underbrace{\overset{\Psi}{\mathcal{Q}}_{\text{pmort}}}_{\mathcal{Q}} \frac{\partial \overset{\Psi}{\mathcal{P}}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S}}}{\partial t} \bigg|_{\text{lys mort}} + \sum_{\Psi} \left(1 - \overset{\Psi}{q}_{\text{dloss}} \right) \frac{\partial \overset{\Psi}{Z}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{mort}} ,$$

$$(63)$$

where $p_{\text{cyto}_{\mathbb{N},\mathbb{P}}}^{\text{lab}}$ reflects the relative nitrogen or phosphorus content of cytoplasm with respect to the structural components assuming that the dissolved losses of zooplankton through excretion are largely of cytoplasm origin and q_{dloss}^{Ψ} is the dissolved fraction of zooplankton losses. The partition of phytoplankton lysis for each functional type is given as

$$\mathcal{Q}_{\mathsf{pmort}} = \min \begin{pmatrix} \chi \\ q_{\mathsf{min}_{\mathbb{N}:\mathbb{C}}}, \chi \\ q_{\mathbb{N}:\mathbb{C}}, q_{\mathbb{P}:\mathbb{C}} \end{pmatrix}$$

The size classes of particulate organic matter χ in these equations originate from the phytoplankton types $\stackrel{\psi}{P}$ and zooplankton types $\stackrel{\psi}{Z}$ as given in Table 5.

39

(65)

Scavenging of mesozooplankton on medium size particulate organic matter results from Eq. (30):

$$\frac{\partial \overset{\text{med}}{R}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S}}}{\partial t} \bigg|_{\substack{\text{scav}}} = \mathcal{F} \big|_{\substack{Z \\ \text{med} \\ R}}^{\substack{\text{MESO} \\ \text{med} \\ R}} \overset{\text{med}}{R'}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S}}.$$
(66)

Additional large particulate organic matter may result from the mesozooplankton $= \frac{\frac{\partial Z_{\mathbb{C}}}{\partial t}}{\partial t}$ -release flux $\frac{\partial R_{\mathbb{C}}}{\partial A_{\mathcal{T}}}$ exudation flux $\frac{\partial R_{C}}{\partial t}$ (Eq. 264). exu rel rel exu

The decomposition of particulate matter is dependent on the bacteria sub-model applied. In case of the standard bacteria model (Sect. 3.3.1) it is converted to dissolved organic matter proportionally to the amount of substrate available by the rate $\overset{\chi}{r}_{\rm decomp}$ and modified by the nutritional status of the substrate in relation to the Redfield Ratio $q_{ref_{CN}}$:

$$\frac{\partial \hat{R}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{\text{decomp}} = q_{\text{ref}_{\mathbb{C}:\mathbb{N}}} q_{\mathbb{N}:\mathbb{C}} \, \stackrel{\chi}{r}_{\text{decomp}} \stackrel{\chi}{R'}_{\mathbb{C},\mathbb{P},\mathbb{N},\mathbb{F}}.$$
(67)

For the model with dynamic decomposition (Sect. 3.3.2) directly mediated by bacteria, the decomposition fluxes are given by the bacterial uptake resulting from Eqs. (55), (56), (57) as:

$$\frac{\partial \overset{\chi}{R}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \bigg|_{\text{decomp}} = -\overset{B}{\mathcal{S}_{\text{growth}}} \overset{\chi}{}_{M}^{\chi} \overset{\chi}{R'}_{\mathbb{C},\mathbb{P},\mathbb{N},\mathbb{F}}.$$
(68)

The iron and silicate component of phytoplankton taken up by zooplankton in Eqs. (20) and (24) are for simplicity directly converted to particulate matter:

$$\frac{\partial \hat{R}_{\mathbb{F}}}{\partial t}\bigg|_{\text{excr}} = \sum_{\psi, \Psi} \mathcal{F}|_{P}^{\Psi} \stackrel{\psi'}{P}_{\mathbb{F}}$$

$$\frac{\partial \hat{R}_{\mathbb{S}}}{\partial R_{\mathbb{S}}}\bigg|_{\mathcal{F}} = \sum_{\psi, \Psi} \frac{\psi'}{P}_{\mathbb{F}}$$
(69)

$$\frac{\partial R_{\mathbb{S}}}{\partial t} \bigg|_{\text{excr}} = \sum_{\psi, \Psi} \mathcal{F} \big|_{P}^{\mathcal{F}} \stackrel{\psi}{P}_{\mathbb{S}}.$$
(70)

In the case of silicate the particulate organic matter types are given by the size relation determined by the predator that ingested the prey and directly releases the silicate contained in the frustule. They are consequently distributed analogous to the zooplankton excretion:

- Small particulate organic matter $\begin{pmatrix} small \\ R \end{pmatrix}$: heterotrophic flagellates $\begin{pmatrix} Z \\ Z \end{pmatrix}$,
- med MICRO - Medium size particulate organic matter (R): microzooplankton (Z),
- Large particulate organic matter (R): mesozooplankton (Z),

while for ironthey are For iron, on the contrary, the size of particulate iron is given by the prey size class and taken analogous to phytoplankton lysis reflecting the assimilation of iron into the cytoplasm:

small nano pico - Small particulate organic matter (R): nano- and picophytoplankton (P, P),

- Medium size particulate organic matter ($\stackrel{\text{med}}{R}$): microphytoplankton and diatoms ($\stackrel{\text{micro}}{P}$, $\stackrel{\text{dia}}{P}$),
- large – Large particulate organic matter (\vec{R}): none.

3.5 **Dissolved organic matter**

The fluxes of dissolved organic matter are affected by excretion, mortality and decomposition. The partition of labile dissolved, semi-labile and semi-refractory carbon originating from bacteria substantially differs in between the standard bacteria model (Sect. 3.3.1) and the bacteria model with dynamic decomposition (Sect. 3.3.2).

For the standard bacteria model the fluxes of dissolved organic matter are affected by uptake, excretion, mortality, decomposition and remineralisation:



The losses of bacteria, phytoplankton and zooplankton in dissolved carbon are fractionated at a constant quota q_{dis} in between labile and semi-labile DOC. Excretion towards the dissolved forms of organic matter may originate from phytoplankton (Eq. 11), or zooplankton



(Eq. 33):

$$\frac{\partial R_{\mathbb{C}}}{\partial t}\bigg|_{\text{excr}} = q_{\text{dis}}\left(\sum_{\psi} \left.\frac{\partial P_{\mathbb{C}}}{\partial t}\right|_{\text{excr}} + \sum_{\Psi} \left.\frac{\Psi}{q_{\text{dloss}}} \left.\frac{\partial Z_{\mathbb{C}}}{\partial t}\right|_{\text{excr}}\right)$$
(73)

$$\frac{\frac{\partial^{\text{slab}}}{\partial t}}{\partial t}\bigg|_{\text{excr}} = (1 - q_{\text{dis}})\left(\sum_{\psi} \frac{\partial^{\psi}}{\partial t}\bigg|_{\text{excr}} + \sum_{\Psi} \left.\frac{\Psi}{q_{\text{dloss}}} \frac{\partial^{\psi}Z_{\mathbb{C}}}{\partial t}\bigg|_{\text{excr}}\right),$$
(74)

where $\overset{\Psi}{q}_{\text{dloss}}$ is the dissolved fraction of the zooplankton losses. Mortality input may originate from all three trophic levels (Eqs. 48, 13, 36, 42):

$$\frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} = q_{\text{lab}} \left(\frac{\partial B_{\mathbb{C}}}{\partial t} \Big|_{\text{mort}} + \sum_{\psi} \left(1 - \frac{\psi}{q_{\text{plys}}} \psi_{\mathcal{Q}_{\text{pmort}}} \right) \frac{\partial P_{\mathbb{C}}}{\partial t} \Big|_{\text{mort}} + \sum_{\psi} \left. \psi_{q_{\text{closs}}} \frac{\partial Z_{\mathbb{C}}}{\partial t} \right|_{\text{mort}} \right)$$

$$\frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} = (1 - q_{\text{ch}}) \left(\frac{\partial B_{\mathbb{C}}}{\partial t} \Big|_{\text{mort}} + \sum_{\psi} \left(1 - \frac{\psi}{q_{\text{plys}}} \psi_{\mathcal{Q}_{\text{pmort}}} \right) \frac{\partial P_{\mathbb{C}}}{\partial t} \Big|_{\text{mort}} + \sum_{\psi} \left. \psi_{q_{\text{closs}}} \frac{\partial Z_{\mathbb{C}}}{\partial t} \right|_{\text{mort}} \right)$$

$$(75)$$

$$\frac{\partial R_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} = (1 - q_{\text{lab}}) \left(\frac{\partial B_{\mathbb{C}}}{\partial t} \Big|_{\text{mort}} + \sum_{\psi} \left(1 - \frac{\psi}{q_{\text{plys}}} \mathcal{Q}_{\text{pmort}} \right) \frac{\partial F_{\mathbb{C}}}{\partial t} \Big|_{\text{mort}} + \sum_{\Psi} \left| \frac{\psi}{q_{\text{closs}}} \frac{\partial Z_{\mathbb{C}}}{\partial t} \right|_{\text{mort}} \right).$$
(76)

In addition, the decomposition of the particulate matter types ($\overset{\Psi}{R}$: Ψ = small, medium or large, Eq. 67) and of semi-labile dissolved organic carbon $\stackrel{\rm slab}{R}_{\mathbb{C}}$ is directly converted to labile

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dissolved organic matter $\stackrel{lab}{(R)}$ according to

$$\frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{decomp}} = \sum_{\Psi} \frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{decomp}} + \frac{\partial R_{\mathbb{C}}}{\partial t} \bigg|_{\text{decomp}}$$
(77)
$$\frac{\partial R_{\mathbb{C}}}{\partial t} \bigg|_{\text{decomp}} = \frac{\text{slab}}{r} \frac{\text{slab}}{\text{decomp}} R'_{\mathbb{C}}$$
(78)

without explicit mediation of bacteria.

In the **dynamic decomposition model** the fluxes of dissolved organic matter are a result of uptake, excretion, mortality and remineralisation:

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Here, the fractionation of dissolved organic matter originating from bacteria and phytoplankton is based on the originating process. This reflects the capacity of bacteria to utilise different forms of substrate and discarding the less digestible forms adding semi-refractory organic matter to the set of state variables. This is reflected in with lysis/mortality contributing to the labile DOM pool, while excretion of carbon occurs in semi-labile form, and discarding the less digestible forms adding semi-refractory organic matter to the set of state variables. Zooplankton losses are treated identically with respect to the standard bacteria model.

Excretion of DOC may originate from the phyto- and zooplankton excretion (Eqs. 11 and 33), the regulation of the bacterial stoichiometric quota (Eq. 58) and excess bacterial growth:

$$\frac{\partial R_{\mathbb{C}}}{\partial t} \bigg|_{\text{excr}} = \sum_{\Psi} q_{\text{dis}} \left. \frac{\Psi}{q_{\text{dloss}}} \frac{\partial Z_{\mathbb{C}}}{\partial t} \right|_{\text{excr}}$$
(82)

$$\frac{\partial B_{\mathbb{C}}}{\partial t}\bigg|_{\text{excr}} = \frac{\partial B_{\mathbb{C}}}{\partial t}\bigg|_{\text{rel}} + \sum_{\psi} \frac{\partial P_{\mathbb{C}}}{\partial t}\bigg|_{\text{excr}} + \sum_{\Psi} (1 - q_{\text{dis}}) \psi_{\text{dloss}} \frac{\partial Z_{\mathbb{C}}}{\partial t}\bigg|_{\text{excr}}$$
(83)

$$\frac{\frac{\partial R_{\mathbb{C}}}{\partial t}}{\partial t}\bigg|_{\text{excr}} = p_{\text{srefr}} \left(1 - \frac{B}{q_{\text{high}\mathbb{O}}} \quad \frac{B}{l_{\mathbb{O}}} - \frac{B}{q_{\text{low}\mathbb{O}}} \left(1 - \frac{B}{l_{\mathbb{O}}}\right)\right) \frac{\partial B_{\mathbb{C}}}{\partial t}\bigg|_{\text{growth}},$$
(84)

while the non-particulate part of mortality/lysis is split according to:

$$\frac{\partial R_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} = \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} + \sum_{\psi} \left(1 - \frac{\psi}{q_{\text{plys}}} \psi_{\mathcal{Q}_{\text{pmort}}}\right) \frac{\partial P_{\mathbb{C}}}{\partial t}\Big|_{\text{lysis}} + \sum_{\Psi} q_{\text{dis}} \psi_{q_{\text{dloss}}} \frac{\partial Z_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}}$$
(85)
$$\frac{\partial R_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} = \sum_{\Psi} (1 - q_{\text{dis}}) \psi_{q_{\text{dloss}}} \frac{\partial Z_{\mathbb{C}}}{\partial t}\Big|_{\text{mort}} .$$
(86)

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Uptake of labile dissolved matter by bacteria is given by

$$\frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{upt}} = \overset{B}{\mathcal{S}_{\text{growth}}} \overset{\text{lab}}{R'_{\mathbb{C},\mathbb{N},\mathbb{P}}}, \tag{87}$$

where the substrate-specific substrate mass specific uptake of bacteria $\overset{B}{\mathcal{S}_{growth}}$ is given in Eq. (46) for the standard decomposition model and in Eq. (56) for the dynamic decomposition model.

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All other The remaining terms are identical for both decomposition sub-models. Excretion and mortality of nitrogen and phosphorus result in the dissolved fluxes

$$\frac{\frac{\partial^{\text{lab}}}{\partial t}}{\frac{\partial R_{\mathbb{N},\mathbb{P}}}{\partial t}}\bigg|_{\text{excr}} = \sum_{\Psi} \left. \frac{\Psi}{q_{\text{closs}}} \right|_{p_{\text{cyto}_{\mathbb{N},\mathbb{P}}}} \frac{\frac{\Psi}{\partial t}}{\frac{\partial Z_{\mathbb{N},\mathbb{P}}}{\partial t}}\bigg|_{\text{excr}}$$

$$\frac{\frac{\partial^{\text{lab}}}{\partial R_{\mathbb{N},\mathbb{P}}}}{\frac{\partial R_{\mathbb{N},\mathbb{P}}}{\partial t}}\bigg|_{\text{mort}} = \frac{\frac{\partial B_{\mathbb{N},\mathbb{P}}}{\partial t}}{\frac{\partial t}{|_{\text{mort}}}} + \sum_{\Psi} \left(1 - \frac{\frac{\Psi}{q_{\text{plys}}}}{\frac{\Psi}{q_{\text{plys}}}}\right) \frac{\frac{\partial P_{\mathbb{N},\mathbb{P}}}{\partial t}}{\frac{\partial t}{|_{\text{mort}}}} + \sum_{\Psi} \left. \frac{\Psi}{q_{\text{closs}}} \frac{\frac{\partial Z_{\mathbb{N},\mathbb{P}}}{\partial t}}{\frac{\partial t}{|_{\text{mort}}}} \right|_{\text{mort}} .$$

$$(89)$$

Remineralisation of dissolved organic nutrients into inorganic form is given by fixed mass specific remineralisation rates $r_{\text{rem}_{N,\mathbb{P}}}$:

$$\frac{\partial R_{\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{remin}} = r_{\text{rem}_{\mathbb{N},\mathbb{P}}} \stackrel{\text{dis}}{R'_{\mathbb{N},\mathbb{P}}}.$$
(90)

In summary, for the **standard model** the balance equations for dissolved organic matter are given as:

$\frac{\frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}}{\partial t}\Big _{\mathrm{bgc}}$	$= \frac{\partial \overset{\mathrm{lab}}{R}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}$	$+\frac{\partial I}{\partial I}$	$\left\ \frac{\frac{b}{\mathcal{R}_{\mathbb{C},\mathbb{N},\mathbb{P}}}}{\partial t} \right\ _{mor}$	$+rac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{N},\mathbb{N},\mathbb{N},\mathbb{N},\mathbb{N},\mathbb{N},N$	P decomp
$\begin{bmatrix} lab \\ \partial R_{\mathbb{C} \mathbb{N} \mathbb{P}} \end{bmatrix}$	lab $\partial R_{\mathbb{C} \mathbb{N}}$				
$-\frac{\partial t}{\partial t}\Big _{t}$	$-\frac{\partial t}{\partial t}$	remin			
$\frac{\partial \overset{\text{slab}}{R}_{\mathbb{C}}}{\partial t} =$	$\frac{\partial R_{\mathbb{C}}}{\partial k}$	+ $\frac{\partial R_{\mathbb{C}}}{\partial I}$	$-\frac{\partial R}{\partial R}$	$\frac{\mathcal{C}}{\mathbb{C}}$,	
0t bgc	Ot excr	$\frac{\partial t}{ _{n}}$	nort	decomp	

while for the dynamic model they are given by:

$$\begin{split} \frac{\partial \overset{\text{lab}}{R}}{\partial t} & = \frac{\partial \overset{\text{lab}}{R}}{\partial t} & + \frac{\partial \overset{\text{lab}}{R}}{\partial t} & \\ - \frac{\partial \overset{\text{lab}}{R}}{\partial t} & = \frac{\partial \overset{\text{lab}}{R}}{\partial t} & \\ - \frac{\partial \overset{\text{lab}}{R}}{\partial t} & & \\ \frac{\partial \overset{\text{lab}}{R} & & \\ \frac{\partial \overset{\text{lab}}{R}}{\partial t} & & \\ \frac{\partial \overset{\text{lab}}{R} & & \\ \frac{\partial \overset{\text{lab}}{R}}{\partial t} & & \\ \frac{\partial \overset{\text{lab}}{R} & & \\ \frac{\partial \overset{\text{lab}}{R} & & \\ \frac{\partial \overset{\text{lab}}{R}}{\partial t} & & \\ \\ \frac{\partial \overset{\text{lab}}{R} & & \\ \frac{\partial \overset{\text{lab}}{R}$$

3.6 Calcification

The model in its current form does not include calcifiers as a dedicated functional group . Nevertheless given the limited knowledge of the physiological constraint of calcification. Therefore, the process of calcification is not directly modelled, but is treated implicitly by considering part of the nanophytoplankton to act as calcifiers. Calcification processes are inferred from the system dynamics based on the assumption of a given quota-ratio between particulate inorganic carbon over particulate organic carbon in sedimenting material, usually referred to as rain-ratio. Here this ratio is used as a proxy for the calcite production matching the local increase of POC originating from nanophytoplankton. Since the rain ratio has been defined for the sinking fluxes and calcite is the more resistant mineral, we limit the description to calcite in this part of the model, neglecting aragonite. This approach is similar to the implementations in other biogeochemical models, e.g. PISCES (Gehlen et al., 2007) or MEDUSA (Yool et al., 2013)

In this context the local rain-ratio is based on a reference ratio q_{rain0} that varies according to the regulating factors $l_{\mathbb{C}}^{calc}$, l_{T}^{calc} and $l_{\langle \mathbb{NP} \rangle}^{calc}$ given in Eqs. (256) or (258), (260) and (261):

$$q_{\text{rain}} = \max\left(\frac{1}{200}, q_{\text{rain0}} \begin{array}{c} \text{calc calc calc} \\ l_{\mathbb{C}} \end{array} \begin{array}{c} l_{\mathsf{T}} \end{array} \begin{array}{c} l_{\langle \mathbb{NP} \rangle} \end{array}\right),$$

where-

 $\frac{\partial R_{\mathbb{C}}^{\text{calc}}}{\partial t} \Bigg|_{\text{bgc}} = \left. \frac{\partial R_{\mathbb{C}}^{\text{calc}}}{\partial t} \right|_{\text{lys}} + \left. \frac{\partial R_{\mathbb{C}}^{\text{calc}}}{\partial t} \right|_{\text{pred}} + \left. \frac{\partial R_{\mathbb{C}}^{\text{calc}}}{\partial t} \right|_{\text{sed}} - \left. \frac{\partial R_{\mathbb{C}}^{\text{calc}}}{\partial t} \right|_{\text{dis}}$

$$q_{\text{rain}} = \max\left(\frac{1}{200}, q_{\text{rain0}} \quad l_{\mathbb{C}} \quad l_{\mathsf{T}} \quad l_{\langle \mathbb{NP} \rangle}\right).$$
(91)

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The calcite dynamics are then described by the equation:

$\partial L_{\mathbb{C}}$	$\begin{bmatrix} calc & \\ & \partial L_{\mathbb{C}} \end{bmatrix}$	$\partial L_{\mathbb{C}}$	$\partial L_{\mathbb{C}}$	$\partial L_{\mathbb{C}}$		(02)
$\overline{\partial t}$	$-\overline{\partial t}$	$\neg \overline{\partial t}$	$\top \overline{\partial t}$	$-\overline{\partial t}$		(52)
	bgc	mort	pred	sed	dis	



(93)

The contribution of nanophytoplankton lysis to calcite production is proportional to the particulate fraction of lysis (compare Eq. 64) by the rain ratio

$\frac{\frac{\operatorname{calc}}{\partial R_{\mathbb{C}}}}{\frac{\partial t}{\partial t}}$		$= q_{rain}$	nano q plys	$\frac{\frac{\partial P_{\mathbb{C}}}{\partial P_{\mathbb{C}}}}{\partial t}$	
	lys				lys

rain-ratio

$$\frac{\frac{\partial L_{\mathbb{C}}}{\partial t}}{\frac{\partial t}{\operatorname{mort}}} = q_{\operatorname{rain}} \left. \frac{\mathcal{Q}_{\operatorname{pmort}}}{\mathcal{Q}_{\operatorname{pmort}}} \frac{\frac{\partial P_{\mathbb{C}}}{\partial t}}{\frac{\partial t}{\operatorname{mort}}} \right|_{\operatorname{mort}}$$

Ingestion of nanophytoplankton and subsequent dissolution in zooplankton guts contributes with a fraction $q_{gutdiss}$ of the excreted part of nanophytoplankton uptake by the various zooplankton groups (compare Eqs. 14 and 33):

$$\frac{\partial \underline{\underline{RL}}_{\mathbb{C}}}{\partial t} \bigg|_{\text{pred}} = q_{\text{rain}} q_{\text{gutdiss}} \left(1 - \frac{\chi}{q_{\text{eff}}} \right) \overset{\chi}{\underline{q}}_{\text{excr}} \sum_{\Psi} \mathcal{F} |_{\underline{P}}^{\Psi} \stackrel{\text{nano}}{P'_{\mathbb{C}}} P'_{\mathbb{C}}$$
(94)

As sedimentation of nanophytoplankton contributes to the organic carbon considered in the rain-ratio the matching contribution to calcite production is computed as

$$\frac{\partial \underline{\underline{RL}}_{\mathbb{C}}}{\partial t} \bigg|_{\text{sed}} = q_{\text{rain}} \frac{\partial \underline{P}_{\mathbb{C}}}{\partial t} \bigg|_{\text{sed}}$$
(95)

with the sinking rate $\frac{\partial \dot{P}_{C}}{\partial t}\Big|_{sed}$ given in Eq. (139).



Dissolution of calcite is proportional to the current concentration of calcite with a maximum rate of $r_{\rm dis}$, regulated by $l_{\mathbb{C}}$ (Eqs. 257 or 259):

$$\frac{\partial \underline{\underline{RL}}_{\mathbb{C}}}{\partial t} = r_{\text{dis}} \begin{array}{c} \underset{l_{\mathbb{C}}}{\text{dis}} & \underset{\mathcal{C}}{\text{calc}} \\ \underset{\mathcal{C}}{\text{dis}} \end{array}$$
(96)

Note, that while the calcification rates are implicitly derived from the rain-ratio and not directly modelled processes, this formulation is still conservative as all sources and sinks of calcite are balanced by dissolved inorganic carbon (DIC, see Eq.s 117 and 118).

The solution of the calcite dynamics is optional and activated by the preprocessing switch CALC.

3.7 Inorganic components

The dynamics of dissolved inorganic nutrients in the model are given by uptake of phytoplankton and bacteria and are resupplied locally by remineralisation and excretion. Dissolved inorganic iron is additionally subject to scavenging.

$$\frac{\partial \tilde{N}_{\mathbb{N}}}{\partial t}\bigg|_{\text{bgc}} = \frac{\partial \tilde{N}_{\mathbb{N}}}{\partial t}\bigg|_{\text{nitr}} - \frac{\partial \tilde{N}_{\mathbb{N}}}{\partial t}\bigg|_{\text{upt}},$$
(97)

$$\frac{\partial N_{\mathbb{N}}}{\partial t}\bigg|_{\text{bgc}} = \frac{\partial N_{\mathbb{N}}}{\partial t}\bigg|_{\text{remin}} + \frac{\partial N_{\mathbb{N}}}{\partial t}\bigg|_{\text{rel}} - \frac{\partial N_{\mathbb{N}}}{\partial t}\bigg|_{\text{upt}} - \frac{\partial N_{\mathbb{N}}}{\partial t}\bigg|_{\text{nitr}},$$
(98)

$$\frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{remin}} + \frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{rel}} - \frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{upt}},$$
(99)

$$\frac{\partial N_{\rm S}}{\partial t}\Big|_{\rm bgc} = \frac{\partial N_{\rm S}}{\partial t}\Big|_{\rm rel} - \frac{\partial N_{\rm S}}{\partial t}\Big|_{\rm upt},\tag{100}$$

$$\frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\mathrm{bgc}} = \frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\mathrm{remin}} + \frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\mathrm{rel}} - \frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\mathrm{upt}} - \frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\mathrm{scav}}.$$
(101)

Oxidised nitrogen in the water-column is taken up only by the four phytoplankton types $\overset{\psi}{P}$ following Eq. (15) according to external availability:

$$\frac{\partial N_{\mathbb{N}}}{\partial t} \bigg|_{\text{upt}} = \sum_{\psi} \frac{\frac{\psi}{r_{\text{aff}_n}} \frac{\partial N}{N'_{\mathbb{N}}}}{\left(\frac{\psi}{r_{\text{aff}_n}} \frac{\partial N}{N'_{\mathbb{N}}} + \frac{\psi}{r_{\text{aff}_a}} \frac{\text{amm}}{N'_{\mathbb{N}}} \right)} \max \left(0, \frac{\partial P_{\mathbb{N}}}{\partial t} \bigg|_{\text{upt}} \right)$$

$$\frac{\partial N_{\mathbb{N}}^{\text{ox}}}{\partial t}\bigg|_{\text{upt}} = \sum_{\psi} \frac{\frac{\psi}{r_{\text{aff}_n}} N'_{\mathbb{N}}}{\left(\frac{\psi}{r_{\text{aff}_n}} N'_{\mathbb{N}} + \frac{\psi}{r_{\text{aff}_a}} N'_{\mathbb{N}}\right)} \frac{\partial P_{\mathbb{N}}}{\partial t}\bigg|_{\text{upt}}$$
(102)

and regenerated exclusively by nitrification:

$$\frac{\partial N_{\mathbb{N}}}{\partial t} \bigg| = \stackrel{B}{r_{\text{nitr}}} \stackrel{B \text{ nitrnitr}}{l_{\mathsf{T}}} \stackrel{\text{amm}}{l_{\mathbb{O}}} \stackrel{53}{l_{\mathbb{N}}} I_{\mathsf{pH}} N'_{\mathbb{N}},$$
(103)

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depending on multiple environmental factors, based on temperature, oxygen and availibility ammonium taking into account the poor competitiveness of nitrifying microbes with respect to other pelagic consumers of ammonium (Ward, 2008). The various regulation and limitation factors $l_{\rm T}^B$, $l_{\rm D}$, $l_{\rm N}$ and $l_{\rm pH}$ are given in Sect. 6.1.

Ammonium is taken up by phytoplankton as the reduced part of total nitrogen uptake (Eq. 15) and bacteria when nitrogen limited

$$\frac{\frac{\partial N_{\mathbb{N}}}{\partial t}}{\frac{\partial t}{\partial t}} \bigg|_{\text{upt}} = \sum_{\psi} \frac{\frac{\psi}{r_{\text{aff}_n}} \frac{n}{N'_{\mathbb{N}}}}{\left(\frac{\psi}{r_{\text{aff}_n}} \frac{n}{N'_{\mathbb{N}} + r_{\text{aff}_n}} \frac{n}{N'_{\mathbb{N}}}\right)} \max\left(0, \frac{\partial P_{\mathbb{N}}}{\partial t}\bigg|_{\text{upt}}\right) - \min\left(0, \frac{\partial B_{\mathbb{N}}}{\partial t}\bigg|_{\text{rel}}\right)$$

$$\frac{\partial N_{\mathbb{N}}^{\operatorname{amm}}}{\partial t}\Big|_{\operatorname{upt}} = \sum_{\psi} \frac{\psi \quad \operatorname{amm}}{\begin{pmatrix} r_{\operatorname{aff}_{n}} & N'_{\mathbb{N}} \\ r_{\operatorname{aff}_{n}} & N'_{\mathbb{N}} + r_{\operatorname{aff}_{a}} & N'_{\mathbb{N}} \end{pmatrix}}{\frac{\psi}{\partial t}} \frac{\partial P_{\mathbb{N}}}{\partial t}\Big|_{\operatorname{upt}} + \frac{\partial B_{\mathbb{N}}}{\frac{\partial t}{\partial t}}\Big|_{\operatorname{upt}}$$
(104)

and remineralised according to Eq. (90)

$$\frac{\partial N_{\mathbb{N}}}{\partial t} \bigg|_{\text{remin}} = r_{\text{rem}_{\mathbb{N}}} \stackrel{\text{lab}}{R'_{\mathbb{N}}}.$$
(105)

Ammonium is released by the phytoplankton types ψ (Eq. 15) when respiration exceeds photosynthesis or when above their luxury storage capacity and by the zooplankton types Ψ (Eqs. 35 and 265) and bacteria (Eq. 51) when above their optimal quota





Ammonium concentrations may be further reduced by nitrification:

$$\frac{\partial N_{\mathbb{N}}}{\partial t} \bigg|_{\text{nitr}} = \frac{B}{r_{\text{nitr}}} \frac{B}{l_{\text{T}}} l_{\mathbb{O}_{\text{nitr}}} l_{\mathbb{N}_{\text{nitr}}} l_{\text{pH}} N'_{\mathbb{N}}.$$
(107)

Phosphorus dynamics are analogous to nitrogen dynamics but simplified with only one dissolved inorganic pool being considered in the model. It is taken up according to Eqs. (15)

$$\frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{upt}} = \sum_{\psi} \max\left(0, \frac{\partial P_{\mathbb{P}}}{\partial t}\Big|_{\text{upt}}\right) - \min\left(0, \frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{\text{rel}}\right),$$

$$\frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{upt} = \sum_{\psi} \frac{\partial P_{\mathbb{P}}}{\partial t}\Big|_{upt} + \frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{upt},$$
(108)

released following Eqs. (15), (50), (35) and (36)

$$\frac{\frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{rel}}}{\frac{1}{2}} = \sum_{\Psi} \frac{\frac{\partial Z_{\mathbb{P}}}{\partial t}\Big|_{\text{rel}} - \sum_{\psi} \min\left(0, \frac{\partial P_{\mathbb{P}}}{\partial t}\Big|_{\text{upt}}\right)}{+ \max\left(0, \frac{\partial B_{\mathbb{P}}}{\partial t}\Big|_{\text{rel}}\right)}$$

$$\frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{rel}} = \sum_{\Psi} \frac{\partial Z_{\mathbb{P}}}{\partial t} \Big|_{\text{rel}} - \sum_{\psi} \frac{\partial P_{\mathbb{P}}}{\partial t} \Big|_{\text{upt}} + \frac{\partial B_{\mathbb{P}}}{\partial t} \Big|_{\text{rel}}$$

and remineralised as given in Eq. (51)

$$\frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{remin}} = r_{\text{rem}_{\mathbb{P}}} \stackrel{\text{lab}}{R'_{\mathbb{P}}}.$$
(110)

56

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(109)

Iron is taken up only by phytoplankton (Eq. 15)

$\left.\frac{\partial N_{\mathbb{F}}}{\partial t}\right _{upt} = \sum_{\psi} \max\left $	$\left(0, \frac{\partial P}{\partial t}\right)$	$\left \frac{\mathbb{F}}{\mathbb{F}} \right _{\text{upt}}$
------------------------------------------------------------------------------------------	-------------------------------------------------	-------------------------------------------------------------

$$\frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\rm upt} = \sum_{\psi} \left. \frac{\partial P_{\mathbb{F}}}{\partial t} \right|_{\rm upt} \tag{111}$$

and subject to scavenging due to hydroxide, treated similarly as in Aumont et al. (2003) and Vichi et al. (2007):

$$\left. \frac{\partial N_{\mathbb{F}}}{\partial t} \right|_{\text{scav}} = r_{\mathbb{F}\text{scav}} \max\left(0, N_{\mathbb{F}}'\right), \tag{112}$$

where $r_{\mathbb{F}scav}$ is a threshold concentration over which scavenging occurs, here fixed at $0.6\frac{\mu mol}{m^3}.$
Iron is released by phytoplankton (Eq. 15)

$\left.\frac{\partial N_{\mathbb{F}}}{\partial t}\right _{\mathbf{I}}$	$rel = -\sum_{\psi}$, min	0,	$\frac{\partial \overset{\psi}{P}_{\mathbb{F}}}{\partial t}$	upt	
					apt	

$$\left. \frac{\partial N_{\mathbb{F}}}{\partial t} \right|_{\mathsf{rel}} = \sum_{\psi} \left. \frac{\partial P_{\mathbb{F}}}{\partial t} \right|_{\mathsf{rel}}$$

(113)

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and implicitly remineralised by mesozooplankton scavenging of particulate organic matter (Eq. 66) and bacterial consumption of particulate matter (Eqs. 67 and 68)

$$\frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\text{remin}} = \mathcal{F}\Big|_{\mathbb{R}}^{\text{MESO}} \frac{\text{med}}{R'} \left[+ \frac{\partial R_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F}}}{\partial t} \right]_{\text{decomp}}.$$

$$\frac{\partial N_{\mathbb{F}}}{\partial t}\Big|_{\text{remin}} = \mathcal{F}\Big|_{\mathbb{R}}^{\text{MESO}} \frac{\text{med}}{R'} \left[+ \frac{\partial R_{\mathbb{F}}}{\partial t} \right]_{\text{decomp}}.$$
(114)

It is assumed here that the feeding activity of scavenging zooplankton increases the bio-availability and accelerates the decomposition of particulate iron.

Silicate is taken up

$$\left. \frac{\partial N_{\mathbb{S}}}{\partial t} \right|_{\mathrm{uptake}} = \max\left(\mathbf{0}, \stackrel{\mathrm{dia}}{q} \stackrel{\mathrm{dia}}{_{\mathrm{ref}_{\mathbb{S}:\mathbb{C}}}} \mathcal{S}_{\mathrm{growth}} \right)$$

and released

$$\left. \frac{\partial N_{\mathbb{S}}}{\partial t} \right|_{\mathrm{rel}} = \max \left(0, P_{\mathbb{S}}^{\mathrm{dia}} - \stackrel{\mathrm{dia}}{q} \stackrel{\mathrm{dia}}{_{\mathrm{ref}_{\mathbb{S}:\mathbb{C}}}} \right. P_{\mathbb{C}}^{\mathrm{dia}} \right)$$

$$\left.\frac{\partial N_{\mathbb{S}}}{\partial t}\right|_{\mathrm{uptake}} = \stackrel{\mathrm{dia}}{q} \mathop{\mathrm{ref}}_{\mathbb{S}:\mathbb{C}} \overset{\mathrm{dia}}{\mathcal{S}}_{\mathrm{growth}}$$

and released

$$\frac{\partial N_{\mathbb{S}}}{\partial t} \bigg|_{\text{rel}} = \frac{\text{dia}}{P_{\mathbb{S}}^{\prime}} - \frac{\text{dia}}{q} \frac{\text{dia}}{\text{ref}_{\mathbb{S}:\mathbb{C}}} P_{\mathbb{C}}^{\prime}$$

exclusively by diatoms (Eq. 21). It is not remineralised in the pelagic part of the system.

This neglection of silicate conversion into inorganic form in the water column is based on observations that the recycling of this element in particulate form while sinking down the water column is much lower than for the other nutrients, such that most of its remineralisation is confined to the sea-floor (Broecker and Peng, 1982; Dugdale et al., 1995). Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

(115)

(116)

The dynamics of DIC are given by photosynthesis and respiration of the organisms considered and calcification and dissolution of calcite:

$$\frac{\partial O_{\mathbb{C}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}} + \sum_{\psi} \frac{\partial P_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}} + \sum_{\Psi} \frac{\partial Z_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}} - \sum_{\psi} \frac{\partial P_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}} + \frac{\partial R_{\mathbb{C}}}{\partial t}\Big|_{\text{dis}} - \frac{\partial R_{\mathbb{C}}}{\partial t}\Big|_{\text{calc}},$$
$$\frac{\partial O_{\mathbb{C}}}{\partial t}\Big|_{\text{bcc}} = \frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}} + \sum_{\psi} \frac{\partial P_{\mathbb{C}}}{\partial t}\Big|_{\text{dis}} + \sum_{\Psi} \frac{\partial Z_{\mathbb{C}}}{\partial t}\Big|_{\text{calc}}$$

$$\frac{\tau}{\psi} \frac{\partial t}{\partial t} = \frac{2}{\psi} \frac{\partial t}{\partial t} \frac{1}{|resp} \frac{\omega}{\psi} \frac{\partial t}{\partial t} \frac{1}{|resp} \frac{\omega}{\psi} \frac{\partial t}{\partial t} \frac{1}{|resp} \frac{\partial t}{|resp} \frac{\partial t}{|$$

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where the respiration terms $\frac{\partial B_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}}$, $\frac{\partial P_{\mathbb{C}}^{\psi}}{\partial t}\Big|_{\text{resp}}$ and $\frac{\partial Z_{\mathbb{C}}}{\partial t}\Big|_{\text{resp}}$ are given in Eqs. (49), (12), (34) and (42), synthesis of carbon is given in Eq. (8), the dissolution of calcite is given in



- Toda

Eq. (96) and precipitation of DIC into calcite is given by the sum of the calcification terms



$\frac{\operatorname{calc}}{\partial L_{\mathbb{C}}}$	$-\frac{\partial L_{\mathbb{C}}}{\partial L_{\mathbb{C}}}$	$ + \frac{\partial L_{\mathbb{C}}}{\partial L_{\mathbb{C}}} $	$+ \frac{\partial L_{\mathbb{C}}}{\partial L_{\mathbb{C}}}$	(11	18)
∂t	$- \partial t$	$\begin{vmatrix} & & \\ & & & \\ & & & \partial t \end{vmatrix}$	$ $ $ $ ∂t		0)
~~~~~		mort	lgraz	sed	

given in Eqs. (93), (94) and (95).

Rates of change of oxygen are implied from the corresponding carbon fluxes converted by stoichiometric factors taking into account different efficiencies for respiration  $p_{\mathbb{O}}^{\text{resp}}$  and photosynthesis  $p_{\mathbb{O}}^{\text{syn}}$ .

The pelagic oxygen cycle is reduced to the consumption of dissolved oxygen in respiration (Eqs. 49, 12, 34 and 42) and the production of dissolved oxygen in photosynthesis (Eq. 8):

$$\frac{\partial O_{\mathbb{O}}}{\partial t}\Big|_{\text{bgc}} = -p_{\mathbb{O}}^{\text{resp}} \left. \frac{\partial B_{\mathbb{C}}}{\partial t} \right|_{\text{resp}} - p_{\mathbb{O}}^{\text{resp}} \sum_{\psi} \left. \frac{\partial P_{\mathbb{C}}}{\partial t} \right|_{\text{resp}} - p_{\mathbb{O}}^{\text{resp}} \sum_{\Psi} \left. \frac{\partial Z_{\mathbb{C}}}{\partial t} \right|_{\text{resp}} + p_{\mathbb{O}}^{\text{syn}} \sum_{\psi} \left. \frac{\partial P_{\mathbb{C}}}{\partial t} \right|_{\text{gpp}}.$$
(119)

### 3.8 The carbonate system

The model for the carbonate system incorprated in ERSEM was introduced in Blackford and Burkill (2002) and further developed in Blackford and Gilbert (2007); Artioli et al. (2012). In this model, the speciation of carbon is calculated from dissolved inorganic carbon  $O_{\mathbb{C}}$ , total alkalinity  $\mathbb{A}_{tot}$  (which is calculated from a regression of temperature and salinity complemented by modifications due to the biological processes in Eq. 130, if activated can

be computed diagnostically, semi-diagnostically or prognostically, see below) and total boron  $\mathbb{B}_{tot}$  (which is calculated from a linear regression of salinity). It assumes chemical equilibrium between the inorganic carbon species justified by the fast reaction time scales of the underlying chemical reaction compared to the biological and physical rates on the spatial scales the model operates on. The comprehensive set of equations to describe the carbonate system and ways to solve it given specific subsets of known quantities have been extensively described elsewhere (Dickson et al., 2007; Zeebe and Wolf-Gladrow, 2001), here we use a simplified set omitting the components that contribute less under general sea-water conditions (Takahashi et al., 1982).

The three quantities  $O_{\mathbb{C}}$ ,  $\mathbb{A}_{tot}$  and  $\mathbb{B}_{tot}$  are used to derive the partial pressure of carbon dioxide  $p_{CO_2} p_{CO_2}$ , carbonic acid, carbonate and bicarbonate concentrations ( $c_{IH_2CO_3}$ ),  $c_{[CO_3^{2-}]}$  and  $c_{[HCO_3^{-}]}$ ) and pH (using the seawater scale) at chemical equilibrium. These utilise the four equilibrium constants for solubility of carbon dioxide and for the dissociation of carbonic acid, bicarbonate and boric acid derived from empirical environmental relationships (Millero, 1995; Mehrbach et al., 1973; Weiss, 1974; Dickson, 1990) that are detailed in the Supplement for reference. The resulting set of equations to solve is then given by:

$$O_{\mathbb{C}} = c_{[\mathsf{CO}_3^{2-}]} + c_{[\mathsf{HCO}_3^{-}]} + c_{[\mathsf{CO}_2^{*}]}$$
(120)

$$\mathbb{A}_{\text{tot}} = c_{[\text{HCO}_3^-]} + 2c_{[\text{CO}_3^{2-}]} + c_{[\text{B}(\text{OH})_4^-]}$$
(121)

$$\mathbb{B}_{\text{tot}} = c_{[\mathsf{B}(\mathsf{OH})_3]} + c_{[\mathsf{B}(\mathsf{OH})_4^-]}$$
(122)  
$$c_{[\mathsf{H}^+]} c_{[\mathsf{B}(\mathsf{OH})^-]}$$

$$c_{\mathsf{B}(\mathsf{OH})_3} = \frac{\frac{1}{k_{\mathsf{b}}} - \frac{1}{k_{\mathsf{b}}}}{k_{\mathsf{b}}}$$
(123)

$$c_{\rm CO_2^*} = \frac{c_{\rm [H^+]}c_{\rm [HCO_3^-]}}{k_1} \tag{124}$$

$$c_{\rm HCO_3^-} = \frac{c_{\rm [H^+]}c_{\rm [CO_3^{2-}]}}{k_2} \tag{125}$$

$$pH = -\log_{10} \left( c_{[H^+]} \right)$$
(126)

$$p_{CO_2} = k_0 c_{[CO_2^*]}$$
(127)

The system is solved using the HALTAFALL algorithm (Ingri et al., 1967) by using the equilibrium relations 123 to 125 to eliminate the unknowns  $c_{[B(OH)_3]}$ ,  $c_{[CO_2^*]}$  and  $c_{[HCO_3^-]}$ . The balance equations for DIC and total boron are then used to express  $c_{[CO_3^{2-}]}$  and  $c_{[B(OH)_4^{-}]}$ in the balance equation for alkalinity (Eq. 121) as functions of the only remaining unknown  $c_{[H^+]}$ . This equation is solved for the logarithm of the unknown variable (allowing only positive real numbers as solution) applying a combination of the bisection method to narrow down the solution to a sufficiently small interval in  $c_{[H^+]}$  to permit linear approximation followed by the bisection method reducing the solution residual to the desired tolerance.

(128)

Calcite saturation is computed from the product of calcium and carbonate concentrations  $(c_{[Ca^{2+}]} \text{ and } c_{[CO_3^{2-}]})$  divided by their product in chemical equilibrium  $k_{calc}$ 

$$\Omega_{\text{calc}} = \frac{{}^{C} \left[ \text{Ca}^{2+} \right]^{C} \left[ \text{CO}_{3}^{2-} \right]}{k_{\text{calc}}}$$

$$\Omega_{\text{calc}} = \frac{c[\text{Ca}^{2+}]^{c}[\text{CO}_3^{2-}]}{k_{\text{calc}}}$$

The variability of this ratio is dominated by  $c_{[GO_3^2-]}$  as  $c_{[Ca^{2+}]}$  is nearly constant in sea water (Kleypas et al., 1999) and therefore fixed in the model at the oceanic mean value of  $0.01028 \text{ mol kg}^{-1}$ .

Similarly, the aragonite saturation state is determined by the equation

$$\Omega_{\text{calc}} = \frac{c[\text{Ca}^{2+}]^{c}[\text{CO}_{3}^{2-}]}{k_{\text{arag}}}$$
(129)

The different variants of alkalinity regressions available from the scientific literature (Borges and Frankignoulle, 1999; Bellerby et al., 2005; Millero et al., 1998; Lee et al., 2006), the total boron regression and the empirical equilibrium constants k are given in the Supplement. Two different modes to compute total alkalinity are provided with the model:

- A diagnostic mode, that computes alkalinity from salinity or salinity and temperature. This mode is non conservative and the field of alkalinity is recomputed at each time step without physical tranport. It does not include changes to alkalinity by the biogeochemical processes of the model.
- A prognostic model, that includes biogeochemical changes to alkalinity. It is fully conservative and adds a state variable for alkalinity that is subject to physical transport.

As a third semi-diagnostic option, these two modes can be combined as a sum by setting the prognostic alkalinity state to 0, so that the diagnostic mode provides the backgound field and the prognostic mode gives a trace of the contribution of biogeochemical processes to the total alkalinity.

The recommended option is the semi-diagnostic option for coastal applications and shelf seas, where reliable and robust regressions exist or the fully prognostic mode, where no single reliable regression is available, e.g. in global simulations. (For further detail the reader is referred to Artioli et al., 2012)

The changes of alkalinity due to biological processes can be traced in the model (activated by the preprocessor definition BIOALK) using a dedicated state variable. Its changes are given by sources and sinks of phosphate, oxidised nitrogen and ammonium as well as calcification and dissolution of calcite:

$$\frac{\partial A_{\rm bio}}{\partial t}\Big|_{\rm bgc} = \frac{\partial \overset{\rm amm}{N_{\rm N}}}{\partial t}\Big|_{\rm bgc} + 2 \left.\frac{\partial \overset{\rm calc}{L_{\rm C}}}{\partial t}\right|_{\rm diss} - \left.\frac{\partial R_{\mathbb P}}{\partial t}\right|_{\rm bgc} - \left.\frac{\partial \overset{\rm ox}{R_{\rm N}}}{\partial t}\right|_{\rm bgc} - 2 \left.\frac{\partial \overset{\rm calc}{R_{\rm C}}}{\partial t}\right|_{\rm calc}$$

$$\frac{\partial A_{\text{bio}}}{\partial t}\Big|_{\text{bgc}} = \frac{\partial \overline{N_{\mathbb{N}}}}{\partial t}\Big|_{\text{bgc}} + 2\frac{\partial \overline{L_{\mathbb{C}}}}{\partial t}\Big|_{\text{diss}} - \frac{\partial N_{\mathbb{P}}}{\partial t}\Big|_{\text{bgc}} - \frac{\partial \overline{N_{\mathbb{N}}}}{\partial t}\Big|_{\text{bgc}} - 2\frac{\partial \overline{L_{\mathbb{C}}}}{\partial t}\Big|_{\text{calc}}.$$
(130)

In three dimensional simulations, these changes are accompanied by the effect of riverine inputs (see Artioli et al., 2012).

The different variants of alkalinity regressions available from the scientific literature (Borges and Frankignoulle, 1999; Bellerby et al., 2005; Millero et al., 1998; Lee et al., 2006), the total boron regression and the empirical equilibrium constants k are given in the Supplement.

(131)

## 3.9 Light extinction

Light in the water column is attenuated according to the Beer–Lambert formulation computing PAR as:

$$\mathsf{E}_{\mathsf{PAR}} = q_{\mathsf{PAR}} \mathsf{I}_{\mathsf{surf}} e^0$$

where I_{surf} is the short-wave radiation at sea-surface level, q_{PAR} is a parameter for the photosynthetically active fraction and  $K_d$  is the spatially varying attenuation coefficient. The latter incorporates light attenuation by the modelled living and non-living optically active components as well as background extinction due to clear sea-water and other components not explicitly modelled. Two alternative models are available for the computation of  $K_d$ :

- 1. a model based on mass specific attenuation coefficients for the relevant functional types, not modelled non-modelled forms of inorganic matter and the background attenuation of clear sea water; this model is used in previous ERSEM versions (Blackford et al., 2004) and is the default choice,
- 2. a model based on broadband inherent optical properties (absorption and backscatter), activated by the preprocessing definition IOPMODEL.

For the default model based on specific attenuation coefficients  $K_d$  is computed according to:

$$K_{d} = \sum_{\chi} \lambda_{P}^{\chi} \stackrel{\chi}{P}_{\mathbb{C}} + \sum_{\Psi} \lambda_{R} \stackrel{\Psi}{R}_{\mathbb{C}} + \lambda_{R_{susp}} R_{susp} + \Lambda_{sea},$$
(132)

where the  $\lambda$ s are the specific attenuation coefficients of the optically active components, i.e. the phytoplankton types  $\chi$  and the particulate organic matter types  $\Psi$ .  $\Lambda_{sea}$  is the background attenuation of sea water and  $R_{susp}$  is the concentration of non-modelled optically active substances, mostly suspended matter.

The model based on inherent optical properties (activated by the preprocessing switch IOPMODEL) uses the light attenuation model proposed in Lee et al. (2005):

$$K_d = (1 + 0.005\theta_{\text{zen}})a + 4.18(1.0 - 0.52e^{-10.8a})b_b,$$
(133)

where  $\theta_{zen}$  is the zenith angle at the given time and location. Absorption *a* and back-scatter  $b_{\rm b}$  are composed as:

$$a = \sum_{\chi} a_{\chi}^* P_{\mathcal{C}}^{\chi} + \sum_{\Psi} a_{W}^* R_{\mathbb{C}}^{\Psi} + a_{M_{\text{susp}}} + a_{\text{sea}}, \qquad (134)$$

$$b_{\mathbf{b}} = \sum_{\chi} b_{\chi}^* P_{\mathcal{C}}^{\chi} + \sum_{\Psi} b_{R}^* R_{\mathbb{C}}^{\Psi} + b_{k} + b_{\text{sea}}$$
(135)

with  $a^*$  and  $b^*$  being the mass specific absorption and back-scatter coefficients of the respective components,  $a_{sea}$  and  $b_{sea}$  being the broadband absorption and back-scatter of clear sea-water,  $a_{M_{susp}}$  the constant absorption of non-modelled suspended matter and  $b_k$ a constant amount of background back-scatter in the water column.

In both optical models the attenuation of optically active matter that is not modelled by ERSEM (R_{susp}, mostly inorganic suspended particulate matter) can be provided homogeneously through a namelist parameter or spatially variable through the physical driver by filling and updating the ESS variable.

The combination of the attenuation of particulate organic matter and the non-modelled particles may be provided externally through the physical driver using the preprocessing definition ADYTRACER. This option introduces the state variable  $a_{ady}$  and Eq. (132) reduces

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to

$$K_d = \sum_{\chi} \lambda_P^{\chi} P_{\mathbb{C}}^{\chi} + a_{\text{ady}} + \Lambda_{\text{sea}}, \qquad (136)$$

or in case of the model based on inherent optical properties

$$a = \sum_{\chi} a_{\psi}^* \stackrel{\chi}{P_{\mathcal{C}}} + a_{\mathsf{ady}} + a_{\mathsf{sea}},$$
(137)

$$b_{\mathbf{b}} = \sum_{\chi} b^*_{\mathbf{b},P} \stackrel{\chi}{P_{\mathcal{C}}} + b_{\mathbf{b},k} + b_{\mathbf{b},\text{sea}},$$
(138)

neglecting the backscatter component of particulate and non-modelled matter (see Eqs. 134 and 135).

The two models can be calibrated to give comparable results, but the latter formulation based on inherent properties has the advantage to be based on quantaties that are frequently measured, which helps in constraining the parameterisation, validation and enables the direct assimilation of optical data.

## 3.10 Gravitational sinking

The sinking of model states is incorporated using a simple upwind scheme for the equation

$$\left. \frac{\partial c_{\mathbf{p}}}{\partial t} \right|_{\mathsf{sed}} = \overset{c_{\mathbf{p}}}{w_{\mathsf{sed}}} \cdot \frac{\partial c_{\mathbf{p}}}{\partial z} \tag{139}$$

and adding the resulting rate to the biogeochemical rates that are passed to the physical driver for integration.

The sedimenting states in the model are given by the particulate organic types  $\overset{\bullet}{R}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S}}$ , the phytoplankton types  $\overset{\chi}{P}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S},\mathcal{C}}$  and calcite  $\overset{calc}{L}_{\mathbb{C}}$ . Sinking velocities are constant velocities  $\overset{\psi}{w}_{0}$  for each particulate matter type  $\psi$ , while for the phytoplankton states  $\chi$  they are

composed of a constant velocity complemented by a variable component subject to nutrient limitation beyond the threshold  $p_{sink}$ :

$$\overset{\chi}{w}_{\text{sed}} = \overset{\chi}{w}_{0} + \overset{\chi}{w}_{\text{lim}} \max\left(0, \overset{\chi}{p}_{\text{sink}} - \overset{\chi}{l}_{\langle \mathbb{NP} \rangle}\right)$$
(140)

#### The benthic system 4

Two benthic models are currently included in ERSEM . The first one is a full benthic model The benthic model in ERSEM is predicated on muddy sediments of the continental shelf, including zoobenthos, bacteria, different forms of organic matter and implicit vertical distribution of material within the sea-bed. The second one is a remineralisation modelthat adsorbs deposing It explicitly describes the main functions of the sediment such as benthic predation, decomposition and recycling of organic matter, bioirrigation and bioturbation. As an alternative to using a full benthic model, the benthic-pelagic interface can be described by a simple benthic closure given in Sect. 5.1.5. This scheme adsorbs depositing particulate matter and phytoplankton and returns dissolved inorganic nutrients and carbon to the water column at a given time scale reducing the sediments to a simple buffer layer of organic matter recyclingin the sediments., that however does not involve any explicit benthic processes. It is computationally considerably lighter compared to the full model, but the computational effort in both cases is neglectible compared to the pelagic component. While the full benthic model is more adequate for shelf seas application that are dominated by the sediment type it represents with a close connection to the productive upper ocean, the simplified closure scheme is more suitable in deep domains under oligotrophic conditions, where the sediment processes are of lesser importance.

#### 4.1 **Benthic model structure**

The full benthic model is a simplified version (Blackford, 1997; Kohlmeier, 2004) of the more complex original model introduced in the original version of ERSEM (Ruardij and

Van Raaphorst, 1995; Ebenhöh et al., 1995) assuming near-equilibirum conditions for the inorganic components. Organisms are distinguished in classes on a more functional and less size oriented base than in the pelagic part.

The model includes the functional types of aerobic and anaerobic bacteria as decomposers of organic material, three types of zoobenthos benthic predators (suspension feeders, deposit feeders and meiobenthos), dissolved organic matter and three forms of particulate detritus classified according to their availability and decomposition time scales into slowly degradable, available refractory and buried refractory matter. The model considers three distinct layers

Benthic state variables are vertically integrated contents (in mass per area) whose vertical distributions are constrained by the following simplifying assumptions: Three distinct layers are considered in the model, a top, aerobic layer that is oxygenated and delimited by the horizon of dissolved oxygen, an intermediate anaerobic oxidised layer with no free oxygen, but oxidised nitrogen available (also referred to as denitrification layer) and delimited by the horizon of oxidised nitrogen, and a completely anoxic deep sediment layer. Given its very shallow penetration into the sediments, for simplicity, also dissolved organic matter is assumed to be restricted to the aerobic layer. Below these layers, limited by the total depth horizon of the model, no biogeochemical processes take place and only buried refractory matter exists. The vertical distribution of matter is implicitly resolved assuming near-equilibrium conditions for the inorganic components determining the diffusion rate with the overlying water body for the inorganic forms.

The chemical components of the types are identical to the pelagic part consisting of carbon, nitrogen, phosphorus, silicate and iron; the silicate and iron cycles are simplified, bypassing the living functional types, similar in a similar manner to the pelagic part of the model. The silicate contained in detritus is remineralised implicitly into inorganic state form in the sediments, while the iron in detritus is directly recycled and returned to the water column. A particularity of the benthic model are the

The vertical distribution of dissolved inorganic and particulate organic matter is crucial in determining the availability of food and resources to the benthic organisms. It is implicitly

resolved assuming near-equilibrium conditions for the inorganic components determining the diffusion rate with the overlying water body for the inorganic forms and assumes exponentially decaying distributions for particalute organic mattter. The vertical dynamics of these distributions are described by dedicated state variables describing the that describe the structure of the sediments. These are given by the oxygen horizon (the lower limit of the oxygenated layer and the upper limit of the anaerobic denitrification layer), the oxidised nitrogen horizon (the lower limit of the denitrification layer and the upper limit of the strictly anoxic layer) and the mean penetration depths for available refractory carbon, nitrogen and phosphorus and slowly degradable carbon, nitrogen, phosphorus and silicate.

A complete list of benthic state variables is given in Table 8.

#### 4.2 Implicit vertical distribution of inorganic states in the benthos

In order to determine the dynamics of the oxygen and oxidised nitrogen horizons as well as the inorganic fluxes across the seabed (Sect. 5.1.3), the inorganic components of the benthos are assumed to be close to their equilibrium distributions, in which all source and sink terms of the pore water concentrations of the inorganic components  $c_{pw}$  inside the sediments are perfectly balanced by diffusion:

$$\nu_{\text{idiff}} \frac{\partial^2 c_{\text{pw}}}{\partial \zeta^2} = \frac{1}{\Delta d} \left. \frac{\partial c_{\text{b}}}{\partial t} \right|_{\text{bgc}} \tag{141}$$

where  $c_{\rm b}$  is the layer content. This partial differential equation has a general parabolic solution in  $\frac{\partial c_b}{\partial t}\Big|_{bgc}$  as a fixed equilibrium rate independent of time. This is a reasonable assumption when the diffusive rates are significantly faster than the biogeochemical processes ( $\nu_{idiff}$  is the diffusivity of dissolved inorganic components in the benthos depending on bioirrigation, see Eq. 210). The equations apply to each of the three sediment layers and the resulting system of piece-wise parabolic continuous profiles can be solved using two boundary conditions per layer: the surface concentration at the upper boundary starting with sediment surface concentrations the sediment surface

concentration and the flux across the lower boundary which is equal to the sum of all source and sink processes below the layer under consideration (by definition, no fluxes of dissolved matter can occur across the bottom of the sediments so that all sources and sinks have to be compensated from above).

The sediment surface concentrations are estimated from the corresponding pelagic concentration modified by diffusive correction for the non homogenous distribution towards the seabed. In cases when the benthic biogeochmical rates of the inorganic state  $c_{\rm b}$ result in a net source the concentration at the sea bed cbed is approximated from the pelagic concentration nearest to the sea bed (required as a boundary condition to the production-diffusion balance above is generally not equal to the concentration at the centre of the lowest pelagic discretisation cell  $c_{p}$ ) by

$$\underline{c_{\mathrm{bed}} = c_{\mathrm{p}} + p_{\mathrm{vmix}} \left. \frac{\partial c_{\mathrm{b}}}{\partial t} \right|_{\mathrm{bgc}}}$$

while for cases when they act as net sink it is given by

$$c_{\text{bed}} = c_{\text{p}} \frac{c_{\text{p}}}{c_{\text{p}} - p_{\text{vmix}} \left. \frac{\partial c_{\text{b}}}{\partial t} \right|_{\text{bgc}}}$$

, as diffusion across the sediment surface will be attenuated by the bottom boundary layer. In the simplest case the difference between cell centre and sediment surface concentrations can be estimated assuming a linear diffusive flux as positively proportional to the biogeochemical net change in the sediments. However, a problem arises for this formulation when the sediments act as net sink, as the calculated differences may exceed the cell centre concentration suggesting negative concentrations at the sediment interface. Therefore, for negative net sinks in the sediments the formulation suggested by

(142)

Patankar (1980); Burchard et al. (2003) is applied, leading to the equation:

$c_{bed} = \langle$	$\left( c_{p} + p_{Vmix} \left. \frac{\partial c_{b}}{\partial t} \right _{bgc} \right)$	if	$\left. \frac{\partial c_{\rm b}}{\partial t} \right _{\rm bgc} > 0$
	$c_{\rm p} \frac{c_{\rm p}}{c_{\rm p} - p_{\rm vmix} \frac{\partial c_{\rm b}}{\partial t}} \Big _{\rm bgc}$	if	$\left. \frac{\partial c_{\rm b}}{\partial t} \right _{\rm bgc} < 0  ,$

where  $p_{\text{vmix}}$  is an inverse mixing velocity constant.

The resulting equilibrium pore water concentrations  $\tilde{c}_{pw}$  in each layer are converted into the full equilibrium layer contents using the layer thickness and the conversion factor

$$\nu_{\mathbb{N},\mathbb{P}} = p_{\mathsf{poro}} p_{\mathsf{ads}} \,, \tag{143}$$

where  $p_{poro}$  and  $p_{ads}$  are porosity and adsorption factors that may vary spatially in case of porosity and adsorption of phosphorus while they are constants for all other adsorptions.

The dynamics of the oxygen and oxidised nitrogen horizons are determined by a relaxation towards their equilibrium values  $d_{eq}^{oxy}$  and  $d_{eq}^{denit}$ , which are the depths where the pore water equilibrium concentrations are 0. Their time evolution is then described by

$$\frac{\partial D}{\partial t} = \frac{1}{\tau_{\text{oxy}}} \begin{pmatrix} \text{oxy} & \text{oxy} \\ d_{\text{eq}} - D \end{pmatrix}$$
(144)  
$$\frac{\partial D}{\partial t} = \frac{1}{\tau_{\text{denit}}} \begin{pmatrix} \text{denit} & \text{denit} \\ d_{\text{eq}} - D \end{pmatrix},$$
(145)

where  $\tau_{ox}$  and  $\tau_{denit}$  are the respective relaxation time scales.

#### 4.3 Implicit vertical distribution of organic matter in the benthos

The penetration of organic matter type  $\psi$  into the sediments is assumed as exponential decay of a concentration  $\gamma_{c}^{\psi}(\zeta)$  from a sediment surface value  $\frac{c_0}{c_0}$  as a function of the

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mean penetration depth  $\stackrel{\psi}{D}$  of matter  $\psi$ . e-folding depth  $\lambda$ :

$$\underbrace{\overset{\psi}{c}(\zeta) = \overset{\psi}{c_0} e^{-\frac{\zeta}{\lambda}}}_{c_0,c_0,\ldots,c_{n-1}}.$$
(146)

Total content  $\frac{c}{c}$  and mean penetration depth are  $\frac{\psi}{c_b}$  is then given by the integrals-

 $\underline{c_{\mathsf{b}} = c_0 \int\limits_{0}^{d_{\mathsf{tot}}} e^{-\frac{\zeta}{\psi}} \mathsf{d}\zeta}$ 

and-

$$\overset{\psi}{D} = \frac{1}{c_{\rm b}} c_0 \int\limits_0^{d_{\rm tot}} \zeta e^{-\frac{\zeta}{\psi}} \mathrm{d}\zeta \,. \label{eq:Deltaconstraint}$$

integral

and the penetration depth  $\stackrel{\psi}{D}$  of matter  $\psi$  is defined accordingly as

$$\overset{\psi}{D} = \frac{1}{\underset{c_{\mathbf{b}}}{\psi}} \overset{\psi}{\underset{c_{\mathbf{b}}}{\int}} \overset{d_{\text{tot}}}{\underset{c_{\mathbf{b}}}{\int}} \zeta e^{-\frac{\zeta}{\lambda}} \mathsf{d}\zeta.$$
(148)

For  $d_{\text{tot}} \rightarrow \infty$  follows

$$\underline{c_{\mathsf{b}} = c_0 \ \overset{\psi}{D},}$$

so assuming  $D \ll d_{tot}$  the vertical distribution of detritus can be expressed as-

$$\underline{c(\zeta)=c_0e^{-\frac{\zeta}{\psi}}}$$

and the two integrals of Eq.s 147 and 148 yield

$\lambda - \frac{\psi}{D} - \frac{\psi}{c_{b}}$	(149)
$\chi = D = \frac{\psi}{\psi}$ ,	(140)
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	

i.e. the mean penetration depth is given by the e-folding depth of the distribution function-:

 ${}^{\psi}_{c}(\zeta) = {}^{\psi}_{c0} e^{-\frac{\zeta}{\psi}}_{D} = {}^{\psi}_{\frac{c_{b}}{\psi}} e^{-\frac{\zeta}{\psi}}_{D} .$ (150)

The change of penetration depth due to sources or sink fluxes f_i occurring at depth d_i and bioturbation vertically distributed sources and sinks $f(\zeta)$ can then be approximated by the equation

$$\frac{\partial \overset{\psi}{D}}{\partial t} = \sum_{i} (d_{i} - \overset{\psi}{D}) \frac{f_{i}}{c_{\mathsf{b}}} + \left. \frac{\partial \overset{\psi}{D}}{\partial t} \right|_{\mathsf{bturb}}$$

calculated by the formula:

Bioturbation is acting over a characteristic length scale δ_{bturb} and assumed of

$$\frac{\mathrm{d}D}{\mathrm{d}t} = \int_{0}^{\infty} (\zeta - D) \frac{f(\zeta)}{c_{\mathrm{b}}} \mathrm{d}\zeta.$$

As the model is not vertically explicit, but, based on the model assumptions, processes can be attributed to layers (e.g. activity of aerobic bacteria to the aerobic layer), the changes \mathcal{F}_i caused in a given layer can be attributed to discrete depth levels being the centre of the layer ζ_i .

The changes of penetration depth due to source and sink terms are complemented by the physical displacement of organic matter by the process of bioturbation, so that the shape

$$\gamma = \nu_{\text{bturb}} \frac{1}{c_{\text{b}}} (c_0 - \gamma(\delta_{\text{bturb}})),$$

which, still assuming that $\stackrel{\psi}{D} \ll d_{\rm tot}$, takes the form-

$$\left. \frac{\partial D}{\partial t} \right|_{\text{bturb}} = \frac{\nu_{\text{bturb}}}{D} \left(1 - e^{-\frac{\phi_{\text{bturb}}}{\psi}} \right),$$

total change is given by the equation:

 $\frac{\partial D}{\partial t} = \sum_{i} (d_{i} - D) \frac{f_{i}}{\psi} + \frac{\partial D}{\partial t} \bigg|_{\text{bturb}}.$ (152)

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(151)



Bioturbation smoothes the concentration gradient and is therefore implemented as diffusive flux proportional to the difference in concentrations between 0 and a bioturbatation

length scale δ_{bturb}

$$\frac{\partial D}{\partial t} \bigg|_{\text{bturb}} = \frac{\nu_{\text{bturb}}}{\frac{\psi}{c_{\text{b}}}} \begin{pmatrix} \psi & \psi \\ c_{0} - c \\ \delta_{\text{bturb}} \end{pmatrix},$$
(153)

where ν_{bturb} is the bioturbation diffusivity of particulate matter (Eq. 212). <u>Still assuming that</u> $\overset{\psi}{D} \ll d_{\text{tot}}$, this takes the form

$$\frac{\partial D}{\partial t} = \frac{\nu_{\text{bturb}}}{D} \left(1 - e^{-\frac{\delta_{\text{bturb}}}{\psi}}\right).$$
(154)

The fraction of organic matter contained between two given depth levels can then be computed as

$$\frac{\frac{c_{\rm b}}{d_{\rm up}}}{c_{\rm b}} = \frac{1}{c_{\rm b}} \int_{d_{\rm up}}^{d_{\rm low}} \gamma(z) dz = \frac{e^{-\frac{d_{\rm up}}{\psi}} - e^{-\frac{d_{\rm low}}{\psi}}}{1 - e^{-\frac{d_{\rm low}}{D}}}, /$$

$$\frac{\frac{\psi}{c_{\rm b}}}{d_{\rm up}} = \frac{1}{\frac{\psi}{c_{\rm b}}} \int_{d_{\rm up}}^{d_{\rm low}} \gamma(\zeta) d\zeta = \frac{e^{-\frac{d_{\rm up}}{\psi}} - e^{-\frac{d_{\rm low}}{\psi}}}{1 - e^{-\frac{d_{\rm low}}{D}}},$$
(155)

where the total content was approximated as

For consistency with the model assumptions and to avoid numerical issues the penetrations depths are constrained to values between D_0 and $d_{\rm tot}$.

Dissolved organic matter is assumed to reside entirely in the oxygenated layer.

4.4 Heterotrophic bacteria

Benthic decomposers consist of aerobic bacteria living in the upper sediment layer down to the oxygen horizon and anaerobic bacteria living in the denitrification layer and anoxic layer. Their dynamics are summarised by the equations



Specific Substrate mass-pecific bacterial uptake is regulated by the sediment surface temperature, oxygen availability (in free or bound form) and the nutritional state of the substrate (through the regulating factors l_T^{χ} , l_0^{χ} and $l_{\langle \mathbb{NP} \rangle}^{\chi}$, Eqs. 235, 248, 243) and the amount of bacteria in the given location:

$$\frac{\mathcal{F}|_{dg}^{\overset{\chi}{H}} = r_{up}|_{Q}^{\overset{\chi}{H}} \quad \overset{\chi}{l_{T}} \quad \overset{\chi}{l_{O}} \quad \overset{\chi}{H_{C}}}{\mathcal{F}|_{refr}^{\overset{\chi}{H}} = r_{up}|_{refr}^{\overset{\chi}{H}} \quad \overset{\chi}{l_{T}} \quad \overset{\chi}{l_{O}} \quad \overset{\chi}{H_{C}}}{\mathcal{F}|_{slow}^{\overset{\chi}{H}} = \left(r_{fast}|_{slow}^{\overset{\chi}{H}} \quad \overset{\chi}{l_{\langle \mathbb{NP} \rangle}} + r_{up}|_{slow}^{\overset{\chi}{H}}\right) \overset{\chi}{l_{T}} \quad \overset{\chi}{l_{O}} \quad \overset{\chi}{H_{C}},$$

$$\mathcal{F}|_{dis}^{\overset{\chi}{H}} = r_{up}|_{Q}^{\overset{\chi}{H}} \overset{\chi}{l_{\mathsf{T}}} \overset{\chi}{l_{\mathsf{D}}} \overset{\chi}{H_{\mathsf{C}}} \overset{\chi}{l_{\mathsf{C}}}$$
(159)

$$\mathcal{F}|_{Q}^{\overset{\chi}{H}} = r_{up}|_{Q}^{\overset{\chi}{H}} \stackrel{\chi}{l_{T}} \stackrel{\chi}{l_{0}} \stackrel{\chi}{H_{C}}$$
(160)

$$\mathcal{F}|_{degr}^{\overset{X}{H}} = \begin{pmatrix} r_{fast}|_{degr}^{\overset{X}{H}} & \overset{X}{l}_{\langle \mathbb{NP} \rangle} + r_{up}|_{degr}^{\overset{X}{H}} \end{pmatrix} \overset{X}{l_{\mathsf{T}}} \overset{X}{l_{\mathbb{O}}} \overset{X}{H_{\mathbb{C}}},$$
(161)

where $r_{up}|_{Q}^{H}$ are the bacteria and substrate mass specific reference uptake rates. These are generally high for the dissolved form and low for refractory matter. Decomposition of slowly degradable matter has a slow basal component complemented by a fast component $r_{tast}|_{Q}^{H}$ subject to nutrient regulation.

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(162)

To obtain the uptake rates these <u>substrate mass</u> specific rates are multiplied by the substrate concentrations available in the respective layer (given by Eq. 155):





where the layer limits $d_{\text{low}}, d_{\text{up}}$ are 0, $\stackrel{\text{oxy}}{D}$ for aerobic bacteria and $\stackrel{\text{oxy}}{D}$, d_{tot} for anaerobic bacteria ria. Aerobic bacteria feed on dissolved and particulate substrate, while anaerobic bacteria feed exclusively on the particulate form.

The uptake of organic nitrogen and phosphate phosphorus is enhanced by a nutrient preference factor $\overset{\chi}{p}_{nup}$ and supported by observations that the relative nutrient content of benthic DOM decreases under bacteria production (van Duyl et al., 1993). It is complemented by the uptake of inorganic forms when organic matter is nutrient-poor with respect to the fixed bacterial stoichiometric ratio. Inorganic uptake of nutrients by each bacteria type is regulated by Michaelis–Menten terms of the pore water inorganic nutrient content within the oxygenated or anaerobic oxidised layer with the Redfield equivalent of carbon uptake

as the half-saturation term:

$$\frac{\partial \tilde{H}_{\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{upt} = \sum_{\psi} \left| \sum_{p \in \mathbb{N}}^{\chi} \tilde{P}_{\mathsf{nup}} \mathcal{F} \right|_{Q}^{\chi} \underbrace{H}_{Q}^{\psi}_{\mathbb{N},\mathbb{P}} \bigg|_{d_{up}}^{d_{\mathsf{low}}} + \frac{q}{q_{\mathsf{ref}_{\mathbb{N},\mathbb{P}:\mathbb{C}}}} \left| \frac{\partial \tilde{H}_{\mathbb{C}}}{\partial t} \right|_{upt} \frac{\frac{1}{\nu_{\mathbb{N},\mathbb{P}}} \left| \frac{K_{\mathbb{N},\mathbb{P}}}{K_{\mathbb{N},\mathbb{P}}} \right|_{d_{up}}^{d_{\mathsf{low}}}}{\frac{1}{\nu_{\mathbb{N},\mathbb{P}}} \left| \frac{K_{\mathbb{N},\mathbb{P}}}{K_{\mathbb{N},\mathbb{P}}} \right|_{d_{up}}^{d_{\mathsf{low}}} + q_{\mathsf{ref}_{\mathbb{N},\mathbb{P}:\mathbb{C}}}} \left| \frac{\partial \tilde{H}_{\mathbb{C}}}{\partial t} \right|_{upt}},$$
(163)

where $K_{\mathbb{N}} \Big|_{d_{up}}^{d_{low}}$, $K_{\mathbb{P}} \Big|_{d_{up}}^{d_{low}}$ are the respective layer contents of ammonium or phosphate between the depth d_{up} and d_{low} and $\nu_{\mathbb{N},\mathbb{P}}$ is a volume correction factor (Eq. 143) reducing the total layer content to the pore water content.

Anaerobic bacteria is feeding on and excreting only in particulate form, so that the above rates are for gross uptake in the case of aerobic bacteria followed by excretion in dissolved form, while for anaerobic bacteria they are net rates with no subsequent excretion. Excretion occurs at fixed fractions $\frac{\text{aer}}{q \text{ sexcr}} \frac{\text{aer}}{q \text{ cexcr}}$, $\frac{\text{aer}}{q \text{ rexcr}}$ of the aerobic bacteria uptake according to:

$$\frac{\frac{\partial H}{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{excr}} = \stackrel{\text{aer}}{q}_{\text{sexcr}} \mathcal{F} \bigg|_{\substack{W \\ \text{slow}}}^{\text{aer}} Q_{\mathbb{C},\mathbb{N},\mathbb{P}}^{(a_{\text{low}})} \bigg|_{\substack{d_{\text{up}}}}^{a_{\text{low}}} + \stackrel{\text{aer}}{q}_{\text{rexcr}} \mathcal{F} \bigg|_{\substack{H \\ \text{refr}}}^{\text{aer}} Q_{\mathbb{C},\mathbb{N},\mathbb{P}}^{(a_{\text{low}})} \bigg|_{\substack{d_{\text{up}}}}^{a_{\text{low}}}.$$

$$\frac{\partial H_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\substack{\text{excr}}} = \stackrel{\text{aer}}{q} \stackrel{\mathcal{F}}{}_{\substack{H \\ Q}} \stackrel{\text{degr}}{Q} \stackrel{\mathcal{O}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{Q} \bigg|_{\substack{d_{\text{up}}}}^{d_{\text{low}}} + \stackrel{\text{aer}}{q} \stackrel{\mathcal{F}}{}_{\substack{rexcr}} \stackrel{\text{aer}}{\mathcal{F}} \stackrel{\text{refr}}{}_{\substack{Q}} \stackrel{\mathcal{O}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{Q} \bigg|_{\substack{d_{\text{up}}}}^{d_{\text{low}}}.$$
(164)

$$\frac{\partial H^{\text{anaer}}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\bigg|_{\text{excr}} = 0.$$
(165)

Respiration of bacteria is given by activity respiration as a fraction of gross uptake q_{aresp}^{χ} and temperature regulated basal respiration at rest proportional to the bacteria biomass by the factor r_{resp}^{χ} :

$$\frac{\partial \hat{H}_{\mathbb{C}}}{\partial t}\bigg|_{\text{resp}} = \frac{\chi}{q_{\text{aresp}}} \frac{\partial \hat{H}_{\mathbb{C}}}{\partial t}\bigg|_{\text{upt}} + \frac{\chi}{r_{\text{resp}}} \hat{l}_{\mathsf{T}}^{\chi} \hat{H}_{\mathbb{C}}^{\chi}$$
(166)

Bacterial mortality is fully regulated by oxygen (see Eq. 248) and proportional to the bacteria biomass by factor r_{mort}^{χ} :

$$\frac{\partial \hat{H}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{mort}} = \stackrel{\chi}{r_{\text{mort}}} \left(1 - \stackrel{\chi}{l_{\mathbb{O}}} \right) \stackrel{\chi}{H'}_{\mathbb{C},\mathbb{N},\mathbb{P}} , \qquad (167)$$

where aerobic bacteria use oxygen in dissolved form while anaerobic bacteria satisfy their oxygen requirements from oxidised nitrogen.

Benthic bacteria are held at a fixed stoichiometric quota $\overset{\chi}{q}_{\mathsf{ref}_{\mathbb{N},\mathbb{P}:\mathbb{C}}}$, so that any chemical component flux in excess of the reference quota is exudated released according to Eqs. (264) and (265), in dissolved form for the nutrients and in the form of organic matter for carbon.

4.5 Predators

The general biogeochemical dynamics of the zoobenthos types χ are given by the equations



The benthic predators considered in ERSEM are deposit feeders, suspension feeders and meiobenthos, distinguished by their prey fields and preferences, the depth section they live in and their respective metabolic rates. The prey fields available to each type are given in Table 9Fig. 5, where organic matter is scavenged only in the accesible depth sections indicated for each predator type and depth sections accessible to each predators given by three parameters as follows:

- suspension feeders:
$$0 \leq \zeta \leq d_Y$$
,

- deposit feeders: $d_Y \leq \zeta \leq d_Y$,

(170)

- meiobenthos: $0 \leq \zeta \leq \frac{d_Y}{d_Y}$.

An additional parameter d_{SUSP} indicates the range of suspension feeders into the water column assuming homogenous prey distribution over this scale and $\frac{d_Z}{d_Z}$, $\frac{d_Z}{d_Z}$ are parameters describing the depth sections where the predators reside.

The total prey available to each zoobenthos type χ is composed of the individual preys prey types ψ as

$$\overset{\chi}{\mathrm{Pr}}_{\mathbb{C},\mathbb{N},\mathbb{P}} = \sum_{\psi} \left. f_{\mathrm{pr}} \right|_{\psi}^{\chi} \frac{f_{\mathrm{pr}} |_{\psi}^{\hat{Z}} \psi_{\mathbb{C}}'}{f_{\mathrm{pr}} |_{\psi}^{\chi} \psi_{\mathbb{C}}' + f_{\mathrm{min}}^{\chi}} \psi_{\mathbb{C},\mathbb{N},\mathbb{P}}',$$

where $f_{pr}|_{u}^{\chi}$

$$\overset{\chi}{\Pr}_{\mathbb{C},\mathbb{N},\mathbb{P}} = \sum_{\psi} f_{\mathsf{pr}}|_{\psi}^{\chi} \frac{f_{\mathsf{pr}}|_{\psi}^{\hat{Y}} \psi_{\mathbb{C}}'}{f_{\mathsf{pr}}|_{\psi}^{\chi} \psi_{\mathbb{C}}' + h_{\mathsf{min}}^{\chi}} \psi'_{\mathbb{C},\mathbb{N},\mathbb{P}},$$

where $f_{pr}|_{tr}^{\tilde{Y}}$ are the food preferences and $\frac{\chi}{f_{min}} h_{min}$ is a food half-saturation constant limiting the detection capacity of predator χ of individual prey types similar to the zooplankton predation (Eq. 28). In contrast to the pelagic form the detection capability for the benthic fauna is assumed to vary by food-source assuming that benthic predators search their food more actively. The prey contents in the half-saturation term are consequently multiplied by the food-preferences.

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The prey mass specific uptake capacity for each zooplanton type χ is then given by:

$$\overset{\chi}{S}_{upt} = \overset{\chi}{g}_{max} \overset{\chi}{l_{T}} \overset{\chi}{l_{O}} \overset{\chi}{l}_{crowd} \frac{\overset{\chi}{Y_{C}}}{\overset{\chi}{\mathsf{Pr}_{C} + h_{up}}},$$

$$(171)$$

where $\overset{\chi}{g}_{max}$ is the maximum uptake capacity of each type at reference temperature, $\overset{\chi}{l}_{T}$ is the metabolic temperature response (Eq. 235), $\overset{\chi}{l}_{\mathbb{O}}$ is the limitation of oxygen (Eq. 246), $\overset{\chi}{l}_{crowd}$ is a growth limiting penalty function accounting for overcrowding effects (Eq. 263, absent for meiobenthos as this type is capable to feed of feeding on itself), h_{up}^{χ} is a predation efficiency limiting the chances of encountering the prey available ($P_{r_{c}}^{\chi}$).

Introducing the prey mass specific fluxes from prey ψ to predator $\stackrel{\star}{Y}$

$$\mathcal{F}|_{\psi}^{\tilde{Y}} = \overset{\chi}{\mathcal{S}}_{upt} f_{pr}|_{\psi}^{\tilde{Y}} \frac{f_{pr}|_{\psi}^{\tilde{Y}} \psi_{\mathbb{C}}'}{f_{pr}|_{\psi}^{\tilde{Y}} \psi_{\mathbb{C}}' + \frac{f_{min}}{f_{min}} h_{min}^{\chi}}$$
(172)

with $f_{\rm pr}|_{\psi}^{\chi}$ being the food preference of predator $\overset{\chi}{Y}$ for prey ψ , $\overset{\chi}{f_{\rm min}} \overset{\chi}{h_{\rm min}}$ being a half-saturation constant reflecting the detection capacity of predator χ , the zooplankton uptake

can then be written as:

.

$$\frac{\partial Y_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\text{upt}} = \sum_{\psi} \mathcal{F}|_{\psi}^{\chi} \psi_{\mathbb{C},\mathbb{N},\mathbb{P}}^{\chi}.$$
(173)

Zoobenthos excretion is given by:

$$\frac{\partial \overset{\chi}{\mathbb{T}}}{\partial t} = \underbrace{\sum_{\psi}^{\text{slow med}}}_{\psi \neq Q, R} \overset{\chi}{q_{\text{excr}}} \frac{\partial \overset{\chi}{\mathbb{T}}}{\partial t} + \underbrace{\sum_{\psi}^{\psi = Q, R}}_{\psi = Q, R} \overset{\chi}{q_{\text{pexcr}}} \frac{\partial \overset{\chi}{\mathbb{T}}}{\partial t} \Big|_{\text{upt}} \frac{\partial \overset{\chi}{\mathbb{T}}}$$

$$\frac{\partial Y_{\mathbb{C}}^{\chi}}{\partial t} = \sum_{\substack{\psi \neq Q, R \\ = \sum_{\psi} \\ \psi \neq Q, R \\ \psi \neq Q, R \\ \psi \neq Q, R \\ \psi = Q, R \\ \psi$$

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$$\frac{\partial Y_{\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\underline{excr}} = q_{dil}^{\chi} \left(\sum_{\psi \neq Q, R}^{\psi \neq Q, R} q_{\underline{excr}} \mathcal{F}|_{\psi}^{Y} \psi_{\mathbb{N},\mathbb{P}}' + \sum_{\psi \neq Q, R}^{\psi \neq Q, R} q_{\underline{pexcr}} \mathcal{F}|_{\psi}^{Y} \psi_{\mathbb{N},\mathbb{P}}' \right)$$
(175)

where q_{excr}^{χ} is a fixed proportion of gross uptake excreted and q_{dil}^{χ} an additional dilution coefficient taking into account a reduced amount of nutrients in the fecal pellets with respect to the uptake quota.

Respiration of zoobenthos is given by activity respiration as a fraction of net uptake $\overset{\chi}{q}_{\mathsf{aresp}}$ and temperature regulated respiration at rest proportional to the zoobenthos biomass by the factor r_{resp}^{χ} :

$$\frac{\partial Y_{\mathbb{C}}^{\chi}}{\partial t}\bigg|_{\text{resp}} = \overset{\chi}{q}_{\text{aresp}} \left(1 - \overset{\chi}{q}_{\text{excr}}\right) \left. \frac{\partial Y_{\mathbb{C}}^{\chi}}{\partial t} \right|_{\text{upt}} + \overset{\chi}{r}_{\text{resp}} \left. \overset{\chi}{l}_{\mathsf{T}} \right|_{\mathsf{Y}_{\mathbb{C}}^{\chi}}$$
(176)

Zoobenthos mortality is regulated by temperature and oxygen and composed of a basal part enhanced under oxygen deficiency and cold temperatures by the factors $\overset{\chi}{r}_{mort\mathbb{O}}, \overset{\chi}{r}_{mort\mathbb{T}}$:

$$\frac{\partial \hat{Y}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\bigg|_{\text{mort}} = \left(\hat{x}_{\text{mort}} \quad \hat{l}_{\text{T}}^{\chi} + \hat{x}_{\text{mort}\mathbb{O}} \quad \hat{l}_{\text{T}}^{\chi} \left(1 - \hat{l}_{\mathbb{O}}^{\chi} \right) + \hat{x}_{\text{mort}\text{T}} e^{-\frac{\mathsf{T}}{\chi}} \right) \hat{Y}'_{\mathbb{C},\mathbb{N},\mathbb{P}}.$$
(177)

Also, zoobenthos types are kept at a fixed stoichiometric quota $\overset{\chi}{q}_{\mathsf{ref}_{\mathbb{N},\mathbb{P}:\mathbb{C}}}$ according to Eqs. (264) and (265) resulting in the exudation release of nutrients in inorganic form and carbon in the form of slowly degradable organic matter.

4.6 Organic matter

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The cycling of carbon, nitrogen and phosphorus through the benthic food web by the processes of uptake, scavenging, excretion, mortality, exudation release and burial results in the following organic matter fluxes:

The dissolved organic matter is produced by excretion and mortality and reduced by bacterial uptake





Degradable matter is generated by excretion and mortality and release fluxes, taken up by bacteria, and scavenged by zoobenthos



Refractory matter is taken up by bacteria and modified by burying across the total depth horizon



The abbreviated cycles for iron and silicate condensate all biogeochemical processes in the benthos into a simple remineralisation of degradable organic matter into dissolved inorganic iron or silicate at a fixed rate $r_{\mathbb{F}remin}$ or $r_{\mathbb{S}remin}$:



In these equations the partioning in between the different forms of organic matter occurs in the following manner:

Uptake of all forms of organic matter by bacteria is given by Eqs. (159)-(161) as

$$\frac{\partial \overset{\psi}{Q}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\bigg|_{\text{upt}} = \mathcal{F}|_{\overset{W}{Q}}^{\overset{\text{arr}}{H}} Q_{\mathbb{C},\mathbb{N},\mathbb{P}}^{\overset{\psi}{D}}\bigg|_{0}^{\overset{\text{ox}}{D}} + \mathcal{F}|_{\overset{W}{Q}}^{\overset{\text{anaer}}{H}} Q_{\mathbb{C},\mathbb{N},\mathbb{P}}^{\overset{\psi}{D}}\bigg|_{D}^{d_{\text{tot}}}.$$
(183)

The excretion of aerobic bacteria is directed to dissolved organic matter, while for the zoobenthos types $\overset{\Psi}{Y}$ it is directed to slowly degradable matter:

$$\frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{excr} = \frac{\partial H_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{excr}$$
(184)
$$\frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{excr} = \sum_{\Psi} \frac{\partial Y_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{excr} ,$$
(185)

using Eqs. (164), (165), (174), (175).

excr

The mortality of aerobic bacteria is partioned between a particulate part directed to slowly degradable matter and a dissolved part $\overset{\rm aer}{q}_{\rm dmort}$, while for the zoobenthos types $\overset{\Psi}{Y}$ and anaerobic bacteria it is entirely directed to slowly degradable matter:

$$\frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{mort}} = \frac{\operatorname{aer}}{q_{\text{dmort}}} \frac{\partial H_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{mort}}$$

$$\frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{mort}} = \left(1 - \frac{\operatorname{aer}}{q_{\text{dmort}}}\right) \frac{\partial H_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{mort}} + \frac{\partial H_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{mort}} + \sum_{\Psi} \frac{\partial Y_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{mort}}$$

$$+ \sum_{\Psi} \frac{\partial Y_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \left|_{\text{mort}} \right|_{\text{mort}}$$
(186)

using Eqs. (167) and (177).

Slowly degradable Degradable matter is scavenged by zoobenthos according to Eq. (172)

$$\frac{\frac{\operatorname{slow}\operatorname{degr}}{\widetilde{Q}}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \bigg|_{\operatorname{scav}} = \sum_{\Psi} \mathcal{F}|_{\widetilde{Q}}^{\Psi} \overset{\operatorname{slow}\operatorname{degr}}{\widetilde{Q}}_{\mathbb{C},\mathbb{N},\mathbb{P}}^{\Psi}.$$
(188)

In addition, slowly degradable carbon may be produced by the stoichiometric adjustment (Eq. 264) of bacteria or zoobenthos:

$$\frac{\frac{\partial \log \deg r}{\partial Q_{\mathbb{C}}}}{\partial t} \bigg|_{\text{rel}} = \sum_{\chi} \frac{\partial \hat{H}_{\mathbb{C}}}{\partial t} \bigg|_{\text{rel}} + \sum_{\Psi} \frac{\partial Y_{\mathbb{C}}}{\partial t} \bigg|_{\text{rel}}.$$
(189)

Refractory organic matter may be buried by the transfer of matter across the total depth horizon d_{tot} resulting from the redistribution of organic matter by diffusion and bioturbation (Eq. 212). Note, The diffusive process of bioturbation leads to the downward displacement

of refractory material. The resulting flux of refractory organic matter across the total depth horizon of living organisms in the model d_{tot} may be interpreted as burial flux (activated by the ISWbur switch), as material is removed from the biogeochemical active part of the model.

To derive this flux we use a simple geometric argument here: it is assumed that the diffusive process will preserve the vertically exponential distribution of refractory organic matter (Eq. 150), stretching it. Consequently the flux across any horizontal interface can be

expressed as the product of the local concentration ${}^{\text{refr}}_{\mathcal{C},\mathbb{N},\mathbb{P}}$ and the displacement rate of the exponential profile at the given level. Specifically, we know that the local displacement rate at the level of the penetration depth is precisely the change of penetration depth due to

bioturbation $\frac{\partial D}{\partial t}$ bturb

To derive the local displacement rate of the exponential profile at the total depth we can use the displacement time scale at d_{tot} , that is independent of the local concentration:

$$\frac{1}{\tau_{\mathsf{bur}}(\zeta)} = \frac{1}{\Pr_{\mathcal{C}_{\mathbb{C},\mathbb{N},\mathbb{P}}(\zeta)}} \frac{\partial \overset{\mathsf{refr}}{c} \overset{\mathsf{refr}}{c}_{\mathbb{C},\mathbb{N},\mathbb{P}}(\zeta)}{\partial t} = \frac{\zeta}{\Pr_{\mathcal{C}_{\mathbb{C},\mathbb{N},\mathbb{P}}^2}} \frac{\partial \overset{\mathsf{refr}}{D}}{\partial t} \Big|_{\mathsf{bturb}} , \qquad (190)$$
Scaling the disclacement rate using this scale the flux of matter at d_{tot}, and hence the burial flux, can be computed as:

$$\frac{\partial \overset{\text{refr}}{Q}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} = \overset{\text{refr}}{c} \overset{\text{refr}}{c}_{\mathbb{C},\mathbb{N},\mathbb{P}} (d_{\text{tot}}) \frac{\tau_{\text{bur}}(\overset{\text{refr}}{D})}{\tau_{\text{bur}}(d_{\text{tot}})} \frac{\partial \overset{\text{refr}}{D}}{\partial t} = \overset{\text{refr}}{c} \overset{\text{refr}}{c}_{\mathbb{C},\mathbb{N},\mathbb{P}} (d_{\text{tot}}) \frac{d_{\text{tot}}}{refr_{\mathbb{C},\mathbb{N},\mathbb{P}}}}{D} \underbrace{\frac{\partial \overset{\text{refr}}{D}}{\partial t}}{D}_{\text{bturb}} = \overset{\text{refr}}{c} \overset{\text{refr}}{c}_{\mathbb{C},\mathbb{N},\mathbb{P}} (d_{\text{tot}}) \frac{d_{\text{tot}}}{refr_{\mathbb{C},\mathbb{N},\mathbb{P}}}}{D} \underbrace{\frac{\partial \overset{\text{refr}}{D}}{\partial t}}{D}_{\text{bturb}}$$
(191)

This result can be formally confirmed by a straight-forward, but fairly lengthy derivation of the time derivative of the integrated content of refractory matter between the sediment surface and d_{tot} using Eq. 150 and Eq. 156.

Note that this process (activated by the ISWbur switch) removes biomass from the biogeochemically active part of the model, as there are no processes connected to buried organic matter and the model currently doesn't does not consider remobilisation. This means that during long term simulations the loss of nutrients needs to be compensated, e.g. by riverine inputs or atmospheric deposition (carbon is restored by air-sea exchange). The amount of material buried may be approximated by the product of the concentration at the total depths and the burial velocity by which this level is shifted by the diffusive processes. The concentration at the total depths is computed using Eq. (150) with $z = d_{\text{tot}}$. while the burial velocity may be approximated in first order from the rate of change of the

refractory organic matter penetration depth $\frac{\partial D}{\partial t}$. The rate of vertical displacement diff

is not homogeneous over depth, as the concentrations are generally not identical along z. The characteristic time scale τ_{bur} of redistribution at any depth z can be computed using

Eq. (150) as:

$$\frac{1}{\tau_{\mathsf{bur}}(z)} = \frac{1}{\Pr[\substack{\mathsf{refr}\\ q \in \mathbb{N}, \mathbb{N}, \mathbb{P}}(\zeta)} \frac{\partial \overset{\mathsf{refr}}{q \in \mathbb{C}, \mathbb{N}, \mathbb{P}}(z)}{\partial t} = \frac{z}{\Pr[\substack{t \in \mathbb{N}, \mathbb{N}, \mathbb{P}\\ D}} 2} \frac{\partial \overset{\mathsf{refr}_{\mathbb{C}, \mathbb{N}, \mathbb{P}}}{D}}{\partial t},$$

where $q_{\mathbb{C},\mathbb{N},\mathbb{P}}(\zeta)$ is the concentration of refractory organic carbon at sediment depth ζ . The burial velocity can then be estimated scaling the rate of change of the penetration Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |

depth with
$$\frac{\tau_{\text{bur}}(D)}{\tau_{\text{bur}}(d_{\text{tot}})} = \frac{d_{\text{tot}}}{D}$$
 resulting in a burial flux of:

$$\frac{\frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}}{\partial t} \Bigg|_{\text{bur}} = \frac{\frac{\operatorname{refr}}{Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}}{D} \left(\begin{array}{c} -\frac{d_{\text{tot}}}{\operatorname{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}} \\ 1-e \end{array} \right) e^{-\frac{d_{\text{tot}}}{\operatorname{refr}_{\mathbb{C},\mathbb{N},\mathbb{P}}}} \frac{d_{\text{tot}}}{D} \frac{\partial D}{\partial t} \Bigg|_{\text{diff}}$$

using again Eqs. (150) and (156).

In summary, the dissolved organic matter is produced by excretion and mortality and reduced by bacterial uptake-

$$\begin{array}{c|c} \frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \\ \end{array} & = \left. \frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{excr}} + \left. \frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{mort}} \\ \\ & - \left. \frac{\partial Q_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t} \right|_{\text{upt}}, \end{array}$$

slowly degradable matter is generated by excretion and mortality of zoobenthos and aerobic bacteria and exudation fluxes, taken up by bacteria, and scavenged by zoobenthos-

and refractory matter is taken up by bacteria and modified by burying across the total depth horizon-

$$\frac{\partial \overset{\text{refr}}{Q}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\Bigg|_{\text{bgc}} = - \left.\frac{\partial \overset{\text{refr}}{Q}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\right|_{\text{upt}} - \left.\frac{\partial \overset{\text{refr}}{Q}_{\mathbb{C},\mathbb{N},\mathbb{P}}}{\partial t}\right|_{\text{bur}} \mathbf{96}.$$

The abbreviated cycles for iron and silicate simplify all biogeochemical processes in the benthos into a simple remineralisation of slowly degradable organic matter into dissolved inorganic iron or silicate at a fixed rate r_{Fremin} or r_{Sremin} :

$$\begin{split} \frac{\partial \overset{\mathrm{slow}}{Q_{\mathbb{F}}}}{\partial t} \Bigg|_{\mathrm{bgc}} = -r_{\mathbb{F}\mathrm{remin}} \overset{\mathrm{slow}}{Q'_{\mathbb{F}}} \\ \frac{\partial \overset{\mathrm{slow}}{Q_{\mathbb{S}}}}{\partial t} \Bigg|_{\mathrm{bgc}} = -r_{\mathbb{S}\mathrm{remin}} \overset{\mathrm{slow}}{Q'_{\mathbb{S}}}. \end{split}$$

4.7 Inorganic components

The dynamics of benthic nutrients are given by the following equations (see Eq. 192 for the remineralisation of silicate):

$$\frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{bgc}} = \frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{nitr}} - \frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{denit}}$$
(192)

$$\frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{bgc}} = -\frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{nitr}} -\frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{upt}} + \frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{ext} \text{ rel}}$$
(193)

$$\frac{\partial K_{\mathbb{P}}}{\partial t}\Big|_{\text{bgc}} = -\frac{\partial K_{\mathbb{P}}}{\partial t}\Big|_{\text{upt}} + \frac{\partial K_{\mathbb{P}}}{\partial t}\Big|_{\text{exu rel}}$$
(194)
$$\frac{\partial K_{\mathbb{S}}}{\partial t}\Big|_{\text{bgc}} = -\frac{\partial K_{\mathbb{P}}}{\partial t}\Big|_{\text{exu rel}}$$
(195)

$$\frac{\partial K_{\mathbb{S}}}{\partial t}\Big|_{\mathsf{bgc}} = r_{\mathsf{Sremin}} \quad Q'_{\mathbb{S}} \tag{195}$$

while the biogeochemistry of dissolved carbon, oxygen and dinitrogen are given by

$$\frac{\partial G_{\mathbb{C}}}{\partial t} \bigg|_{t} = \frac{\partial G_{\mathbb{C}}}{\partial t} \bigg|$$
(196)

$$\frac{\partial G_{\mathbb{O}}}{\partial t}\Big|_{\text{bgc}} = -\frac{\partial G_{\mathbb{O}}}{\partial t}\Big|_{\text{resp}} - \frac{\partial G_{\mathbb{O}}}{\partial t}\Big|_{\text{nitr}}$$
(197)

$$\frac{\partial G_{\mathbb{N}}}{\partial t}\Big|_{\mathsf{bgc}} = \frac{\partial G_{\mathbb{N}}}{\partial t}\Big|_{\mathsf{denit}}.$$
(198)

The respiration terms of dissolved inorganic carbon and dissolved oxygen are given by Eqs. (166) and (176) as

$$\frac{\partial G_{\mathbb{C}}}{\partial t}\Big|_{\mathsf{resp}} = \sum_{\chi} \frac{\partial \tilde{H}_{\mathbb{C}}}{\partial t}\Big|_{\mathsf{resp}} + \sum_{\Psi} \frac{\partial \tilde{Y}_{\mathbb{C}}}{\partial t}\Big|_{\mathsf{resp}}$$
(199)

$$\frac{\partial G_{\mathbb{O}}}{\partial t}\Big|_{\mathsf{resp}} = -q_{\mathbb{O}:\mathbb{C}} \left(\left. \frac{\partial H_{\mathbb{C}}}{\partial t} \right|_{\mathsf{resp}} + \sum_{\Psi} \left. \frac{\partial Y_{\mathbb{C}}}{\partial t} \right|_{\mathsf{resp}} \right)$$
(200)

where $q_{\mathbb{O}:\mathbb{C}}$ is the oxygen to carbon conversion coefficient.

Nitrification in the benthos is computed similar to the pelagic nitrification from a maximum ammonium mass specific nitrification rate $\begin{array}{c} \mathcal{B} & H\\ \mathcal{T}_{\text{nitr}} & \mathcal{T}_{\text{oitr}} \end{array}$ at reference temperature depending on the ammonium available in the oxygenated layer, approximated as $\begin{array}{c} \frac{\partial \mathcal{B}}{\partial t} & \mathcal{H}\\ \frac{\partial \mathcal{B}}{\partial t} & \mathcal{H}'_{\mathbb{N}} \end{array}$:

$$\frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{nitr}} = \frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{nitr}} = \frac{H}{r_{\text{nitr}}} \frac{\text{bnitr bnitr bnitr}}{l_{\text{T}}} \frac{D}{l_{\mathbb{N}}} \frac{\text{amm}}{d_{\text{tot}}} K'_{\mathbb{N}}, \qquad (201)$$

$$\frac{\partial G_{\mathbb{O}}}{\partial t}\Big|_{\text{nitr}} = 2 \left. \frac{\partial K_{\mathbb{N}}}{\partial t} \right|_{\text{nitr}}$$
(202)

where l_N^{bnitr} and l_T^{bnitr} are the nitrification limitation factors due to the presence of high concentrations of oxidised nitrogen and temperature regulation the temperature regulation factor (Eqs. 253 and 235).

Denitrification is calculated from the oxidised nitrogen reduction equivalent required for anaerobic bacteria respiration:

$$\overset{\text{anaer}}{\mathcal{F}}_{\text{req}} = \frac{1}{2\left(1 - \frac{H}{q_{\text{denit}}}\right) + \frac{5}{4}} \frac{H}{q_{\text{denit}}} \frac{H}{q_{\text{red}}q_{\mathbb{O}:\mathbb{C}}} \left. \frac{\partial H_{\mathbb{C}}}{\partial t} \right|_{\text{resp}} ,$$
(203)

where $\overset{H}{q}_{\text{red}}$ is the maximum fraction of anaerobic bacteria respiration resulting in oxidised nitrogen reduction, $\overset{H}{q}_{\text{denit}}$ is the fraction of reduction subject to denitrification as opposed to ammonification and 2, $\frac{5}{4}$ are the stoichiometric coefficients of oxygen demand per reduction equivalent for the ammonification and denitrification reactions respectively.

The actual reduction of oxidised nitrogen by denitrification is then further limited by availability of oxidised nitrogen ($l_{\mathbb{N}}^{\text{denit}}$, Eq. 254) resulting in the following denitrification fluxes:

$\frac{\partial K_{\mathbb{N}}}{\partial t}$ denit anaer $= l_{\mathbb{N}} ~~ {\mathcal F}$ _{req} (204)

$$\frac{\partial \overline{K_{\mathbb{N}}}}{\partial t} \bigg|_{\text{denit}} = (1 - q_{\text{red}N_2}) \frac{\partial \overline{\mathbb{K}_{\mathbb{N}}}}{\partial t} \bigg|_{\text{denit}}$$
(205)
$$\frac{\partial G_{\mathbb{N}}}{\partial t} \bigg|_{\text{bgc}} = q_{\text{red}G} \frac{\partial \overline{K_{\mathbb{N}}}}{\partial t} \bigg|_{t=1}$$
(206)

denit

where q_{redG} is the fraction of reduction directed to di-nitrogen. As nitrogen fixation is currently not considered in the model, losses of oxidised nitrogen by denitrification are removed from the active cycle and need to be compensated in long term runs by riverine or atmospheric inputsor, otherwise denitrification needs to be switched off.

Exudation Release of nutrients caused by stoichiometric adjustment (Eq. 264) of bacteria or zoobenthos are given by:

$$\frac{\partial K_{\mathbb{N}}}{\partial t} \bigg|_{\text{exu rel}} = \sum_{\chi} \frac{\partial H_{\mathbb{N}}}{\partial t} \bigg|_{\text{exu rel}} + \sum_{\Psi} \frac{\partial Y_{\mathbb{N}}}{\partial t} \bigg|_{\text{exu rel}}$$
(207)
$$\frac{\partial K_{\mathbb{P}}}{\partial t} \bigg|_{\text{exu rel}} = \sum_{\chi} \frac{\partial H_{\mathbb{N}}}{\partial t} \bigg|_{\text{exu rel}} = \sum_{\chi} \frac{\partial Y_{\mathbb{N}}}{\partial t} \bigg|_{\text{exu rel}}$$
(207)

$$\frac{\partial K_{\mathbb{P}}}{\partial t}\Big|_{\text{exu rel}} = \sum_{\chi} \left. \frac{\partial \hat{H}_{\mathbb{P}}}{\partial t} \right|_{\text{exu rel}} + \sum_{\Psi} \left. \frac{\partial Y_{\mathbb{P}}}{\partial t} \right|_{\text{exu rel}} .$$
(208)

4.8 **Bioirrigation**

The diffusivity of dissolved inorganic states is given by a basal diffusivity ϑ_{χ} for each layer χ : aer, den, anox that is increased for bioirrigation by the factor p_{bimin} . The activity of deposit feeders and meiofauna cause further enhancement to yield the total bioirigation diffusivity ν_{idiff} (used in Eq. 141):

$$S_{\text{birr}} = \frac{\mathsf{DEPO}}{q} \frac{\partial Y_{\mathbb{C}}}{\partial t} \bigg|_{\text{upt}} + \frac{\mathsf{MEIO}}{q} \frac{\partial Y_{\mathbb{C}}}{\partial t} \bigg|_{\text{upt}}$$
(209)

$$\nu_{\text{idiff}} = \vartheta_{\chi} \left(p_{\text{bimin}} + p_{\text{bienh}} \frac{\mathcal{S}_{\text{birr}}}{\mathcal{S}_{\text{birr}} + h_{\text{birr}}} \right), \tag{210}$$

where $\stackrel{\text{DEPO}}{q}_{\text{birr}}$ and $\stackrel{\text{MEIO}}{q}_{\text{birr}}$ are the fractions of deposit feeder and meiobenthos uptake contributing to bioirrigation, h_{birr} is a half-saturation rate for bioirrigation enhancement and p_{bienh} is the maximum bioturbation enhancement factor of dissolved inorganic diffusion in the benthos.

4.9 Bioturbation

For particulate matter in the benthos sediment diffusion $\nu_{\rm bturb}$ in Eq. (154) is based on a background diffusivity ϑ_{part} and an enhancement factor of Michaelis-Menten type depending on the bioturbation caused by deposit feeder activity (see Eq. 173):

$$S_{\text{bturb}} = \frac{\mathsf{DEPO}}{q} \frac{\partial Y_{\mathbb{C}}}{\partial t} \bigg|_{\text{upt}}$$
(211)

$$\nu_{\text{bturb}} = \vartheta_{\text{part}} \left(1 + p_{\text{btenh}} \frac{\mathcal{S}_{\text{bturb}}}{\mathcal{S}_{\text{bturb}} + h_{\text{bturb}}} \right),$$
(212)

where $\overset{\text{DEPO}}{q}_{\text{bturb}}$ is the fraction of deposit feeder uptake contributing to bioturbation, h_{bturb} is a half-saturation rate for bioturbation enhancement and p_{btenh} is the maximum bioturbation enhancement factor of particulate matter diffusion in the benthos.

5 Horizontal interfaces

5.1 The benthic-pelagic interface

The boundary condition at the seabed is given by the deposition of sinking particulate organic material, phytoplankton and calcite on the seafloor, the diffusion of inorganic chemical components between the pore water and the pelagic water column and resuspension of organic matter. All other state variables generally have no flux conditions at the pelagicbenthic interface.

5.1.1 Deposition of organic matter and phytoplankton

Deposition fluxes are taken analogous to the gravitational sinking rates in Eq. (139) where the sinking velocity is replaced by the deposition velocity $\stackrel{\text{dep}}{w_{c_p}}$ according to the seabed shear stress τ_{bed} :

$$\frac{\substack{\text{depo}\\w_{c_{p}}}}{w_{c_{p}}} = \max\left(1 - \frac{\tau_{\text{bed}}}{\tau_{\text{crit}}}, 0\right) \stackrel{\text{sed}}{w_{c_{p}}},$$

$$\frac{\substack{\text{c}_{p}\\w_{\text{depo}}}}{w_{\text{depo}}} = \max\left(1 - \frac{\tau_{\text{bed}}}{\tau_{\text{crit}}}, 0\right) \stackrel{c_{p}}{w_{\text{sed}}},$$

leading to the deposition fluxes

$$\mathcal{F}|_{c_{\mathsf{p}}}^{\mathsf{ben}} = \overset{\mathsf{depo}}{w_{c_{\mathsf{p}}}} c'_{\mathsf{p}} \,.$$

$$\mathcal{F}|_{c_{\mathsf{p}}}^{\mathsf{ben}} = \overset{c_{\mathsf{p}}}{w_{\mathsf{depo}}} c'_{\mathsf{p}} \,. \tag{2}$$

As for gravitational sinking the only state variables sedimenting onto the seafloor are particulate organic matter, the phytoplankton components and calcite $(\stackrel{\Psi}{M}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S}},\stackrel{\chi}{P}_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{F},\mathbb{S},\mathcal{C}},$ 102

(213)

214)

 $_{L\mathbb{C}}^{\rm calc}$). The absorption of deposited carbon, nitrogen and phosphorus components into the sediments then results in separation of the organic material into dissolved, slowly degradable and refractory matter according to

$$\mathcal{F}|_{\mathsf{pel}}^{\frac{\mathsf{stow degr}}{Q_{\mathbb{C}}^{\circ}}} = \left(1 - \overset{\chi}{q}_{\mathsf{ddepo}} - \overset{\chi}{q}_{\mathsf{rdepo}}\right) \sum_{\chi} \mathcal{F}|_{P_{\mathbb{C}}}^{\mathsf{ben}} + \overset{\mathsf{part}}{q}_{\mathsf{rdepo}} \sum_{\chi} \mathcal{F}|_{R_{\mathbb{C}}}^{\mathsf{ben}}$$
(215)

$$\begin{split} \mathcal{F}|_{\text{pel}}^{\text{refr}} &= \overset{\chi}{q}_{\text{rdepo}} \sum_{\chi} \mathcal{F} \bigg|_{P_{\mathbb{C}}}^{\text{ben}} + \overset{\text{part}}{q}_{\text{rdepo}} \sum_{\chi} \mathcal{F} \bigg|_{R_{\mathbb{C}}}^{\text{ben}} \\ \mathcal{F}|_{\text{pel}}^{\text{dis}} &= \overset{\chi}{q}_{\text{ddepo}} \sum_{\chi} \mathcal{F} \bigg|_{P_{\mathbb{C}}}^{\text{ben}}, \end{split}$$
(216) (217)

where $\overset{\chi}{q}_{\text{ddepo}}$ and $\overset{\chi}{q}_{\text{rdepo}}$ are the dissolved and refractory fractions of deposing material. For nitrogen and phosphorus the portioning is modified according to the relative cytoplasm $\text{nutrient contents } \stackrel{\text{lab}}{p} _{\text{cyto}_{\mathbb{N},\mathbb{P}}}, \stackrel{\text{part}}{p} _{\text{cyto}_{\mathbb{N},\mathbb{P}}}:$

$$\mathcal{F}|_{\mathsf{pel}}^{\overset{\mathsf{slow degr}}{Q}} = \sum_{\chi} \left(1 - \overset{\chi}{q}_{\mathsf{ddepo}} \overset{\mathsf{lab}}{p}_{\mathsf{cyto}_{\mathbb{N},\mathbb{P}}} - \overset{\chi}{q}_{\mathsf{rdepo}} \overset{\mathsf{part}}{p}_{\mathsf{cyto}_{\mathbb{N},\mathbb{P}}} \right) \mathcal{F}|_{\chi}^{\mathsf{ben}}$$
(218)

$$+\sum_{\psi} \left(1 - \stackrel{\text{part}}{q}_{\text{rdepo}}\right) \mathcal{F}|_{\substack{\psi \\ R_{\mathbb{N},\mathbb{P}}}}^{\text{ben}}$$
(219)

$$\mathcal{F}|_{\mathsf{pel}}^{\mathsf{refr}} = \sum_{\chi} \begin{array}{c} \chi \\ q_{\mathsf{rdepo}} \end{array} \stackrel{\mathsf{part}}{p} \begin{array}{c} \mathsf{part} \\ p_{\mathsf{cyto}_{\mathbb{N},\mathbb{P}}} \end{array} \mathcal{F}|_{\mathcal{P}_{\mathbb{N},\mathbb{P}}}^{\mathsf{ben}} + \sum_{\psi} \begin{array}{c} p_{\mathsf{rdepo}} \\ q_{\mathsf{rdepo}} \end{array} \mathcal{F}|_{\psi}^{\mathsf{ben}} \\ R_{\mathbb{N},\mathbb{P}} \end{array}$$
(220)

$$\mathcal{F}|_{\mathsf{pel}}^{\mathsf{ols}} = \sum_{\chi} \begin{array}{c} \chi \\ q_{\mathsf{ddepo}} \end{array} \begin{array}{c} \mathsf{lab} \\ p_{\mathsf{cyto}_{\mathbb{N},\mathbb{P}}} \end{array} \mathcal{F}|_{P_{\mathbb{N},\mathbb{P}}}^{\mathsf{ben}} \end{array} .$$
(221)

The iron and silicate components and phosphorus are entirely directed to slowly degradable matter, the only state considered for these components in the benthic model:

$$\mathcal{F}|_{\mathsf{pel}}^{\mathsf{slow degr}} = \sum_{\chi} \mathcal{F}|_{R_{\mathbb{F}}}^{\mathsf{ben}} + \mathcal{F}|_{R_{\mathbb{F}}}^{\mathsf{ben}} + \mathcal{F}|_{R_{\mathbb{F}}}^{\mathsf{ben}}$$
(222)

$$\mathcal{F}|_{\mathsf{pel}}^{Q_{\mathbb{S}}} = \mathcal{F}|_{\substack{\mathsf{dia}\\P_{\mathbb{S}}}}^{\mathsf{ben}} + \mathcal{F}|_{\substack{\mathsf{med}\\R_{\mathbb{S}}}}^{\mathsf{ben}} + \mathcal{F}|_{\substack{\mathsf{large}\\R_{\mathbb{S}}}}^{\mathsf{ben}}$$
(223)

Calcite deposition is given by

$$\mathcal{F}|_{\substack{C_{\mathbb{C}}\\calc}}^{calc} = \underset{L_{\mathbb{C}}}{\overset{depo}{w_{calc}}} \underset{L_{\mathbb{C}}}{\overset{calc}{u_{\mathbb{C}}}} L_{\mathbb{C}}^{calc}$$
(224)

5.1.2 Resuspension

In the case of strong shear stress τ_{bed} at the seafloor part of the sediments may get resuspended into the water column. The erosion flux is calculated proportional to the excess

shear stress over a critical threshold $\tau_{\rm crit}$ by a reference erosion flux $r_{\rm er}$. Erosion in terms of particulate organic matter is then approximated as a fraction of the total sediment matter $p_Q^{\rm sed} + Q_{\mathbb{C}}^{\rm slow degr}$:

The values and approximations used for the three parameters $\tau_{\rm crit}$, $r_{\rm er}$ and $\overset{\rm sed}{p_Q}$ are given in the Supplement.

5.1.3 Inorganic fluxes across the seabed

The diffusion of dissolved inorganic states across the benthos is derived from the equilibrium conditions described in Sect. 4.2. Based on the tendency of the system towards the equilibrium the total flux across the sea-bed is then given by the sum of all sources and sinks and a relaxation towards equilibrium.

$$- \left. \frac{\chi}{\mathcal{F}} \right|_{\text{ben}}^{\text{pel}} = \left. \frac{\partial \chi}{\partial t} \right|_{\text{bgc}} + \frac{1}{\frac{\chi}{\tau_{\text{eq}}}} \left(\chi - p_{\text{poro}} p_{\text{Cads}} \tilde{\chi}_{\text{pw}} \right),$$
(227)

where χ represents the inorganic states of oxygen, DIC, oxidised nitrogen, ammonium, phosphate and silicate.

For phosphorus, ammonium, silicate and DIC the excess is distributed in parabolic form relaxtion fluxes towards equilibrium are computed by assuming a parabolic vertical distribution of excess biomass with 0 surface concentrations concentration and 0 bottom

(228)

flux, so that the relaxation time scale τ_{eq}^{χ} towards equilibrium conditions is given by the parabolic slope at the surface. and assuming contributions to the generation of the excess proportional to the layer depth. The compensation flux across the seabed is then again computed from the production-diffusion balance in Eq. 141. For oxidised nitrogen and oxygen the procedure requires modification for two reasons: the separation depths of the oxygenated layer and denitrification layer given by the dissolved oxygen horizon and the horizon of oxidised nitrogen may be considered as fixed parameters for the diffusion-production balance of the other state variables, but not so for dissolved oxygen and oxidised nitrogen whose biogeochemical changes affect the dynamics of these horizons directly. In addition, the system imposes a third boundary condition on the balance equation, i.e. that the concentration at the respective horizon has to be zero by definition (and no sources and sinks exist below these limits), which renders the system overdetermined. For these two variables the relaxation time scale is therefore approximated by the fixed parameters τ_{ox} and τ_{denit} also used to determine the dynamical evolution of oxygen and oxidised nitrogen horizon in Eqs. (144) and (145).

The recycling of iron in the benthos is abbreviated, as there is very little information on the iron cycle in the sea-bed. The only form of iron considered in the benthos is the slowly degradable matter, which is implicitly remineralised and returned to the water column in dissolved form at a fixed remineralisation rate $\overset{\chi}{r_{\text{remin}}}$:

$$\left. \begin{array}{c} {}^{\mathrm{remin}} \\ \mathcal{F}_{\mathbb{F}} \end{array} \right|_{Q_{\mathbb{F}}}^{N_{\mathbb{F}}} = r_{\mathrm{remin}\mathbb{F}} \ \begin{array}{c} \chi \\ Q'_{\mathbb{F}} \end{array}$$

5.1.4 Remineralistion of calcite

No processes related to the formation or dissolution of calcite in the benthos are currently included in the model, the benthic cylce cycle of calcite is resolved purely implicitly similar to iron as simple linear release to the water column of the calcite deposited onto the

(229)

sediments: calc

$$\left. \begin{array}{c} \operatorname{remin}_{\mathcal{F}_{\text{calc}}} \right|_{C_{\mathbb{C}}}^{L_{\mathbb{C}}} = \begin{array}{c} \operatorname{calc}_{r} & \operatorname{calc}_{\mathbb{C}} \\ \operatorname{calc}_{C_{\mathbb{C}}} & \operatorname{calc}_{r} \end{array} \right. \\ \end{array}$$

5.1.5 Benthic remineralisation sub-model

As an alternative to the full benthic model described in the Sect. 4, a simple benthic closure is available, that implicitly remineralises benthic substrate into dissolved inorganic states, analogous to the treatment of iron and calcite above. The treatment of deposition and resuspension of organic matter on the sea floor in this case is identical to the full benthic model, while the recycling of organic matter occurs as a linear function of the benthic content at a given remineralisation rate r_{remin}^{χ} :

$$\mathcal{F}_{\mathbb{C},\mathbb{P},\mathbb{S}} \Big|_{\substack{\chi \\ Q_{\mathbb{C},\mathbb{P},\mathbb{S}}}}^{G_{\mathbb{C}},N_{\mathbb{P}},N_{\mathbb{S}}} = \stackrel{\chi}{r_{\mathsf{remin}}} \stackrel{\chi}{Q'}_{\mathbb{C},\mathbb{P},\mathbb{S}}$$

$$(230)$$

For nitrogen the remineralisition flux is split regenerating oxidised nitrogen and ammonium using the fixed fraction $\overset{\chi}{q}_{\text{remin}}$:

$$\mathcal{F}_{\mathbb{N}}^{\mathsf{remin}} \Big|_{\substack{\chi \\ Q_{\mathbb{N}}}}^{\stackrel{\mathsf{ox}}{\mathsf{N}}} = \stackrel{\mathsf{ox}}{q}_{\mathsf{remin}} \stackrel{\chi}{r}_{\mathsf{remin}} \stackrel{\chi}{Q'_{\mathbb{N}}}$$
(231)

$$\mathcal{F}_{\mathbb{N}}^{\mathsf{remin}} \Big|_{\substack{\chi \\ Q_{\mathbb{N}}}}^{N_{\mathbb{N}}} = \left(1 - \stackrel{\mathsf{ox}}{q_{\mathsf{remin}}}\right) \stackrel{\chi}{r_{\mathsf{remin}}} \stackrel{\chi}{Q'_{\mathbb{N}}}$$
(232)

With this option no other biogeochemical processes are considered in the benthos. The treament of iron and calcite is identical in between the full benthic model and this simplified benthic closure.

(233)

(234)

5.2 Sea surface fluxes

The only two boundary fluxes computed in the standard set-up at the air-sea interface are the exchange of oxygen and carbon dioxide. Other processes like atmospheric deposition of nutrients and riverine inputs require spatially varying surface fields and are best provided thourgh through the physical driver. (Implementations of this type have been used in Artioli et al., 2012; Edwards et al., 2012; Holt et al., 2012; Wakelin et al., 2012.)

Oxygen is exchanged based on the difference from the saturation state

 $\mathcal{F}_{\mathbb{O}}|_{\mathsf{sea}}^{\mathsf{air}} = k_{\mathsf{air}\mathbb{O}}\left(\mathsf{T},\mathsf{S},\boldsymbol{u}_{\mathsf{wind}}\right)(G_{\mathbb{O}}-s_{\mathbb{O}})$

while the, which is estimated according to Weiss (1970):

 $\mathcal{F}_{\mathbb{O}}|_{sea}^{air} = k_{air\mathbb{O}}(\mathsf{T},\mathsf{S},\boldsymbol{u}_{wind})(O_{\mathbb{O}}-s_{\mathbb{O}})$.

The regression formula for $s_{\mathbb{Q}}$ is given in the Supplement.

The exchange of carbon dioxide is based on the difference in partial pressures

$$\mathcal{F}_{\mathbb{C}}|_{\text{sea}}^{\text{air}} = \rho_{\text{sea}} k_{\text{air}\mathbb{C}} (\mathsf{T}, \boldsymbol{u}_{\text{wind}}) \left(p_{\text{CO}_2} - \stackrel{\text{air}}{p}_{\text{CO}_2} \right),$$

where $p_{CO_2}^{air}$

$$\mathcal{F}_{\mathbb{C}}|_{\text{sea}}^{\text{air}} = \rho_{\text{sea}} k_{\text{air}\mathbb{C}} \left(\mathsf{T}, \boldsymbol{u}_{\text{wind}}\right) \left(\mathsf{p}_{\text{CO}_2} - \overset{\text{air}}{\mathsf{p}}_{\text{CO}_2}\right)$$

where $p_{CO_2}^{air}$ maybe be provided by the physical driver or a constant parameter $\frac{air}{p_{CO_2}}$ The empirical gas transfer coefficients $k_{air\mathbb{O}}$ and $k_{air\mathbb{C}}$ are taken from Weiss (1970); Nightingale et al. (2000) and given in the Supplement.

Generic terms 6

Regulation and limitation factors 6.1

The regulation of metabolic processes by temperature is modelled using the Q_{10} function introduced in Blackford et al. (2004) that strongly increases at low temperatures and decreases slower at high temperatures representing eznyme enzyme degradation:

$$l_{\rm T}^{\chi} = p_{Q_{10}}^{\chi} \frac{T_{\rm I}^{\circ} c_{\rm I} - 10^{\circ} c}{10^{\circ} c} - p_{Q_{10}}^{\chi} \frac{T_{\rm I}^{\circ} c_{\rm I} - 32^{\circ} c}{3^{\circ} c},$$
(235)

where T [°C] is the water temperature in degrees Celsius and χ represents the respective process or state.

Nitrogen and phosphorus limitation factors for each of the four phytoplankton types are based on Droop-kinetics (Droop, 1974) and computed as:

where χ represents any phytoplankton type (dia, micro, nano, pico), $\overset{\chi}{q}_{ref_{\mathbb{N},\mathbb{P},\mathbb{C}}}$ is its reference internal quota and $\overset{\chi}{q}_{\min_{\mathbb{N},\mathbb{P}:\mathbb{C}}}$ is its minimal internal quota. These two factors are combined to three alternative forms of co-limitation $\overset{\chi}{l}_{\langle \mathbb{NP} \rangle}$

$$\overset{\chi}{l}_{\langle \mathbb{NP} \rangle} = f \begin{pmatrix} \chi & \chi \\ l_{\mathbb{N}}, l_{\mathbb{P}} \end{pmatrix},$$
(238)

switchable through the namelist switch LimnutX:

Limnut X=0: $\overset{\chi}{l}_{\langle \mathbb{NP} \rangle}$ is the geometric mean of $\overset{\chi}{l}_{\mathbb{N}}$ and $\overset{\chi}{l}_{\mathbb{P}}$,

 $\textbf{LimnutX}{=}\,2\textbf{:}\;\stackrel{\chi}{l}_{\langle\mathbb{NP}\rangle}\text{ is the harmonic mean of }\stackrel{\chi}{l}_{\mathbb{N}}\text{ and }\stackrel{\chi}{l}_{\mathbb{P}},$

Limnut X = 1: $\overset{\chi}{l}_{(\mathbb{NP})}$ is the minimum of $\overset{\chi}{l}_{\mathbb{N}}$ and $\overset{\chi}{l}_{\mathbb{P}}$.

The silicate limitation factor for diatoms is computed from the external availability of disdia solved silicate $N_{\mathbb{S}}$, based on a Michaelis–Menten term with half-saturation $h_{\mathbb{S}}^{\text{dia}}$:

$$l_{\mathbb{S}}^{\text{dia}} = \frac{N_{\mathbb{S}}}{N_{\mathbb{S}} + h_{\mathbb{S}}}$$
(239)

The iron limitation factor is computed in the same way as the factors for nitrogen and phosphorus:

$$\overset{\chi}{l}_{\mathbb{F}} = \min\left(1, \max\left(0, \frac{\overset{\chi}{q}_{\mathbb{F}:\mathbb{C}} - \overset{\chi}{q}_{\min_{\mathbb{F}:\mathbb{C}}}}{\underset{q_{\mathsf{ref}_{\mathbb{F}:\mathbb{C}}} - \overset{\chi}{q}_{\min_{\mathbb{F}:\mathbb{C}}}}{}\right)\right),$$
(240)

with $\overset{\chi}{q}_{\mathsf{ref}_{\mathbb{F}:\mathbb{C}}}$ as its reference internal quota and $\overset{\chi}{q}_{\mathsf{min}_{\mathbb{F}:\mathbb{C}}}$ as its minimal internal quota. Phosphorus and nitrogen limitation $\overset{B}{l}_{\mathbb{P}}$, $\overset{B}{l}_{\mathbb{N}}$ for the standard model of bacteria mediated decomposition can be based on the availability of the resource in dissolved inorganic form

(ISWBlimX = 1) and substrate or only in inorganic form (ISWBlimX = 2):

$${}^{B}_{l_{\mathbb{P}}} = \begin{cases} \min\left(\frac{N_{\mathbb{P}}}{B}, \frac{dis}{R_{\mathbb{P}}}\right) & \text{if } \text{ISWBlimX} = 1\\ \frac{dis}{dis} & R_{\mathbb{P}} + h_{\mathbb{P}} \\ \frac{N_{\mathbb{P}} + R_{\mathbb{P}}}{dis} & \text{if } \text{ISWBlimX} = 2\\ N_{\mathbb{P}} + R_{\mathbb{P}} + h_{\mathbb{P}} & \text{if } \text{ISWBlimX} = 2 \end{cases}$$

$$(241)$$

and analogous:

$$B_{\mathbb{N}} = \begin{cases} \min\left(\frac{\operatorname{amm}}{N_{\mathbb{N}}}, \frac{\operatorname{dis}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{dis}}, \frac{B_{\mathbb{N}}}{\operatorname{N}_{\mathbb{N}} + R_{\mathbb{N}}} + h_{\mathbb{N}}} & \text{if } \text{ISWBlim} \mathbb{X} = 2 \end{cases}$$

$$(242)$$

where $h_{\mathbb{P},\mathbb{N}}^B$ are the Michaelis–Menten half–saturation constants for phosphorus and nitrogen limitation.

Nutrient regulation of benthic bacteria occurs based on the nutritional state of the substrate

$$\begin{split} \chi \\ l_{\mathbb{N}}^{\chi} = \min \begin{pmatrix} \left. \frac{s_{\mathsf{low}} \deg r}{Q'_{\mathbb{N}}} \right|_{d_{\mathsf{low}}}^{d_{\mathsf{low}}} \\ 1, \frac{1}{Q'_{\mathbb{N}}} \left|_{d_{\mathsf{low}}}^{\chi} \right|_{d_{\mathsf{low}}}^{d_{\mathsf{low}}} \end{pmatrix} \min \begin{pmatrix} \left. \frac{s_{\mathsf{low}} \deg r}{Q'_{\mathbb{P}}} \right|_{d_{\mathsf{low}}}^{d_{\mathsf{low}}} \\ 1, \frac{1}{Q'_{\mathbb{P}}} \left|_{d_{\mathsf{low}}}^{\chi} \right|_{d_{\mathsf{low}}}^{\chi} \\ q_{\mathsf{ref}_{\mathbb{P}:\mathbb{C}}} \left. Q'_{\mathbb{P}} \right|_{d_{\mathsf{low}}}^{d_{\mathsf{low}}} \end{pmatrix} . \end{split}$$
(243)

where χ are aerobic and anaerobic bacteria within the layers described in Sect. 4.4.

Oxygen limitation of zooplankton (χ : HET, MICRO, MESO) is computed as function of the relative oxygen saturation state

$$s_{\mathsf{rel}\mathbb{O}} = \min\left(1, \frac{G_{\mathbb{O}}}{s_{\mathbb{O}}}\right)$$

$$\sum_{l=1}^{\chi} \frac{s_{\mathsf{rel}\mathbb{O}} + s_{\mathsf{rel}\mathbb{O}}}{h_{\mathbb{O}}} \frac{h_{\mathbb{O}}}{h_{\mathbb{O}}},$$
(244)
(245)

$$s_{\mathsf{rel}\mathbb{O}} + \hat{h_{\mathbb{O}}}$$

where the oxygen saturation concentration $s_{\mathbb{O}}$ is estimated according to Weiss (1970). (The regression formula used is given in the Supplement).

For zoobenthos (χ : DEPO, SUSP, MEIO) it is given by a cubic Michaelis–Menten response to the oxygen concentration in the overlying water body in relation to a minimum oxygen threshold $\overset{\chi}{p}_{\mathbb{O}\mathrm{min}}$ for each species:

$$\overset{\chi}{l_{\mathbb{O}}} = \left(\frac{\max\left(G_{\mathbb{O}}-\overset{\chi}{p_{\mathbb{O}\mathsf{min}}},0\right)}{\max\left(G_{\mathbb{O}}-\overset{\chi}{p_{\mathbb{O}\mathsf{min}}},0\right)+\overset{\chi}{h_{\mathbb{O}}}}\right)^{3}.$$

$$\overset{\chi}{l_{\mathbb{O}}} = \frac{\max\left(G_{\mathbb{O}} - \overset{\chi}{p_{\mathbb{O}}\mathsf{min}}, \mathbf{0}\right)^3}{\max\left(G_{\mathbb{O}} - \overset{\chi}{p_{\mathbb{O}}\mathsf{min}}, \mathbf{0}\right)^3 + \overset{\chi}{h_{\mathbb{O}}}^3}.$$

For pelagic bacteria it is given by a simple Michaelis–Menten term of the relative oxygen saturation state (Eq. 244)

$$l_{\mathbb{D}}^{B} = \frac{s_{\mathsf{rel}\mathbb{D}}}{s_{\mathsf{rel}\mathbb{D}} + h_{\mathbb{D}}}.$$
(247)

For benthic bacteria oxygen regulation occurs through the oxygen and oxidised nitrogen horizons

where d_{ref}^{oxy} is the aerobic half saturation depth and d_{ref}^{denit} the anaerobic oxidised half saturation depth for oxygen regulation.

(246)

 $l_{\mathbb{O}}^{\rm nitr}$ is the oxygen limitation factor for nitrification:

$$l_{\mathbb{D}}^{\text{nitr}} = \frac{O_{\mathbb{D}}^{3}}{O_{\mathbb{D}}^{3} + h_{\mathbb{D}}}$$
(249)

with $h_{\mathbb{O}}$ being the cubic half-saturation constant for oxygen limitation of nitrification, $_{\rm nitr}$

 $l_{\mathbb{N}}$ is the substrate limitation factor for nitrification:

$$_{N}^{\text{nitr}} = \frac{\frac{\text{amm}^{3}}{N_{N}}}{\frac{\text{amm}^{3} \quad \text{nitr}}{N_{N}} + h_{N}}$$
(250)

with $h_{\mathbb{N}\text{nitr}}$ being the cubic half-saturation constant for substrate limitation of nitrification and l_{pH} is the pH-limitation factor for nitrification:

$$l_{pH} = \min(2, \max(0, 0.6111pH - 3.8889)).$$
 (251)

Benthic nitrification is inhibited at high benthic content of oxidised nitrogen according to

$$\overline{k_{N}^{ox}} = \frac{k_{N}^{ox}}{\frac{h_{N}}{D + \frac{D-D}{3}}}$$
(252)
$$\frac{h_{N}^{bnitr}}{l_{N}} = \frac{h_{N}}{\frac{h_{N}}{\frac{h_{N}}{N + K_{N}}}},$$
(253)

bnitr

where $h_{\mathbb{N}}$ is the oxygenated layer concentration of oxidised nitrogen at which nitrifation nitrification is inhibited by 50%.

Here, it is assumed that some oxidised nitrogen penetrates into the denitrification layer, so that the oxygenated layer concentration is on average three times higher compared to the denitrification layer.

Based on the same assumption, denitrification in the oxidised layer uses a Michaelis-Menten response to the assumed layer content of oxidised nitrogen

$$\overline{denitr}_{K_{\mathbb{N}}} = \frac{1}{3} \frac{K_{\mathbb{N}}'}{D + \frac{D - D}{3}}$$

$$\frac{denitr}{l_{\mathbb{N}}} = \frac{\overline{K_{\mathbb{N}}}}{\frac{denitr}{K_{\mathbb{N}}} + h_{\mathbb{N}}},$$
(254)
(255)

denitr

where $h_{\mathbb{N}}$ is a denitrification half saturation constant.

Calcification and dissolution of calcite occur in relation to the calcite saturation state of the water $\Omega_{calc} \ge 0.\Omega_{calc} \ge 1$ (Eq. 128). The regulating factor of the rain ratio for calcification and the regulation factor for dissolution of calcite can be calculated in two alternative ways chosen by the ISWCAL = 1 namelist switch. The first option (ISWCAL = 1) is based on an exponential term:

${}^{ ext{calc}}_{l\mathbb{C}}= ext{max}ig(0,ig(\Omega_{ ext{calc}}-1ig)^{n_{ ext{calc}}}ig)$	(256)
$\stackrel{ ext{dis}}{l_{\mathbb{C}}} = \max ig(0, ig(1 - \Omega_{ ext{calc}} ig)^{n_{ ext{dis}}} ig) ,$	(257)

where $n_{\text{calc.dis}}$ are calcification/dissolution exponents (Ridgwell et al., 2007; Keir, 1980).

The second option (ISWCAL = 2) uses a Michaelis–Menten term:

$$\begin{split} l_{\mathbb{C}}^{\text{calc}} &= \max\left(0, \frac{\Omega_{\text{calc}} - 1}{\Omega_{\text{calc}} - 1 + h_{\text{calc}}}\right) \end{split} \tag{258}$$
$$l_{\mathbb{C}}^{\text{dis}} &= \max\left(0, \frac{1 - \Omega_{\text{calc}}}{1 - \Omega_{\text{calc}} + h_{\text{calc}}}\right) \end{aligned} \tag{259}$$

where h_{calc} is the half-saturation constant for calcification and dissolution of calcite (Blackford et al., 2010; Gehlen et al., 2007).

The rain ratio (Eq. 91) is regulated by nutrient limitation and temperature to reflect the dependency of the calcifying fraction of nanophytoplankton on the environmental conditions. Temperature regulation is given by

$$l_{\mathsf{T}}^{\mathsf{calc}} = \frac{\max(0,\mathsf{T}[^{\circ}\mathsf{C}])}{\max(0,\mathsf{T}[^{\circ}\mathsf{C}]) + h_{T}},$$
(260)

where the half-saturation constant is set to $\stackrel{\text{calc}}{h_T} = 2 \,^{\circ}\text{C}$. As coccolithophores are reported to have generally higher phosphorus affinity but lower nitrogen acquisition capacity with respect to other phytoplankton (Riegman et al., 2000; Paasche, 1998), limitation of these nutrients has an opposed impact on the rain ratio. This is reflected in our combined nutrient limitation factor for calcification which is obtained from the phosphorus and nitrogen

(262)

(263)

limitation of nanophytoplankton (Eqs. 237 and 236) as

$$l_{\langle \mathbb{NP} \rangle}^{\text{calc}} = \min \left(1 - \frac{l_{\mathbb{P}}}{l_{\mathbb{P}}}, l_{\mathbb{N}} \right).$$
(261)

Uptake limitation of suspension and deposit feeders by overcrowding is given by a nested Michaelis-Menten response to the respective biomass:

$$\overset{\chi}{p_{\text{crowd}}} = \begin{pmatrix} \overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p_{\mathbb{C}}} \end{pmatrix} \frac{\overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p_{\text{crowd}}}}{\overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p_{\text{crowd}}} + \overset{\chi}{h_{\text{sat}}}}$$

$$\begin{split} \overset{\chi}{p}_{\text{crowd}} &= \max\left(0, \overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p}_{\mathbb{C}}\right) \frac{\overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p}_{\mathbb{C}}}{\overset{\chi}{Y_{\mathbb{C}}} - \overset{\chi}{p}_{\mathbb{C}} + \overset{\chi}{h}_{\text{sat}}} \end{split}$$

$$\overset{\chi}{l}_{ ext{crowd}} = 1 - rac{\overset{\chi}{p}_{ ext{crowd}}}{\overset{\chi}{p}_{ ext{crowd}} + \overset{\chi}{h}_{ ext{crowd}}} \, .$$

6.2 Stoichiometric adjustments

For states $\overset{\chi}{\varphi}$ with fixed stoichiometric quota $q_{\mathbb{N},\mathbb{P}:\mathbb{C}}^{\chi}$ (mesozooplankton, benthic bacteria and predators) the processes process rates are complemented by exudation release fluxes that regulate imbalances with respect to the in order to preserve the fixed reference quotas as

Discussion Paper Discussion Paper

(266)

follows:

$$\frac{\partial \widehat{\varphi}_{\mathbb{C}}^{\chi}}{\partial t}\Big|_{\substack{\text{exu rel}\\ \overline{\partial t}}} = \max\left(\frac{\widetilde{\partial \varphi_{\mathbb{C}}}}{\partial t}\Big|_{\substack{\text{bgc}}} - \frac{1}{q_{\mathbb{P}:\mathbb{C}}^{\chi}} \frac{\widetilde{\partial \varphi_{\mathbb{P}}}}{\partial t}\Big|_{\substack{\text{bgc}}}, \frac{\widetilde{\partial \varphi_{\mathbb{C}}}}{\partial t}\Big|_{\substack{\text{bgc}}} - \frac{1}{q_{\mathbb{N}:\mathbb{C}}^{\chi}} \frac{\widetilde{\partial \varphi_{\mathbb{N}}}}{\partial t}\Big|_{\substack{\text{bgc}}}, 0\right), \quad (264)$$

$$\frac{\partial \widehat{\varphi}_{\mathbb{N},\mathbb{P}}}{\partial t}\Big|_{\substack{\text{exu rel}\\ \overline{\partial t}}} = \max\left(\frac{\widetilde{\partial \varphi_{\mathbb{N},\mathbb{P}}}}{\partial t}\Big|_{\substack{\text{net}}} - q_{\mathbb{N},\mathbb{P}:\mathbb{C}}^{\chi} \frac{\widetilde{\partial \varphi_{\mathbb{C}}}}{\partial t}\Big|_{\substack{\text{bgc}}}\right) \quad (265)$$

are the comprehensive biogeochemical process rates prior to adjustments

net

$$\left. \frac{\partial \overset{\chi}{\varphi}}{\partial t} \right|_{\rm bgc} = \left. \frac{\partial \overset{\chi}{\varphi}}{\partial t} \right|_{\rm net} - \left. \frac{\partial \overset{\chi}{\varphi}}{\partial t} \right|_{\rm exturned}$$

Implementations 7

exu rel

Most ecosystem models are tightly bound to a specific physical, hydrodynamic driver that is usually three-dimensional and consequently computationally heavy and cumbersome to test and implement. The ERSEM model comes as an independent library and can in principle be coupled to any physical driver with comparatively little effort. In fact, coupled configurations exist for a variety of drivers in one or three-dimensional settings amongst which are the NEMO ocean engine (Madec, 2008), the POLCOMS model for shelf seas (Holt and James, 2001), and the GOTM/GETM model (Burchard et al., 2006). While for realistic implementations a full-scale three-dimensional configuration is required, for the stages of process development and qualitative analysis of the functioning of the modelled ecosystem, zero- or one-dimensional frameworks are often beneficial as they provide a light-weight implementation that is easier to grasp, much faster to run, amenable to sensitivity analysis and quicker to analyse.

The model distribution itself includes drivers for two idealised systems: the first is a simple zero dimensional implementation of mesocosm type called the ERSEM-Aquarium with a pelagic box overlying a benthic box, each of them with internally homogeneous conditions. This is essentially a test environment for new users and fast process assessment requiring no external software for the ocean physics. The second is a driver for the vertical one-dimensional GOTM model (http://www.gotm.net - Burchard et al., 2006). It is a more realistic system allowing for full vertical structures in a comparatively lightweight software environment that is capable of running in serial mode on any standard desktop or laptop. It requires a copy of the GOTM code with minor modifications to accommodate ERSEM, which can be obtained for the stable release or the development release of GOTM (see Sect. 10). Here, we use the 0-D framework to illustrate the carbon fluxes through the model food-web food web under contrasting environmental conditions (Sect. 7.1) and the 1-D implementation to demonstrate the model capacity to reflect the lower trophic level of the marine ecosystem under varying conditions at three different sites, underpinned by a brief validation against in situ time-series data (Sect. 7.2).

Beyond these simpler test cases, the ERSEM model has been implemented in various full-scale three dimensional applications from coastal to global scales, cited above. The descriptions of these configurations would exceed the scope and volume of this paper and are given in the respective publications, but for completeness we give a short example of a simulation based on a previously published configuration in order to illustrate the full potential of the model (Sect. 7.3).

All simulations presented in this section were performed using the same parametrisation, which is given in the Supplement. This parametrisation was developed using size as the main trait to scale the metabolic rates of the pelagic functional groups more widely than in previous parametrisations (Baretta-Bekker et al., 1997; Blackford et al., 2004) and respects the conventional restriction of the food matrix suggested in Eq. (32). A table with all parameter values, their mathematical symbols as used in Sect. 2 to 6 and the corresponding name in the model code and namelists is given in the Supplement.

ERSEM-Aquarium 7.1

The simulation of mesocosm type environments is supported through the ERSEM-Aquarium model. The model simulates two 0-D boxes, a pelagic box, which is characterised by its mid-depth below the surface and by the geographical location, and a benthic box beneath it. Seasonal variations in temperature and salinity can be imposed as cosine functions between an extreme value at the first of January in the beginning of the simulation and a second extreme after half a year. The light field can be imposed in the same way as cosine oscillation between two prescribed extreme values, or extracted from the prescribed geographical position using standard astronomical formula ignoring cloud cover. Additionally diurnal oscillations of temperature and light can be superimposed in cosine form by prescribing a daily excursion between midday and midnight. It should be noted that this framework is not designed to deliver realistic simulations of the marine environment in a particular location, but rather to aid the development and quick evaluation of process studies, or to study the model system behaviour in a simplified context without additional complicating factors.

Figure 6 illustrates the carbon fluxes between model compartments for two different simulations using the ERSEM-Aquarium. The first is configured as a representation of tropical oligotrophic conditions characterised by deep and warm waters with high irradiance and low nutrients, while the second roughly corresponds to the shallow coastal eutrophic waters of the Southern North Sea with strong nutrient supply and comparatively low light. Both configurations are run for a thousand years in order to achieve full equilibrium between the benthic and pelagic environments. The former uses the simple benthic closure scheme for remineralisation (Sect. 5.1.5), which is more appropriate for deep water configurations where the impact of the benthos is of lesser importance, while the latter uses the full benthic model (Sect. 4). All configuration files necessary to replicate these runs are given in the Supplement. Figure 6 gives flux magnitudes in the modelled food-web food web directly scaled from the annual average of the last year of each simulation. The experiment highlights the substantial quantitative production difference in between the two systems. In

addition, it clearly shows the qualitative shift in the model food-web food web under the contrasting conditions. In the oligotrophic case most of the gross production is excreted to dissolved matter due to strong growth-nutrient limitation. This leads to a microbial-microbe dominated scenario with bacteria as the main food-source for the predators and only small amounts of carbon entering the second trophic level leading to negative community production and low deposition of biomass to the sediments. In the eutrophic case production levels are increased by a level an order of magnitude. The assimilated carbon is used more efficiently by phytoplankton fueling substantial secondary production with autotrophs as the main food source of zooplankton and significantly more biomass exported to the sediments resulting in positive community production.

7.2 GotmErsem – a model Framework for the water column

The GotmErsem framework provides the possibility to include a more realistic physical environment into the simulations with opposing gradients of nutrient supply from depth and short-wave radiation attenuated as it penetrates through the water column. The GOTM model is a one-dimensional water column model including a variety of turbulence closure schemes for vertical mixing (Burchard et al., 2006). Here, we show three implementations using this framework in contrasting environments to demonstrate the portability of the ERSEM model, one for the Oyster Grounds in the Southern North Sea, a typical shelf sea site; one at the L4 site in the Western English Channel representative of a midlatitude site with mixed waters of both oceanic and coastal origin; and one in the oligotrophic sub-tropics at the Bermuda Atlantic Time-series Study site. Each of these sites is supported by extensive in situ data sets for model evaluation. Full configuration files to run these simulations are provided in the Supplement. The validation against in situ data was performed by sub-sampling the daily averaged model output for each in situ data sample. It is presented in target diagrams (Jolliff et al., 2009) for each site showing statistically robust metrics (e.g. Daszykowski et al., 2007) to account for the underlying non-Gaussian asymmetric data distributions and in order to avoid spurious overweighting of outliers. The metrics provided are the median bias (median $(M_i - D_i)$; M_i : model sample, D_i data sample) on the ordinate and the unbiased median absolute error (MAE', median [$abs(M_i - D_i - median(M_i - D_i))$]) on the abscissa. Both are normalised with the inter-quartile range (IQR) for the scale of the in situ data and the Spearman or rank correlation is represented by the colour code for each data set. The sign on the abscissa is given by the relation of IQRs (sign (IQR $(M_i) - IQR(D_i))$).

All three sites are forced with data from the ERA-interim reanalysis (Dee et al., 2011) at the atmospheric boundary condition. The L4 and Oyster Ground configurations use surface pressure data to introduce tidal mixing into the idealised one-dimensional set-ups. The BATS and L4 site were additionally relaxed towards temperature and salinity profiles from CTD measurements (BATS - Steinberg et al., 2001, L4 - Harris, 2010) in order to compensate for the missing hydrodynamic impacts of lateral advection and diffusion. Initial conditions for the sites were derived from the concurrent in situ data where available. As for the ERSEM-Aquarium simulations the benthic remineralisation closure was used for the deep, oligotrophic BATS site, while for the shallow eutrophic sites L4 and Oyster Grounds the full benthic model was used.

Oyster Grounds – (54°24'36" N, 4°1'12" E) 7.2.1

This site is located in the Southern North Sea and is influenced by the English Channel and surrounding coastal waters, with seasonal stratification in most summers and an accentuated spring bloom at the onset of stratification that depletes the nutrients from the comparatively stable and isolated water surface layer (Baretta-Bekker et al., 2008).

A comparison with smart buoy data for the years 2000-2009 (Greenwood et al., 2010) reveals a good representation of the local seasonal cycle (Fig. 7). Simulations do not show significant bias in any of the variables, while the MAE' is significantly lower than the in situ data variability (≈ 0.75 of the IQR of the in situ data for chlorophyll $a_1 \approx 0.25$ silicate and phosphate and virtually 0 for oxidised nitrogen). Correlations are high for the nutrients (> 0.6), but comparatively low for chlorophyll a (> 0.2). The lower skill for the latter is partly caused by a weaker secondary bloom in summer in the simulations compared to the observations and comparatively low observational coverage over the first years of the simulation leading to potential overstressing of singular events in the data sampling and giving a spurious picture of the seasonal cycle when compared to the more consistently covered last three years of the period shown. In addition, some deficiencies, in the model simulations are to be expected as the Oyster Ground site is characterised by strong lateral influences including estuarine, coastal and channel waters that include strong direct impacts on the nutrient concentrations in the area that can not be captured in this idealised setting. Particularly in the stratified season in summer these lateral effects are dominating the surface water signal while the deeper part of the depression is essentially isolated from the surface layer (Weston et al., 2008).

7.2.2 L4 – Western English Channel (50°15' N, 4°13' W)

The L4 site is a long-term monitoring station near the Northern coast of the Western English Channel. Similar to the Oyster Grounds site, it is seasonally stratified and generally nutrient depleted in summer, but highly affected by episodic events of freshwater inputs of riverine origin (Smyth et al., 2010).

Figure 8 shows the seasonal cycles of oxidised nitrogen, phosphate and chlorophyll a at the sea surface for the model simulations and for the in situ data (Smyth et al., 2010 - http://www.westernchannelobservatory.org.uk/) for the years 2007-2011. The model follows the seasonal cycle of nutrient depletion in summer and nutrient resupply in winter revealed by the data in all three nutrients shown. Also the results for chlorophyll a follow the bulk seasonality represented by the in situ data, but show deficiencies in capturing the episodic peaks, which appear misplaced with respect to the measurements. Possible reasons for these short-comings include the absence of physical and biogeochemical impacts of lateral processes in such an idealised 1-dimensional setting as well as a sub-optimal representation of the local phytoplankton community by the parametrisation adopted consistently across the contrasting environments. Nevertheless, the model skill expressed in the overall statistics is considerable. The bias and MAE' for all 4 variables falls fall well below the variability of the in situ data. Chlorophyll a shows a relative bias of about 0.25 and

a relative unbiased error of little less than 0.5, while the three nutrients show an error and bias very close to 0.

7.2.3 BATS – Bermuda, Sargasso Sea (31°40' N, 64°10' W)

This site in the Sargasso Sea is characterised by a weak geostrophic flow with net downwelling. Strong stratification separates the nutrient-poor surface waters from the nutrientrich deep water, with the exception of the passing of cold fronts in winter which cause substantial convective mixing with accompanying nutrient entrainment (Steinberg et al., 2001). This is illustrated in the left panel of Fig. 9, which shows the seasonal cycle of chlorophyll a from model simulations (on top) and in situ data. The mixing events triggering autotrophic growth initially spread over the upper part of the water column, but they are limited to a rather marked deep-chlorophyll a maximum at around 100 m depth when stratification sets in. Interannul variability at the site is dominated by the varying strength of the sub-tropical storm events in spring that cause strong vertical mixing which can reach up to 200m depth resulting in variable levels of nutrient entrainment, largely captured by the model. A summary of the validation against the extensive in situ data available at BATS (Bermuda Time Series Study - Steinberg et al., 2001) for the years 1990-2008 is given in the target diagram on the right of Fig. 9. In contrast to the two shallow sites, in situ data in this case is vertically resolved, which was respected in the matching procedure.

Bias and MAE' for all variables do not exceed the variability of the in situ data. Both metrics are very close to zero for the nitrate, phosphate and chlorophyll a and in general most metrics stay below 50% of the in situ variability with the exception of the bias for oxygen and the MAE' for phosphate. The latter are caused by an underestimated aeriation of the water column and a weaker vertical gradient in phosphate for the model (not shown). However, some weakness weaknesses in the simulation of the vertical distributions are to be expected given the absence of explicit lateral dynamics and the resulting vertical flows. Correlations lie between 0.4 and 0.6 reflecting the overall satisfactory model performance.

7.2.4 Properties emerging from simulations at all three sites

In order to give an impression of the functioning of the ecosystem dynamics across the three sites, Fig. 10 shows a comparison between some ecosystem properties emerging from data meta-analysis and model simulations, namely the internal stoichiometric quotas of nutrients with respect to carbon in phytoplankton and the phytoplankton community structure. On the left of Fig. 10 we show the range of the internal stoichiometric quotas of nitrogen, phosphorus, silicate and iron with respect to carbon on the abscissa plotted against the average guotas for phytoplankton on the ordinate as an indicator of the modelled phytoplankton plasticity in response to nutrient limitation. Quotas from the simulations (circles) are compared to the results of a meta-analysis (diamonds) provided by Moore et al. (2013) based on observed internal stoichiometric phytoplankton quotas from scientific literature. Results for the three macronutrients are consistent in that the average quotas are well matched while the stoichiometric range is underestimated by approximately half an order of magnitude. This is to be expected given that the case studies included in the model simulations don't cover the full range of natural variability of marine environments. Results for iron show substantial differences in range and average state. The mismatch in average state can be attributed to the fact that the present parametrisation of the iron cycle took into consideration the works of Timmermans et al. (2005) and Veldhuis et al. (2005), which reported comparatively low iron to carbon quotas, but weren't considered in the above meta-analysis, while the huge discrepancy in range is caused by the absence of substantial iron limitation in the sites of the case studies.

The right hand side panel of Fig. 10 shows the size fractionated contribution of each phytoplankton group to total chlorophyll a across the three sites as a running average over the ordered model samples from all three sites collectively. The procedure is analogous to the meta-analysis provided by Hirata et al. (2011). The results show a domination of the phytoplankton community by picophytoplankton at low chlorophyll a and by large phytoplankton at high chlorophyll a. Nanophytoplankton is present throughout the chlorophyll a range, reaching a maximum at intermediate values. The emerging modelled community structure

compares well to the meta-analysis (compare Fig. 2a-c therein) particularly considering the limited range of marine environments considered in this exercise.

7.3 A full scale implementation for the North-West European Shelf

The previous case studies demonstrate the capability of the model to represent the marine ecosystem with a focus on small scale ecosystem processes. Nevertheless, the full potential of the model unfolds in full-scale applications of coupled dynamical systems linked to hydrodynamic models capturing the full advection and diffusion of the biogeochemical states and thus providing a complete synoptic picture of the large scale biogeochemical cycles and the marine environment. A full description of these systems would exceed the scope of this particular paper. Nevertheless, we give here a brief overview of the model performance on a simulation of the North-West European Shelf Seas using the POLCOMS model for shelf sea circulation (Holt and James, 2001), based on a hindcast configuration identical to the one used and described in Holt et al. (2012) and Artioli et al. (2012), but using the most recent model version presented in this work and the same parametrisation as in the above examples.

The left hand side panel of Fig. 11 shows the mean optical-depth-averaged chlorophyll a field of the area to illustrate the model domain as used in the validation exercise, and also to give an idea of the ecosystem characteristics of the area. Model simulations were validated against in situ data for oxidised nitrogen, phosphorus, chlorophyll a, oxygen and salinity retrieved from the ICES data base (ICES, 2009) for the period of 1970-2004 using the same metrics as above, summarised in a target diagram on the right of Fig. 11. Results are consistent with the validation results of the 1-D sites with both bias and MAE' generally less than 50 % of the in situ variability, and correlations > 0.4 for all variables confirming the good performance of the model dynamics in a realistic large-scale simulation.

Development and testing framework 8

In addition to the 0- and 1-D ERSEM implementations a framework is provided with the model that allows developers and users of the code to analyse and plot the result of calls to individual ERSEM procedures from Python. This facility is supported through Fortran-C interoperability, that arrived with the Fortran 2003 standard (ISO/IEC 1539-1:2004(E)), and the Python Ctypes package. The ERSEM test harnesses consist of the ERSEM library and a set of C wrappers, which are jointly compiled as a shared library. A Python interface to the shared library permits access to Fortran data structures and procedures from Python. This allows developers and users of the code to quickly interrogate the validity and behaviour of individual procedures, without first reimplementing them in a second language, and without running the full model. Here we illustrate this feature by examining the photosynthesis model implemented in ERSEM.

The photosynthesis model used in ERSEM is based on Geider et al. (1997), and is described in Sect. 3.1. In the case of diatoms, the carbon specific rate of photosynthesis, $\tilde{\mathcal{S}}_{gpp}$ (d⁻¹), is a function of temperature, T (°C); PAR, E_{PAR} (Wm); the external silicate concentration, N_S (mmol Si m); and the dynamic cellular chlorophyll a to carbon ratio, $q_{C:C}^{\chi}$ (mg Chl a mg C⁻¹), as given by Eq. (5). The other primary producer groups use the same photosynthesis model, but without silicate limitation. The sensitivity of the maximum, light-saturated carbon specific photosynthesis rate $\frac{\chi}{q}(T)$ to temperature is modelled by a Q_{10} function (Eq. 235), empirically adapted to mimic enzyme inhibition at high temperatures. The reference temperature, T_0 , is set at 10 °C. The model assumes that the light saturated rate of photosynthesis is proportional to the organic carbon content of the cell, while the rate of photosynthesis under light limitation is assumed to be proportional to the product of the chlorophyll a to carbon ratio and PAR (Geider et al., 1997). In the model model, photosynthetic cells are able to regulate the their chlorophyll a to carbon ratio in response to changes in irradiance, temperature and silicate (in the case of diatoms) by modifying the proportion of photosynthate that is directed towards chlorophyll biosynthesis

 $(\stackrel{\chi}{\rho};$ see Eq. 10). Balanced growth is achieved when cells are fully acclimated, in which case:

$$\frac{\mathsf{d}}{\mathsf{d}t} \begin{pmatrix} \frac{\chi}{P_{\mathcal{C}}} \\ P_{\mathbb{C}} \end{pmatrix} = 0 \tag{267}$$

Chlorophyll a biosynthesis is assumed to be up-regulated in response to a reduction in irradiance and down regulated in response to an increase in irradiance. Through this process, cells are able to balance the rate of energy supply through light absorption, and energy demands for growth. The maximum, light saturated photosynthesis rate $g^{\chi}(T)$ is assumed to be independent of changes in irradiance, which is consistent with observations which indicate Rubisco content is relatively invariant with respect to changes in irradiance (Sukenik et al., 1987), and the hypothesis that these cells are adapted to survive and reproduce in dynamic light environments (Talmy et al., 2014).

Using the ERSEM testing framework, model it is possible to investigate this process in isolation. Model cells can be artificially acclimated to a given set of environmental conditions by finding a value for $q_{C:\mathbb{C}}^{\chi}$ which satisfies Eq. (267). Figure 12 shows a plot of $q_{C:\mathbb{C}}^{\chi}$ vs. I_{PAR} for fully photo-acclimated diatoms in ERSEM. Cells were acclimated to a given irradiance by holding cellular carbon fixed and varying the cellular chlorophyll a content within the range $q_{\min_{\mathcal{C}:\mathbb{C}}} \leq q \leq q_{\varphi\max}^{\chi}$ in order to achieve balanced growth. Overlaid are observations Using the testing framework, the model can be compared with observations in order to sanity check the validity of the implementation, or parameterised against observations using curve fitting procedures. In Fig. 12, observations for the diatom T. Pseudonana have been overlaid. No attempt was made to fit the curve to this particular set of observations, although the fit appears reasonable. The parameter set is the same as used in the simulations of Sect. 7 and is given in the Supplement.

Diatoms are a physiologically and morphologically diverse group, which are characterised by their requirement for silicate, which they use to construct their cell wall. It is perhaps unsurprising that model fits to photosynthesis-irradiance curves for different diatom species result in a range of parameter values, including differences in the maximum light saturated carbon specific photosynthesis rate as a function of temperature, and the initial slope of the photosynthesis-irradiance curve (e.g. Geider et al., 1997). Ultimately, many of these differences arise due to differences in organism morphology and physiology, with, for example, different pigment complements complements or levels of investment in biosynthesis, being reflected in derived parameter values. These within group variations pose a perennial problem to the development of marine ecosystem and biogeochemical models. The diatom group in ERSEM is designed to be representative of diatoms as a whole, and to reflect the important biogeochemical role these organisms perform in nature.

ERSEM includes four phytoplankton functional groups: diatoms, which are characterised by their requirement for silicate, and three further groups which are characterised according to their size. These are the pico-, nano-, and microphytoplankton. The choice to characterise groups according to their size reflects the importance of size as a physiological trait (Litchman et al., 2007, 2010), which influences an organism's competitive ability through its effect on nutrient acquisition, carbon and nutrient storage, the intracellular transport of solutes, photosynthesis rates through pigment packaging effects, and susceptibility to predation (e.g. Chisholm, 1992; Finkel et al., 2010).

Using ERSEM's testing framework it is possible to demonstrate how this classification impacts the competitive ability of the four photosynthetic groups represented in the model. Figure 13 shows photosynthesis-irradiance curves for ERSEM's four phytoplankton groups under the condition of balanced growth. As with the diatoms, the use of a single parameter set for each size-based group ignores within group variations that are observed in nature. It is important to take such abstractions into consideration when interpreting model outputs.

This example illustrates how ERSEM's testing framework can be used to study and check the implementation of different processes within the code. Importantly, this is achieved without having to rewrite sections of the code in a second language with visualisation capabilities, which is an inherently error prone procedure. This capability is designed to compliment complement the 0-D and 1-D drivers that simulate more complex time-varying environments, in which it is often difficult to study processes in isolation.
9 Optional Choices

In the following section we provide an overview of the main optional choices in the model configuration. Options that involve major structural changes which alter the number of state variables or add substantial functionality are activated by preprocessor definitions, that need to be included at compile time. These include:

- The model of bacterial decomposition.
- The inclusion of the iron cycle.
- The light attenuation model.
- The calcification model.

Other options can be triggered at run-time via namelist parameters in the files include/ersem_pelagic_switches.nml and include/ersem_benthic_switches.nml without the need for a recompilation of the model code. These include the choice for the alkalinity description of the model and the choice of the benthic model.

9.1 The iron cycle

The use of the iron cycle in the model including growth limitation of phytoplankton by iron is activated by the preprocessor key IRON. It involves additional state variables for dissolved inorganic iron and iron components of the four phytoplankton types, two particulate matter types in the pelagic and one particulate matter type in the benthos.

9.2 Calcification

The use of the calcification sub-module (Sect. 3.6) is activated by the preprocessor key CALC. It's computational impact is limited adding a single pelagic and a single benthic state to the list of state variables.

9.3 The model of bacterial decomposition

Two options are included for the modelling of the decomposition of organic matter (see Sect. 3.3.1). By default, the bacteria sub-model presented in Allen et al. (2002) with a basic microbial food-web and implicit decomposition is used. Enabling the preprocessing key DOCDYN the model for dynamic decomposition of organic matter is activated which uses fully explicit recycling of organic matter and includes the recalcitrant fraction of the DOC pool at the cost of an additional state variable.

9.4 The light attenuation model

Two options for light attenuation are available. The default choice is the legacy model based on apparent optical properties in the form of specific attenuation coefficients, while the recently developed model using inherent optical properties in the from of specific adsoprtion and backscatter coefficients and zenith angle needs to be activated by the IOPMODEL preprocessor key (see Sect. 3.9). The computational effort of the two models is comparable, but the latter involves the computation of the zenith angle and therefore requires the geographical coordinates and the current simulation date and time from the physical driver.

9.5 Alkalinity

The description of alkalinity in the model is given by the combination of two switches. The prognostic mode using an ocean tracer modified by biogeochemical processes affecting alkalinity is activated by setting ISWbioalk in include/ersem_pelagic_switches.nml to 1. The diagnostic mode deriving alkalinity from salinity (and optionally temperature) is enabled by activating an adequate alkalinity regression by setting ISWtalk to a value between 1 and 3. (The different regression options are specified in the Supplement.) The recommended use for these modes is a combination of both modes or the purely progostic option with ISWbioalk = 1and ISWtalk=0 (see Sect. 3.8).

9.6 The benthic model

The full benthic model (Sect. 4) is activated by setting the ibenXin parameter in include/ersem_benthic_switches.nml to 2, while for ibenXin = 1 (see Sect. 5.1.5) the benthic closure scheme is used. While the latter involves considerably less state variables and computations, the computational impact of this choice is largely neglegible in 1D and 3D simulations as the computational cost is dominated by the advection and diffusion of the pelagic states.

Technical Specifications and Code Availability 10

The ERSEM 15.06 model is written in FORTRAN using the 2008 standard. Output is entirely based on ${\tt netCDF}$ and the output parsing scripts generating I/O ${\tt FORTRAN}$ code from plain text lists of variables are written in python.

The model is distributed under the open-source GNU Lesser General Public License through a gitlab server and freely available upon registration through the web-portal www.shelfseasmodelling.org. There are no restrictions or conditions for the registration of individual users, the registration is merely implemented in order to keep track of the user base. The code repository is fully version controlled (using git) and features a bug tracking system open to users. The release code of this publication is available in the master branch of the repository as tag ERSEM-15.06. The GOTM version used in the simulations of this work is also taged tagged as "ERSEM-15.06" on the ERSEM enabled fork of the development version of GOTM which can be downloaded from the same repository server. A quick start guide and user's reference manual are also provided along with the code.

The versioning convention used with this software refers to the year and month of the release.

11 Conclusions

In this paper we have provided a full mathematical description of an updated version of ERSEM, one of the most established marine ecosystem models currently in use in the scientific community and in operational systems. Case studies ranging from a mesocosm type zero-dimensional experiment through three one-dimensional water column implementations to a brief three-dimensional full-scale example have illustrated the model dynamics in varying environments.

Qualitative and quantitative validation with in situ data for the basic ecosystem state variables chlorophyll a and the macronutrients has demonstrated the capability of the model to represent ecosystems ranging from oligotrophic open oceans to eutrophic coastal conditions. An integral validation of each single component would exceed the scope of this paper, the main purpose of which is the detailed description of the model ingredients as a reference for scientists, developers and users. Nevertheless, examples of component validations have been published previously and are available in literature (Artioli et al., 2012; Allen and Somerfield, 2009; Allen et al., 2007; de Mora et al., 2013). In addition the testing framework supplied within the model distribution allows for targeted analysis and validation of individual parts of the model down to the level of single equations directly without rewriting or extracting the model code. We have demonstrated this capability here on the example of the PI-curve for phytoplankton growth.

The ERSEM 15.06 model is to our knowledge the only model currently available that provides the structure for simulating in one coherent system the biogeochemical cycles of carbon, the major macronutrients and iron (using variable stochiometric relationships), the carbonate system and calcification, the microbial food web food web and the benthic biogeochemistry.

While the range of processes included in the model brings the advantage of suitability for a whole range of applications as different as process studies, regional or global budgets of different chemical elements, habitat maps or risk assessment of environmental hazard, it also points to one of the major drawbacks of the model, i.e. a comparatively heavy structure

and high number of parameters, that render it difficult to access for new users and hard to calibrate and parametrise. These problems are being addressed in a fully modular version of the model with streamlined process descriptions that is currently under development. It will allow for an arbitrary number of functional groups and easy replacment of individual submodels, which can be tuned to the specific application at run-time. These developments will be made available with the next release of the model.

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References

Aksnes, D. L. and Egge, J. K.: A theoretical model for nutrient uptake in phytoplankton, Mar. Ecol.-Prog. Ser., 70, 65-72, doi:10.3354/meps070065, 1991.

- Allen, J., Somerfield, P., and Gilbert, F.: Quantifying uncertainty in high-resolution coupled hydrodynamic-ecosystem models, in: Contributions from Advances in Marine Ecosystem Modelling Research, 27-29 June, 2005, Plymouth, UK AMEMR, 64, 3-14, available at: http://www. sciencedirect.com/science/article/pii/S0924796306001035 (last access: 14 August 2015), 2007.
- Allen, J. I.: Simulating the spring phytoplankton bloom in the Humber Plume (UK) with a variable phytoplankton carbon: chlorophyll-a model, in: Elsevier Oceanography Series, edited by: Fiemming, N., Vallerga, S., Pinardi, N., Behrens, H., Manzella, G., Prandle, D., and Stei, J., vol.Somerfield, 66 of Opertional Oceanography Implementation at the European and Regional Scales Proceedings of the second international Conference on EuroGOOS, 11-13 March 1999, Rome, Italy, 497-504, Elsevier, Amsterdam, available at:(last access: 13 August 2015)P. J., and Siddonr, J.: Primary and bacterial production in the Mediterranean Sea: a modelling study, J. Marine Syst., system in the North Sea: sensitivity and model validation, J. Marine Syst., 33-34, 473-495, doi:10.1016/S0924-7963(02)00072-6, 2002.
- Allen, J. I. and Somerfield, P. J.: A multivariate approach to model skill assessment, J. Marine Syst., 76, 83-94, doi:10.1016/j.jmarsys.2008.05.009, 2009.
- Allen, J. I., Blackford, J. C., Holt, J., Proctor, R., Ashworth, M., and Siddorn, J.: A highly spatially resolved ecosystem model for the North West European Continental Shelf, Sarsia, 86, 423-440, 2001.
- Anderson, T. R., Hessen, D. O., Mitra, A., Mayor, D. J., and Yool, A.: Sensitivity of secondary production and export flux to choice of trophic transfer formulation, J. Marine Syst., 125, 41-53, doi:10.1016/j.jmarsys.2012.09.008, 2013.

- Artioli, Y., Blackford, J. C., Butenschön, M., Holt, J. T., Wakelin, S. L., Thomas, H., Borges, A. V., and Allen, J. I.: The carbonate system in the North Sea: sensitivity and model validation, J. Marine Syst., 102–104, 1–13, doi:10.1016/j.jmarsys.2012.04.006, 2012.
- Artioli, Y., Blackford, J. C., Nondal, G., Bellerby, R. G. J., Wakelin, S. L., Holt, J.T., Butenschön, M., and Allen, J. I.: Heterogeneity of impacts of high CO₂ on the North Western European Shelf, Biogeosciences Discuss., 10, 9389-9413, doi:10.5194/bgd-10-9389-2013, 2013.
- Artioli, Y., Blackford, J. C., Nondal, G., Bellerby, R. G. J., Wakelin, S. L., Holt, J. T., Butenschön, M., and Allen, J. I.: Heterogeneity of impacts of high CO₂ on the North Western European Shelf, Biogeosciences, 11, 601-612, doi:10.5194/bg-11-601-2014, 2014.
- Aumont, O., Maier-Reimer, E., Blain, S., and Monfray, P.: An ecosystem model of the global ocean including Fe, Si, P colimitations, Global Biogeochem. Cy., 17, 1–23, doi:10.1029/2001GB001745, 2003.
- Barange, M., Merino, G., Blanchard, J. L., Scholtens, J., Harle, J., Allison, E. H., Allen, J. I., Holt, J., and Jennings, S.: Impacts of climate change on marine ecosystem production in societies dependent on fisheries, Nature Climate Change, 4, 211–216, doi:10.1038/nclimate2119, 2014.
- Baretta, J., Ruardij, P., Billings, W. D., Golley, F., Lange, O. L., Olson, J. S., and Remmert, H. (Eds.): Tidal Flat Estuaries, vol. 71 of Ecological Studies, Springer Berlin Heidelberg, Berlin, Heidelberg, Germany, available at: http://link.springer.com/10.1007/978-3-642-73753-4 (last access: 14 August 2015), 1988.

Baretta, J. W.: Preface, J. Sea Res., 38, 169–171, doi:10.1016/S1385-1101(97)00054-3, 1997.

- Baretta, J. W., Ebenhöh, W., and Ruardij, P.: The European regional seas ecosystem model, a complex marine ecosystem model, Neth. J. Sea Res., 33, 233-246, doi:10.1016/0077-7579(95)90047-0, 1995.
- Baretta-Bekker, H., Bot, P., Prins, T., and Zevenboom, W.: Report on the second application of the OSPAR Comprehensive Procedure to the Dutch marine waters, Tech. rep., OSPAR Comission, London, 2008.
- Baretta-Bekker, J. G.: Note of the editor, Neth. J. Sea Res., 33, 230-231, doi:10.1016/0077-7579(95)90046-2, 1995.
- Baretta-Bekker, J. G., Baretta, J. W., and Rasmussen, E. K.: The microbial food web in the European Regional Seas Ecosystem Model, Neth. J. Sea Res., 33, 363–379, 1995.
- Baretta-Bekker, J. G., Baretta, J. W., and Ebenhöh, W.: Microbial dynamics in the marine ecosystem model ERSEM II with decoupled carbon assimilation and nutrient uptake, J. Sea Res., 38, 195-211, doi:10.1016/S1385-1101(97)00052-X, 1997.

- Bellerby, R. G. J., Olsen, A., Furevik, T., and Anderson, L. G.: Response of the surface ocean CO₂ system in the Nordic Seas and northern North Atlantic to climate change, in: The Nordic Seas: An Integrated Perspective, edited by: Drange, H., Dokken, T., Furevik, T., Gerdes, R., and Berger, W., 189–197, American Geophysical Union, Washington, DC, USA, doi:10.1029/158GM13, 2005.
- Blackford, J., Artioli, Y., Kelly-Gerreyn, B., Martin, A., Tyrrell, T., and Somavilla, R.: Sub-model acidification-sensitive calcification rate, including user guide, Project Report, Plymouth Marine Laboratory, Plymouth, UK, D2.2, EC FP7 MEECE - 212085, 2010.
- Blackford, J. C.: An analysis of benthic biological dynamics in a North Sea ecosystem model, J. Sea Res., 38, 213-230, doi:10.1016/S1385-1101(97)00044-0, 1997.
- Blackford, J. C. and Burkill, P. H.: Planktonic community structure and carbon cycling in the Arabian Sea as a result of monsoonal forcing: the application of a generic model, J. Marine Syst., 36, 239-267, doi:10.1016/S0924-7963(02)00182-3, 2002.
- Blackford, J. C. and Gilbert, F. J.: pH variability and CO(2) induced acidification in the North Sea, Symposium on Advances in Marine Ecosystem Modelling Research, Plymouth, England, 27-29 June 2005, J. Marine Syst., 64, 229–241, doi:10.1016/j.jmarsys.2006.03.016, 2007.
- Blackford, J. C., Allen, J. I., and Gilbert, F. J.: Ecosystem dynamics at six contrasting sites: a generic modelling study, J. Marine Syst., 52, 191-215, 2004.
- Bopp, L., Resplandy, L., Orr, J. C., Doney, S. C., Dunne, J. P., Gehlen, M., Halloran, P., Heinze, C., Ilyina, T., Séférian, R., Tjiputra, J., and Vichi, M.: Multiple stressors of ocean ecosystems in the 21st century: projections with CMIP5 models, Biogeosciences, 10, 6225-6245, doi:10.5194/bg-10-6225-2013, 2013.
- Borges, A. V. and Frankignoulle, M.: Daily and seasonal variations of the partial pressure of CO₂ in surface seawater along Belgian and southern Dutch coastal areas, J. Marine Syst., 19, 251–266, doi:10.1016/S0924-7963(98)00093-1, 1999.

Broecker, W. S. and Peng, T. H.: Tracers in the sea, Eldigio Press, New York, USA, 1982.

- Brzezinski, M. A.: The Si:C:N ratio of marine diatoms: interspecific variability and the effect of some environmental variables, J. Phycol., 36, 87-96, doi:10.1111/j.0022-3646.1985.00347.x, 1985.
- Broekhuizen, N., Heath, M. R., Hay, S. J., and Gurney, W. S. C.: Modelling the dynamics of the North Sea's Mesozooplankton, Neth. J. Sea Res., 33, 381-406, doi:10.1016/0077-7579(95)90054-3, 1995.
- Burchard, H., Deleersnijder, E., and Meister, A.,: A high-order conservative Patankar-type discretisation for stiff systems of production-destruction equations, Appl. Numer. Math., 47, 1-30, doi:10.1016/S0168-9274(03)00101-6, 2003.
 - 137

- Burchard, H., Bolding, K., Kühn, K., Meister, A., Neumann, T., and Umlauf, L.: Description of a flexible and extendable physical-biogeochemical model system for the water column, J. Marine Syst., 61, 180-211, 2006.
- Butenschön, M., Zavatarelli, M., and Vichi, M.: Sensitivity of a marine coupled physical biogeochemical model to time resolution, integration scheme and time splitting method, Ocean Model., 52–53, 36-53, doi:10.1016/j.ocemod.2012.04.008, 2012.
- Chesson, J.: The estimation and analysis of preference and its relatioship to foraging models, Ecology, 64, 1297-1304, doi:10.2307/1937838, 1983.
- Chisholm, S.: Phytoplankton size, in: Primary Productivity and Biogeochemical Cycles in the Sea, edited by: Falkowski, P. and Woodhead, A., 213-237, Plenum Press, New York, 1992.
- Chust, G., Allen, J. I., Bopp, L., Schrum, C., Holt, J., Tsiaras, K., Zavatarelli, M., Chifflet, M., Cannaby, H., Dadou, I., Daewel, U., Wakelin, S. L., Machu, E., Pushpadas, D., Butenschon, M., Artioli, Y., Petihakis, G., Smith, C., Garaçon, V., Goubanova, K., Le Vu, B., Fach, B. A., Salihoglu, B., Clementi, E., and Irigoien, X.: Biomass changes and trophic amplification of plankton in a warmer ocean, Glob. Change Biol., 20, 2124-2139, doi:10.1111/gcb.12562, 2014.
- Daszykowski, M., Kaczmarek, K., Heyden, Y. V., and Walczak, B.: Robust statistics in data analysis - a review: basic concepts, Chemometr. Intell. Lab., 85, 203-219, doi:10.1016/j.chemolab.2006.06.016, 2007.
- de Mora, L., Butenschön, M., and Allen, J. I.: How should sparse marine in situ measurements be compared to a continuous model: an example, Geosci. Model Dev., 6, 533-548, doi:10.5194/gmd-6-533-2013, 2013.
- Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Hólm, E. V., Isaksen, L., Kållberg, P., Köhler, M., Matricardi, M., McNally, A. P., Monge-Sanz, B. M., Morcrette, J.-J., Park, B.-K., Peubey, C., de Rosnay, P., Tavolato, C., Thépaut, J.-N., and Vitart, F.: The ERA-Interim reanalysis: configuration and performance of the data assimilation system, Q. J. Roy. Meteor. Soc., 137, 553-597, doi:10.1002/qj.828, 2011.
- Dickson, A., Sabine, C., and Christian, G.: Guide to Best Practices for Ocean CO₂ Measurements, PICES Special Publication 3, PICES, Sidney, British Columbia, available at: http://cdiac.ornl.gov/ ftp/oceans/Handbook 2007/Guide all in one.pdf (last access: 14 August 2015), 2007.
- Dickson, A. G.: Thermodynamics of the dissociation of boric acid in synthetic seawater from 273.15 to 318.15 K, Deep-Sea Res., 37, 755–766, doi:10.1016/0198-0149(90)90004-F, 1990.

- Doney, S. C., Ruckelshaus, M., Emmett Duffy, J., Barry, J. P., Chan, F., English, C. A., Galindo, H. M., Grebmeier, J. M., Hollowed, A. B., Knowlton, N., Polovina, J., Rabalais, N. N., Sydeman, W. J., and Talley, L. D.: Climate change impacts on marine ecosystems, Annual Review of Marine Science, 4, 11-37, doi:10.1146/annurev-marine-041911-111611, 2012.
- Droop, M. R.: The nutrient status of alga cells in continous culture, J. Mar. Biol. Assoc. U.K., 54, 825-855, doi:10.1016/0924-7963(94)00031-6, 1974.
- Dugdale, R. C., Wilkerson, F. P., and Minas, H. J.: The role of a silicate pump in driving new production, Deep-Sea Res. Pt. I, 42, 697-719, doi:10.1016/0967-0637(95)00015-X, 1995.
- Ebenhöh, W., Kohlmeier, C., and Radford, P. J.: The benthic biological submodel in the European regional seas ecosystem model, Neth. J. Sea Res., 33, 423-452, doi:10.1016/0077-7579(95)90056-X, 1995.
- Edwards, K. P., Barciela, R., and Butenschön, M.: Validation of the NEMO-ERSEM operational ecosystem model for the North West European Continental Shelf, Ocean Sci., 8, 983-1000, doi:10.5194/os-8-983-2012, 2012.
- Falkowski, P. G. and Raven, J. A.: Aquatic photosynthesis, Princeton University Press, Princeton, USA, 2007.
- Fasham, M. J. R., Ducklow, H. W., and McKelvie, S. M.: A nitrogen-based model of plankton dynamics in the oceanic mixed layer, J. Mar. Res., 48, 591-639, 1990.
- Fennel, W.: A model of the yearly cycle of nutrients and plankton in the Baltic Sea, J. Mar. Sys., 6, 313-329, doi:10.1016/0924-7963(94)00031-6, 1995.
- Finkel, Z. V., Beardall, J., Flynn, K. J., Quigg, A., Rees, T. A. V., and Raven, J. A.: Phytoplankton in a changing world: cell size and elemental stoichiometry, J. Plankton Res., 32, 119–137, doi:10.1093/plankt/fbp098, 2010.
- Flynn, K. J.: Ecological modelling in a sea of variable stoichiometry: dysfunctionality and the legacy of Redfield and Monod, Prog. Oceanogr., 84, 52-65, doi:10.1016/j.pocean.2009.09.006, 2010.
- Follows, M. J., Dutkiewicz, S., Grant, S., and Chisholm, S. W.: Emergent biogeography of microbial communities in a model ocean, Science, 315, 1843-1846, doi:10.1126/science.1138544, 2007.
- Franks, P. J., S.: Planktonic ecosystem models: perplexing parameterizations and a failure to fail, J. Plankton Res., 31, 1299-1306, doi:10.1093/plankt/fbp069, 2009.
- Gehlen, M., Gangstø, R., Schneider, B., Bopp, L., Aumont, O., and Ethe, C.: The fate of pelagic CaCO₃ production in a high CO₂ ocean: a model study, Biogeosciences, 4, 505–519, doi:10.5194/bg-4-505-2007, 2007.

- Geider, R. J., MacIntyre, H. L., and Kana, T. M.: A dynamic model of phytoplankton growth and acclimation: responses of the balanced growth rate and chlorophyll a: carbon ratio to light, nutrient limitation and temperature, Mar. Ecol-Prog. Ser., 148, 187–200, doi:10.3354/meps148187, 1997.
- Gentleman, W., Leising, A., Frost, B., Strom, S., and Murray, J.: Functional responses for zooplankton feeding on multiple resources: a review of assumptions and biological dynamics, Deep-Sea Res. Pt. II, 50, 2847-2875, doi:10.1016/j.dsr2.2003.07.001, 2003.
- Gismervik, I.: Implications of zooplankton stoichiometry on distribution of N and P among planktonic size fractions, J. Plankton Res., 19, 343-356, doi:10.1093/plankt/19.3.343, 1997.
- Glibert, P. M., Icarus Allen, J., Artioli, Y., Beusen, A., Bouwman, L., Harle, J., Holmes, R., and Holt, J.: Vulnerability of coastal ecosystems to changes in harmful algal bloom distribution in response to climate change: projections based on model analysis, Glob. Change Biol., 20, 3845-3858, doi:10.1111/gcb.12662, 2014.
- Greenwood, N., Parker, E. R., Fernand, L., Sivyer, D. B., Weston, K., Painting, S. J., Kröger, S., Forster, R. M., Lees, H. E., Mills, D. K., and Laane, R. W. P. M.: Detection of low bottom water oxygen concentrations in the North Sea; implications for monitoring and assessment of ecosystem health, Biogeosciences, 7, 1357–1373, doi:10.5194/bg-7-1357-2010, 2010.
- Hansell, D. A.: Recalcitrant dissolved organic carbon fractions, Annual Review of Marine Science, 5, 421-445, doi:10.1146/annurev-marine-120710-100757, 2013.
- Harris, R.: The L4 time-series: the first 20 years, J. Plankton Res., 32, 577-583, doi:10.1093/plankt/fbg021, 2010.
- Heath, M., Roberston, W., Mardaljevic, J., and Gurney, W. S. G.: Modelling the population dynamics of Calanus in the Fair Isle current of northern Scotland, J. Sea Res., 38, 381-412, doi:10.1016/S1385-1101(97)00047-6, 1997.
- Hirata, T., Hardman-Mountford, N. J., Brewin, R. J. W., Aiken, J., Barlow, R., Suzuki, K., Isada, T., Howell, E., Hashioka, T., Noguchi-Aita, M., and Yamanaka, Y.: Synoptic relationships between surface Chlorophyll-a and diagnostic pigments specific to phytoplankton functional types, Biogeosciences, 8, 311-327, doi:10.5194/bg-8-311-2011, 2011.
- Holt, J., Butenschön, M., Wakelin, S. L., Artioli, Y., and Allen, J. I.: Oceanic controls on the primary production of the northwest European continental shelf: model experiments under recent past conditions and a potential future scenario, Biogeosciences, 9, 97–117, doi:10.5194/bg-9-97-2012, 2012.

- Holt, J. T. and James, I. D.: An s coordinate density evolving model of the northwest European continental shelf: 1. Model description and density structure, J. Geophys. Res.-Oceans, 106, 14015-14034, doi:10.1029/2000JC000304, 2001.
- ICES: ICES Dataset on Ocean Hydrography, The International Council for the Exploration of the SeaCopenhagen, Copenhagen, Denmark, 2009.
- Ingri, N., Kakolowicz, W., Sillén, L. G., and Warnqvist, B.: High-speed computers as a supplement to graphical methods V1: Haltafall, a general program for calculating the composition of equilibrium mixtures, Talanta, 14, 1261–1286, doi:10.1016/0039-9140(67)80203-0, 1967.
- Jassby, A. D. and Platt, T.: Mathematical formulation of relationship between photosynthesis and light for phytoplankton, Limnol. Oceanogr., 21, 540–547, doi:10.4319/lo.1976.21.4.0540, 1976.
- Jiao, N., Herndl, G. J., Hansell, D. A., Benner, R., Kattner, G., Wilhelm, S. W., Kirchman, D. L., Weinbauer, M. G., Luo, T., Chen, F., and Azam, F.: Microbial production of recalcitrant dissolved organic matter: long-term carbon storage in the global ocean, Nat. Rev. Microbiol., 8, 593-599, doi:10.1038/nrmicro2386, 2010.
- Jiao, N., Robinson, C., Azam, F., Thomas, H., Baltar, F., Dang, H., Hardman-Mountford, N. J., Johnson, M., Kirchman, D. L., Koch, B. P., Legendre, L., Li, C., Liu, J., Luo, T., Luo, Y.-W., Mitra, A., Romanou, A., Tang, K., Wang, X., Zhang, C., and Zhang, R.: Mechanisms of microbial carbon sequestration in the ocean - future research directions, Biogeosciences, 11, 5285-5306, doi:10.5194/bg-11-5285-2014, 2014.
- Jolliff, J. K., Kindle, J. C., Shulman, I., Penta, B., Friedrichs, M. A. M., Helber, R., and Arnone, R. A.: Summary diagrams for coupled hydrodynamic-ecosystem model skill assessment, J. Marine Syst., 76, 64-82, doi:10.1016/j.jmarsys.2008.05.014, 2009.
- Keir, R. S.: The dissolution kinetics of biogenic calcium carbonates in seawater, Geochim. Cosmochim. Ac., 44, 241-252, doi:10.1016/0016-7037(80)90135-0, 1980.
- Kleypas, J. A., Buddemeier, R., W., Archer, D., Gattuso, J.-P., Langdon, C., and Opdyke, B., N. : Geochemical consequences of increased atmospheric carbon dioxide on coral reefs, Science, 284, 118-120, doi:10.1126/science.284.5411.118, 1999.
- Kohlmeier, C.: Modellierung des Spiekerooger Rückseitenwatts mit einem gekoppelten Euler-Lagrange-Modell auf der Basis von ERSEM, PhD thesis, Carl von Ossietzky Universität, Oldenburg, 2004.
- Kwiatkowski, L., Yool, A., Allen, J. I., Anderson, T. R., Barciela, R., Buitenhuis, E. T., Butenschön, M., Enright, C., Halloran, P. R., Le Quéré, C., de Mora, L., Racault, M.-F., Sinha, B., Totterdell, I. J., and Cox, P. M.: iMarNet: an ocean biogeochemistry model intercomparison project within a common

physical ocean modelling framework, Biogeosciences, 11, 7291-7304, doi:10.5194/bg-11-7291-2014, 2014.

- Lee, K., Tong, L. T., Millero, F. J., Sabine, C. L., Dickson, A. G., Goyet, C., Park, G.-H., Wanninkhof, R., Feely, R. A., and Key, R. M.: Global relationships of total alkalinity with salinity and temperature in surface waters of the world's oceans, Geophys. Res. Lett., 33, L19605, doi:10.1029/2006GL027207, 2006.
- Lee, Z., Du, K., and Arnone, R.: A model for the diffuse attenuation coefficient of downwelling irradiance, J. Geophys. Res., 110, 1-10, doi:10.1029/2004JC002275, 2005.
- Leeuwen, S. M. v., Molen, J. v. d., Ruardij, P., Fernand, L., and Jickells, T.: Modelling the contribution of deep chlorophyll maxima to annual primary production in the North Sea, Biogeochemistry, 113, 137-152, doi:10.1007/s10533-012-9704-5, 2012.
- Lenhart, H.-J., Mills, D. K., Baretta-Bekker, H., Leeuwen, S. M. v., Molen, J. v. d., Baretta, J. W., Blaas, M., Desmit, X., Kühn, W., Lacroix, G., Los, H. J., Ménesguen, A., Neves, R., Proctor, R., Ruardij, P., Skogen, M. D., Vanhoutte-Brunier, A., Villars, M. T., and Wakelin, S. L.: Predicting the consequences of nutrient reduction on the eutrophication status of the North Sea, J. Marine Syst., 81, 148-170, doi:10.1016/j.jmarsys.2009.12.014, 2010.
- Litchman, E., Klausmeier, C. A., Schofield, O. M., and Falkowski, P. G.: The role of functional traits and trade-offs in structuring phytoplankton communities: scaling from cellular to ecosystem level, Ecol. Lett., 10, 1170–1181, doi:10.1111/j.1461-0248.2007.01117.x, 2007.
- Litchman, E., Pinto, P. d. T., Klausmeier, C. A., Thomas, M. K., and Yoshiyama, K.: Linking traits to species diversity and community structure in phytoplankton, Hydrobiologia, 653, 15-28, doi:10.1007/s10750-010-0341-5, 2010.
- Madec, G.: NEMO Ocean Engine, Note du Pole de modélisation, Institut Pierre-Simon Laplace (IPSL), Paris, France, No 28, 2008.
- Mehrbach, C., Culberson, C. H., Hawley, J. E., and Pytkowicx, R. M.: Measurement of the apparent dissociation constants of carbonic acid in seawater at atmospheric pressure, Limnol. Oceanogr., 18, 897-907, doi:10.4319/lo.1973.18.6.0897, 1973.
- Millero, F. J.: Thermodynamics of the carbon dioxide system in the oceans, Geochim. Cosmochim. Ac., 59, 661-677, doi:10.1016/0016-7037(94)00354-O, 1995.
- Millero, F. J., Lee, K., and Roche, M.: Distribution of alkalinity in the surface waters of the major oceans, Mar. Chem., 60, 111-130, doi:10.1016/S0304-4203(97)00084-4, 1998.
- Moore, C. M., Mills, M. M., Arrigo, K. R., Berman-Frank, I., Bopp, L., Boyd, P. W., Galbraith, E. D., Geider, R. J., Guieu, C., Jaccard, S. L., Jickells, T. D., La Roche, J., Lenton, T. M., Mahowald, N. M.,

Maranon, E., Marinov, I., Moore, J. K., Nakatsuka, T., Oschlies, A., Saito, M. A., Thingstad, T. F., Tsuda, A., and Ulloa, O.: Processes and patterns of oceanic nutrient limitation, Nat. Geosci., 6, 701-710, doi:10.1038/ngeo1765, 2013.

- Nightingale, P. D., Malin, G., Law, C. S., Watson, A. J., Liss, P. S., Liddicoat, M. I., Boutin, J., and Upstill-Goddard, R. C.: In situ evaluation of air-sea gas exchange parameterizations using novel conservative and volatile tracers, Global Biogeochem. Cy., 14, 373-387, doi:10.1029/1999GB900091, 2000.
- Paasche, E.: Roles of nitrogen and phosphorus in coccolith formation in Emiliania huxleyi (Prymnesiophyceae), Eur. J. Phycol., 33, 33-42, 1998.

Patankar, S. V.: Numerical Heat Transfer and Fluid Flow, McGraw-Hill, New York, USA, 1980.

- Platt, T., Harrison, W. G., Irwin, B., Horne, E. P., and Gallegos, C. L.: Photosynthesis and photoadaptation of marine phytoplankton in the arctic, Deep-Sea Res., 29, 1159-1170, doi:10.1016/0198-0149(82)90087-5, 1982.
- Polimene, L., Allen, J. I., and Zavatarelli, M.: Model of interactions between dissolved organic carbon and bacteria in marine systems, Aquat. Microb. Ecol., 43, 127-138, doi:10.3354/ame043127, 2006.
- Polimene, L., Pinardi, N., Zavatarelli, M., Allen, J. I., Giani, M., and Vichi, M.: A numerical simulation study of dissolved organic carbon accumulation in the northern Adriatic Sea, J. Geophys. Res.-Oceans, 112, C03S20, doi:10.1029/2006JC003529, 2007.
- Polimene, L., Archer, S. D., Butenschön, M., and Allen, J. I.: A mechanistic explanation of the Sargasso Sea DMS "summer paradox", Biogeochemistry, 110, 243-255, doi:10.1007/s10533-011-9674-z, 2012.
- Polimene, L., Brunet, C., Butenschön, M., Martinez-Vicente, V., Widdicombe, C., Torres, R., and Allen, J. I.: Modelling a light-driven phytoplankton succession, J. Plankton Res., 36, 214-229, doi:10.1093/plankt/fbt086, 2014.
- Pujo-Pay, M. and Conan, P. and Raimbault, P.:Excretion of dissolved organic nitrogen by phytoplankton assessed by wet oxidation and ¹⁵N tracer procedures, Mar. Ecol.-Prog. Ser., 153, 99-111, doi:10.3354/meps153099, 1997.
- Radford, P. and Joint, I.: The application of an ecosystem model to the Bristol Channel and Severn Estuary, Water Pollut. Control, 2, 244-250, 1980.
- Ridgwell, A., Zondervan, I., Hargreaves, J. C., Bijma, J., and Lenton, T. M.: Assessing the potential long-term increase of oceanic fossil fuel CO₂ uptake due to CO₂-calcification feedback, Biogeosciences, 4, 481-492, doi:10.5194/bg-4-481-2007, 2007.

- Riegman, R., Stolte, W., Noordeloos, A. A. M., and Slezak, D.: Nutrient uptake and alkaline phosphatase (ec 3:1:3:1) activity of emiliania huxleyi (PRYMNESIOPHYCEAE) during growth under n and p limitation in continuous cultures, J. Phycol., 36, 87-96, doi:10.1046/j.1529-8817.2000.99023.x, 2000.
- Ruardij, P. and Van Raaphorst, W.: Benthic nutrient regeneration in the ERSEM ecosystem model of the North Sea, Neth. J. Sea Res., 33, 453-483, doi:10.1016/0077-7579(95)90057-8, 1995.
- Saux Picart, S., Butenschön, M., and Shutler, J. D.: Wavelet-based spatial comparison technique for analysing and evaluating two-dimensional geophysical model fields, Geosci. Model Dev., 5, 223-230, doi:10.5194/gmd-5-223-2012, 2012.
- Shutler, J. D., Smyth, T. J., Saux-Picart, S., Wakelin, S. L., Hyder, P., Orekhov, P., Grant, M. G., Tilstone, G. H., and Allen, J. I.: Evaluating the ability of a hydrodynamic ecosystem model to capture inter- and intra-annual spatial characteristics of chlorophyll-a in the north east Atlantic, J. Marine Syst., 88, 169–182, doi:10.1016/j.jmarsys.2011.03.013, 2011.
- Smyth, T. J., Fishwick, J. R., AL-Moosawi, L., Cummings, D. G., Harris, C., Kitidis, V., Rees, A., Martinez-Vicente, V., and Woodward, E. M. S.: A broad spatio-temporal view of the Western English Channel observatory, J. Plankton Res., 32, 585-601, doi:10.1093/plankt/fbp128, 2010.
- Steinberg, D. K., Carlson, C. A., Bates, N. R., Johnson, R. J., Michaels, A. F., and Knap, A. H.: Overview of the US JGOFS Bermuda Atlantic Time-series Study (BATS): a decade-scale look at ocean biology and biogeochemistry, Deep-Sea Res. Pt. II, 48, 1405-1447, doi:10.1016/S0967-0645(00)00148-X, 2001.
- Stock, C. A., Dunne, J. P., and John, J. G.: Global-scale carbon and energy flows through the marine planktonic food web: an analysis with a coupled physical-biological model, Prog. Oceanogr., 120, 1-28, doi:10.1016/j.pocean.2013.07.001, 2014.
- Sukenik, A., Bennett, J., and Falkowski, P.: Light-saturated photosynthesis Limitation by electron transport or carbon fixation?, BBA-Bioenergetics, 891, 205-215, doi:10.1016/0005-2728(87)90216-7, 1987.
- Takahashi, T., Williams, R. T., and Bos, D. L.: Carbonate chemistry, Chapter 3, in: GEOSECS Pacific Expedition, Hydrographic Data 1973–1974, Vol. 3., U.S. Governemnt Priniting Office, Washington, D.C., USA, 1982.
- Talmy, D., Blackford, J., Hardman-Mountford, N. J., Polimene, L., Follows, M. J., and Geider, R. J.: Flexible C: N ratio enhances metabolism of large phytoplankton when resource supply is intermittent, Biogeosciences, 11, 4881-4895, doi:10.5194/bg-11-4881-2014, 2014.

- Timmermans, K. R., van der Wagt, B., Veldhuis, M. J. W., Maatman, A., and de Baar, H. J. W.: Physiological responses of three species of marine pico-phytoplankton to ammonium, phosphate, iron and light limitation, J. Sea Res., 53, 109–120, doi:10.1016/j.seares.2004.05.003, 2005.
- van der Molen, J., Smith, H. C. M., Lepper, P., Limpenny, S., and Rees, J.: Predicting the large-scale consequences of offshore wind turbine array development on a North Sea ecosystem, Cont. Shelf Res., 85, 60-72, doi:10.1016/j.csr.2014.05.018, 2014.
- van Duyl, F. C., van Raaphorst, W., and Kop, A. J.: Benthic bacterial production and nutrient sediment-water exchange in sandy North-Sea sediments, Mar. Ecol-Prog. Ser., 100, 85-95, doi:10.3354/meps100085, 1993.
- Varela, R. A., Cruzado, A., and Gabaldón, J. E.: Modelling primary production in the North Sea using the European Regional Seas Ecosystem Model, Neth. J. Sea Res., 33, 337-361, doi:10.1016/0077-7579(95)90052-7, 1995.
- Veldhuis, M. J. W., Timmermans, K. R., Croot, P., and van der Wagt, B.: Picophytoplankton; a comparative study of their biochemical composition and photosynthetic properties, J. Sea Res., 53, 7-24, doi:10.1016/j.seares.2004.01.006, 2005.
- Vichi, M., Ruardij, P., and Baretta, J. W.: Link or sink: a modelling interpretation of the open Baltic biogeochemistry, Biogeosciences, 1, 79-100, doi:10.5194/bg-1-79-2004, 2004.
- Vichi, M., Pinardi, N., and Masina, S.: A generalized model of pelagic biogeochemistry for the global ocean ecosystem. Part I: Theory, J. Marine Syst., 64, 89-109, 2007.
- Villarino, E., Chust, G., Licandro, P., Butenschön, M., Ibaibarriaga, L., Larrañaga, A., and Irigoien, X.: Modelling the future biogeography of North Atlantic zooplankton communities in response to climate change, Mar. Ecol.-Prog. Ser., 531, 121-142, doi:10.3354/meps11299, 2015.
- Wakelin, S. L., Holt, J. T., Blackford, J. C., Allen, J. I., Butenschön, M., and Artioli, Y.: Modeling the carbon fluxes of the northwest European continental shelf: validation and budgets, J. Geophys. Res., 117, C05020 -, doi:10.1029/2011JC007402, 2012.
- Walve, J. and Larsson, U.: Carbon, nitrogen and phosphorus stoichiometry of crustacean zooplankton in the Baltic Sea: implications for nutrient recycling, J. Plankton Res., 21, 2309-2321, doi:10.1093/plankt/21.12.2309, 1999
- Ward, B. B.: Chapter 5 Nitrification in marine systems, in: Nitrogen in the marine environment (2nd edition), edited by: Capone, D. G., Bronk, D., A. and Mulholland, M., R., and Carpenter, E., J., 199–261, Plenum Press, New York, 1992.
- Weiss, R. F.: The solubility of nitrogen, oxygen and argon in water and seawater, Deep-Sea Res., 17, 721-735, doi:10.1016/0011-7471(70)90037-9, 1970.

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- Weiss, R. F.: Carbon dioxide in water and seawater: the solubility of a non-ideal gas, Mar. Chem., 2, 203-215, doi:10.1016/0304-4203(74)90015-2, 1974.
- Weston, K., Fernand, L., Nicholls, J., Marca-Bell, A., Mills, D., Sivyer, D., and Trimmer, M.: Sedimentary and water column processes in the Oyster Grounds: A potentially hypoxic region of the North Sea, Mar. Environ. Res., 65, 235-249, doi:10.1016/j.marenvres.2007.11.002, 2008.
- Wild-Allen, K., Herzfeld, M., Thompson, P. A., Rosebrock, U., Parslow, J., and Volkman, J. K.: Applied coastal biogeochemical modelling to quantify the environmental impact of fish farm nutrients and inform managers, J. Marine Syst., 81, 134-147, doi:10.1016/i.jmarsys.2009.12.013, 2010.
- Yool, A., Popova, E. E., and Anderson, T. R.: MEDUSA-2.0: an intermediate complexity biogeochemical model of the marine carbon cycle for climate change and ocean acidification studies, Geosci. Model Dev., 6, 1767-1811, doi:10.5194/gmd-6-1767-2013, 2013.
- Zavatarelli, M. and Pinardi, N.: The Adriatic Sea modelling system: a nested approach, Ann. Geophys., 21, 345-364, doi:10.5194/angeo-21-345-2003, 2003.
- Zeebe, R. W. and Wolf-Gladrow, D.: CO2 in Seawater: Equilibrium, Kinetics, Isotopes, no. 65 in Elsevier Oceanography Series, Elsevier, Amsterdam, the Netherlands, 2001.

Table 1. Pelagic functional types and their components, organic part (squared brackets indicate
option states) - chemical components: \mathbb{C} carbon, \mathbb{N} nitrogen, \mathbb{P} phosphorus, \mathbb{F} iron, \mathbb{S} silicate, \mathcal{C}
chlorophyll a.

Symbol	Code	Description
$\overset{pico}{-P}_{\mathbb{C},\mathbb{N},\mathbb{P}[,\mathbb{F}],\mathcal{C}^{-}}$	P3c,n,p [,f],Chl3	Picophytoplankton (< 2 µm)
$\frac{P}{P}_{\mathbb{C},\mathbb{N},\mathbb{P}[,\mathbb{F}],\mathcal{C}}$	P2c,n,p[,f],Chl2	Nanophytoplankon (2–20 μm)
$\overset{micro}{-P}_{-\mathbb{C},\mathbb{N},\mathbb{P}[,\mathbb{F}],\mathcal{C}}$	- P4c,n,p [,f],Chl4	Microphytoplankton (> 20μm)
dia $P_{\mathbb{C},\mathbb{N},\mathbb{P}[,\mathbb{F}],\mathbb{S},\mathcal{C}}$	Plc,n,P[,f],Chll	Diatoms
$\stackrel{HET}{-Z_{-\mathbb{C},\mathbb{N},\mathbb{P}^{-}}}$	Z6c,n,p	Heterotrophic Flagellates
$\frac{MICRO}{-Z-\mathbb{C},\mathbb{N},\mathbb{P}^{-}}$	Z5c,n,p	Microzooplankton
MESO -ZC BC-ND-	Z4c B1c.n.p	Mesozooplankton Heterotrophic Bacteria
lab $R_{\mathbb{C},\mathbb{N},\mathbb{P}^+}$	R1c,n,p	Labile dissolved organic matter
slab $R_{\mathbb{C}^+}$	R2c	Semi-labile organic matter
srefr $R_{\mathbb{C}^+}$	R3c	Semi-refractory organic matter
small $-R_{\mathbb{C},\mathbb{N},\mathbb{P}[\mathbb{F}]}$	R4c,n,p [,f]	Small particulate organic matter
$\overset{med}{=} \overset{R_{\mathbb{C},\mathbb{N},\mathbb{P}},\mathbb{F},\mathbb{S}^{-}}$	R6c,n,p [,f] ,s	Medium size particulate organic matter
large $R_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{S}}$	R8c,n,p,s	Large particulate organic matter

Symbol	Code	Description
$\begin{bmatrix} calc \\ L_{\mathbb{C}} \end{bmatrix}$	[L2c]	Calcite
$\dot{\Theta}_{\mathbb{O}}$	020	Dissolved oxygen
$\Theta_{\mathbb{C}^+}$	03c	Disolved inorganic carbon (DIC)
$N_{\mathbb{P}}$	N1p	Phosphate
$N_{\mathbb{N}}^{-}$	N3n	Oxidised nitrogen
$N_{\mathbb{N}}$	N4n	Ammonium
$N_{\mathbb{S}^-}$	N5s	Silicate
$[N_{\mathbb{F}}]$	[N7f]	Dissolved iron
[Abio]	[bioAlk]	Bioalkalinity

Table 2. Pelagic functional types and their components, inorganic part (squared brackets indicate optional states) – chemical components: C carbon, N nitrogen, P phosphorus, F iron, S silicate.

Table 3. Pelagic functional types and their components (squared brackets indicate optional states)- chemical components: \mathbb{C} carbon, \mathbb{N} nitrogen, \mathbb{P} phosphorus, \mathbb{F} iron, \mathbb{S} silicate, \mathcal{C} chlorophyll a.



Symbol	Code	Description
pico	D3g n n[f] Ch13	$Picophytoplankton (< 2 \mu m)$
nano	ESCHIPT FIGHTS	
$P_{\mathcal{C},\mathcal{N},\mathcal{P}_{1},\mathcal{F}_{2},\mathcal{C}_{2}}$	P2cinip[if],Ch12	Nanophytoplankon (2–20 µm)
$\underset{\mathcal{I}}{\overset{P}{\longrightarrow}} \mathbb{C}, \mathbb{N}, \mathbb{P}[,\mathbb{F}], \mathcal{L}_{\sim}$	P4c, n, p[, f], Chl4	Microphytoplankton (> 20 µm)
	Plc, n, P[, f], Chll	Diatoms
	Z6c.n.p	Heterotrophic Flagellates
	<u>Z5c, n, p</u>	Microzooplankton
$Z_{\mathbb{C}}$	Z4c	Mesozooplankton
$\underset{\sim}{B}_{\mathbb{C}}$.N.R.	Blcinep	Heterotrophic Bacteria
	Ricinip	Labile dissolved organic matter
$\overset{ ext{slab}}{\underset{ ext{{magenta}}}{\overset{ ext{slab}}{\overset{ ext{{magenta}}}{\overset{ ext{{magenta}}}{$	R2c	Semi-labile organic matter
srefr $\underset{\mathcal{R}_{\mathbb{C}}}{\overset{ ext{srefr}}{\longrightarrow}}$	R3c	Semi-refractory organic matter
small $\ \mathcal{R}_{\mathcal{C},\mathbb{N},\mathbb{P}[\mathbb{F}]_{\mathcal{C}}}$	R4cinip[if]	Small particulate organic matter
$\overset{med}{\underset{\sim}{R}}_{\mathcal{R}} \mathbb{C}, \mathbb{N}, \mathbb{P}[,\mathbb{F}], \mathbb{S}_{\sim}$	R6cenep[ef]es	Medium size particulate organic matter
large $R_{\mathcal{R}}$, $\mathbb{R}_{\mathcal{R}}$, $\mathbb{R}_{\mathcal{R}}$	Rocenepes	Large particulate organic matter
$\mathcal{L}_{\mathbb{C}}$	[<u>L2c</u>]	Calcite
	020	Dissolved oxygen
$\widetilde{O}_{\mathbb{C}}$	<u>03c</u>	Disolved inorganic carbon (DIC)
$N_{\mathbb{R}}$	Nlp	Phosphate
$N_{\mathbb{N}}$	N3n	Oxidised nitrogen
$N_{\mathbb{N}}$	N4n	Ammonium
\widetilde{N}_{S}	N5s	Silicate
$[N_{\mathbb{F}}]$	[<u>N7f</u>]	Dissolved iron
[Abio]	[bioAlk]	Bioalkalinity

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 Table 4. Pelagic predators and their preys.

Predator type	Prey types
Heterotrophic flagellates $(-Z)$	$\begin{array}{llllllllllllllllllllllllllllllllllll$
Microzooplankton (Z)	$\begin{array}{llllllllllllllllllllllllllllllllllll$
Mesozooplankton (Z)	Picophytoplankton, nanophytoplankton, microphytoplankton, diatoms, heterotrophic flagellates, microzooplankton, mesozooplankton, medium size pico nano micro dia HET MICRO MESO med particulate matter (P, P, P, P, Z, Z, R)

 Table 5. Particulate organic matter and its origin.

POM type	Originating from
Small particulate organic matter ($\stackrel{\text{small}}{R}$)	Nano- and picophytoplankton $(\stackrel{\text{nano}}{P}, \stackrel{\text{pico}}{P})$, HET heterotrophic flagellates (Z)
Medium size particulate organic matter $\binom{\text{med}}{(R)}$	Microphytoplankton and diatoms (P , P), MICRO microzooplankton (Z)
Large particulate organic matter $\begin{pmatrix} R \\ R \end{pmatrix}$	Mesozooplankton $\begin{pmatrix} MESO \\ Z \end{pmatrix}$

Symbol	Code	Description
$\stackrel{DEPO}{-Y_{\mathbb{C}}}$	¥2e	Deposit feeders
SUSP $-Y_{\mathbb{C}}$	Y3c	Suspension feeders
$\stackrel{MEIO}{}$	Y4c	Meiobenthos
$H_{\mathbb{C}}^{-}$	Hlc	Aerobic bacteria
anaer $H_{\mathbb{C}}^+$	H2c	Anaerobic bacteria
dis $Q_{\mathbb{C}^+}$	Qlc	Dissolved organic matter
slow $\overline{Q_{\mathbb{C},\mathbb{N},\mathbb{P}[,\mathbb{F}]}}$	Q6c,n,p [,f] ,s	Slowly degradable organic matter
$Q_{\mathbb{C},\mathbb{N},\mathbb{P},\mathbb{S}}^{-}$	Q7c,n,p,s	Refractory organic matter
bur $Q_{\mathbb{C},\mathbb{N},\mathbb{P}^+}$	Q17c,n,p	Buried organic matter

Table 6. Benthic functional types and their components, organic part (squared brackets indicate option states) – chemical components: ℂ carbon, ℕ nitrogen, ℙ phosphorus, ℙ iron, S silicate.

Table	7.	Benthic	functional	types	and th	heir co	mponents	, inorgnic	part	and	states	of	vertical
distrib t	utio	n (squar	ed brackets	indica	e optic	on state	s) - chem	ical compo	onente	s: € c	arbon,	<mark>ℕ ni</mark>	trogen,
<mark>₽ phos</mark>	spho	orus, S s	ilicate.										

Symbol	Code	Description
$\begin{bmatrix} \text{bcalc} \\ -C_{\mathbb{C}} \end{bmatrix}$	[bL2c]	Calcite
$\dot{G}_{\mathbb{O}}$	G20	Dissolved oxygen
$G_{\mathbb{C}^+}$	G3c	Disolved inorganic carbon (DIC)
$G_{\mathbb{N}^+}$	G4n	Dinitrogen
$K_{\mathbb{P}^+}$	K1p	Phosphate
$\frac{K_{\mathbb{N}}}{K_{\mathbb{N}}}$	K3n	Oxidised nitrogen
$\frac{M}{K_{\mathbb{N}}}$	K4n	Ammonium
$K_{\mathbb{S}^+}$	K5s	Silicate
oxy - D	D1m	Depth of oxygen horizon
denit ————	D2m	Depth of oxidised nitrogen horizon
refr _ℂ ─ D ─	D3m	Average penetration depth of refractory carbon
refr _ℕ ─ D ─	D4m	Average penetration depth of refractory nitrogen
refr _ℙ ─ D ─	Ð5m	Average penetration depth of refractory phosphorus
$\stackrel{slow_{\mathbb{C}}}{\longrightarrow}$	D6m	Average penetration depth of slowly degradable carbon
slow _ℕ ─────	D7m	Average penetration depth of slowly degradable nitrogen
slow _ℙ ─────	D8m	Average penetration depth of slowly degradable phosphorus
slow _s ─────	D9m	Average penetration depth of slowly degradable silicate

Table 8. Benthic functional types and their components .(squared brackets indicate option states) –chemical components: \mathbb{C} carbon, \mathbb{N} nitrogen, \mathbb{P} phosphorus, \mathbb{F} iron, \mathbb{S} silicate.

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Symbol	Code	Description
DEPO	X2c	Deposit feeders
SUSP	~~~~	
$Y_{\mathbb{C}}$	<u>Y3c</u>	Suspension feeders
$Y_{\mathbb{C}}$	Y4c	Meiobenthos
$\overset{\mathrm{aer}}{{}{}{}{}{}{}{\overset$	Hlc	Aerobic bacteria
anaer $\underbrace{H_{\mathbb{C}}}$	H2c	Anaerobic bacteria
$\overset{dis}{\mathscr{Q}_{\mathbb{C}}}$	Qlc	Dissolved organic matter
$\overset{\text{degr}}{\sim} \mathcal{Q}_{\mathcal{C},\mathcal{N},\mathbb{R}[,\mathbb{F}]}$	Q6cinip[if]is	Degradable organic matter
$\mathcal{Q}_{\mathcal{C}, \mathbb{N}, \mathbb{P}, \mathbb{S}_{\mathcal{C}}}$	Q7cinipis	Refractory organic matter
bur $\mathcal{Q}_{\mathcal{C},\mathbb{N},\mathbb{P}_{\sim}}$	Q17cenep	Buried organic matter
$\mathcal{C}_{\mathbb{C}}$	[bL2c]	Calcite
$G_{\mathbb{Q}}$	G2o	Dissolved oxygen
$\widetilde{G}_{\mathbb{C}}$	<u>G3c</u>	Disolved inorganic carbon (DIC)
$\underline{G}_{\mathbb{N}}$	<u>G4n</u>	Dinitrogen
$\underbrace{K}_{\mathbb{R}}$	<u>K1p</u>	Phosphate
$\overset{ox}{\overset{K}{\mathbb{N}}}_{\sim}$	<u>K3n</u>	Oxidised nitrogen
$K_{\mathbb{N}}$	K4n	Ammonium
$\widetilde{K}_{\mathbb{S}}$	K5s	Silicate
$\overset{\text{oxy}}{\overset{D}{}}$	Dlm	Depth of oxygen horizon
denit \underbrace{D}	<u>D2m</u>	Depth of oxidised nitrogen horizon
$\overset{refr_{\mathbb{C}}}{\overset{D}{\longrightarrow}}$	<u>D3m</u>	Average penetration depth of refractory carbon
$\overset{refr_{\mathbb{N}}}{\overset{D}{\longrightarrow}}$	<u>D4m</u>	Average penetration depth of refractory nitrogen
$\overset{refr_\mathbb{P}}{\overset{D}{\sim}}$	<u>D5m</u>	Average penetration depth of refractory phosphorus
$\operatorname{degr}_{\mathbb{C}}$	<u>D6m</u>	Averagegrenetration depth of degradable carbon
$\operatorname{degr}_{\mathbb{N}}$	D7m	Average penetration depth of degradable nitrogen

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Table 9. Benthic predators and their preys.

Predator type	Prey types
DEPO	Aerobic and anaerobic bacteria, meiobenthos, available
	$\begin{array}{c} \text{aer anaer MEIO slow} & \overset{d_{\mathcal{Z}}}{\underset{d_{\mathcal{Z}}}{\text{slowly degradable organic matter }}, & \overset{d_{\mathcal{Z}}}{\underset{H}{\text{slow}}, H, Y, Q} \\ \end{array}$
SUSP Suspension feeders (Y)	Aerobic bacteria, picophytoplankton, nanophytoplankton, diatoms, medium size particulate matter and available
	$\begin{array}{c c} \text{Slowly degradable organic matter } (H, a_{\text{SUSP}}, h, a_{\text{SUSP}}, h, h,$
$\frac{\text{MEIO}}{(Y)}$	Aerobic bacteria, anaerobic bacteria, meiobenthos, available aer anaer MEIO slowly degradable organic matter (H, H, Y, Q)









Figure 2. ERSEM schematic showing how model components interact with or influence each other. Blue connectors represent inorganic carbon fluxes, red represents nutrient fluxes, yellow represents oxygen, black represents predator-prey interactions and green represents fluxes of non-living organics. Dashed arrows indicate the influence of carbonate system variables.





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Figure 3. Pelagic predators and their prey.



Figure 4. The microbial cycling of organic material for the standard bacteria model (left) and the dynamic decomposition model (right).





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Figure 5. Benthic predators and their prey.



Figure 6. Carbon fluxes in ERSEM under oligotrophic (left) and eutrophic (right) conditions. The flux amount is proportional to arrow thickness. (Note the different scales of the arrow sizes.)





Figure 7. Simulation results vs. in situ data at the Oyster Grounds - left: model time series (red lines) vs. in situ measurements (black dots) for oxidised nitrogen, phosphate, silicate and chlorophyll a (top to bottom); right: target diagram with bias (abscissa), MAE' (ordinate) and Spearman correlation (colour code) for oxidised nitrogen (NO3), phosphate (PO4), silicate (Sil) and chlorophyll a (Chl). The observations consist of ship-based data collected by Rijkswaterstaat as part of the Dutch national monitoring programme MWTL (see publicwiki.deltares.nl/display/OET/Dataset+documentation+MWTL) and SmartBuoy data collected by Cefas in collaboration with Rijkswaterstaat (Greenwood et al., 2010; http://www.cefas.co.uk/publications-data/smartbuoys).


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Figure 8. Simulation results vs. in situ data at the L4 site – left: model time series (red lines) vs. in situ measurements (black dots) for oxidised nitrogen, phosphate, silicate and chlorophyll *a* (top to bottom); right: target diagram with bias (abscissa), MAE' (ordinate) and Spearman correlation (colour code) for oxidised nitrogen (NO3), phosphate (PO4), silicate (Sil) and chlorophyll *a* (Chl).





Figure 9. Simulation results vs. in situ data at BATS – left: chlorophyll *a* concentrations (Top – model, bottom – interpolated HPLC data); right: target diagram with bias (abscissa), MAE' (ordinate) and spearman correlation (colour code) for oxidised nitrogen (NO3), phosphate (PO4), silicate (Sil), dissolved inorganic carbon (DIC), dissolved oxygen (O₂), chlorophyll a (Chl) and particulate organic carbon (POC).





Figure 10. Emergent properties of the simulations across the three 1-D sites. Left: range (ordinate) and mean (abscissa) of internal stoichiometric ratios of phytoplankton – nitrogen (yellow), silicate (blue), phosphorus (green) and iron (red). Data (diamonds, Moore et al., 2013), assembled 1-D model simulations (circles); right: community fraction of total chlorophyll *a* from assembled 1-D model simulations. Picophytoplankton (red), nanophytoplankton (green) and microphytoplankton and diatoms (cyan).

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Figure 11. The ERSEM model in a simulation for the North West European Shelf Seas – left: optical-depth-averaged chlorophyll *a*; right: hindcast simulation vs. in situ data.





Figure 12. Chlorophyll *a* to carbon ratio of diatoms as a function of PAR under the condition of balanced growth (Eq. 267). The solid line represents output from the model. Black circles show data for nutrient-replete cultures of Thalassiosira pseudonana, digitally extracted from Geider et al. (1997) using Plot Digitizer Version 2.6.6 (see http://plotdigitizer.sourceforge.net).

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Figure 13. Phytoplankton growth over PAR for the four phytoplankton types.



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