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Parameterizing the microbial loop: an experiment in reducing model complexity

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ABSTRACT

The structure of the plankton food web in the upper mixed layer has important implications for the export of biogenic material from the euphotic zone. While the action of the microbial loop causes material to be recycled near the surface, activity of the larger zooplankton leads to a significant downward flux of material. The balance between these pathways must be properly represented in climate models to predict carbon export. However, the number of biogeochemical compartments available to represent the food web is limited by the need to couple biogeochemical models with general circulation models. A structurally simple model is therefore sought, with a number of free parameters, which can be constrained by available observations to produce reliable estimates of export.

A step towards addressing this aim is described: an attempt is made to emulate the behavior of an 11 compartment model with an explicit microbial loop, using a 4 compartment model. The latter, incorporating a basic microbial loop parameterization, is derived directly from the `true' model. The results are compared with equivalent results for a 4 compartment model with no representation of the microbial loop. These non-identical twin experiments suggest that export estimates from 4 compartment models are prone to serious biases in regions where the action of the microbial loop is significant. The basic parameterization shows some promise in addressing the problem but a more sophisticated parameterization would be needed to produce reliable estimates. Some recommendations are made for future research.

KEYWORDS

biogeochemical cycles, data assimilation, ecosystem modelling, model complexity, parameter estimation

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1 Introduction

The experiment described was motivated by the need to find a model of minimal complexity which could adequately represent the observed variability in biogeochemical cycles over an ocean basin. In particular, the number of biogeochemical compartments (representing nitrogen and/or carbon pools) should be as small as is practical to allow the biogeochemical model to be coupled with high resolution general circulation models for climate research.

The model must be able to cope with a range of different environmental conditions spanning eutrophic and oligotrophic regimes. For climate research applications, it is required to produce estimates of carbon export from the upper layers of the ocean associated with sinking particles because of the impact of this process on air-sea CO_2 fluxes. This process is dependent on the structure of the foodweb which controls the balance between recycling of material near the surface and the downward flux of material. Dominance of a linear food chain, in which much of the grazing is done by larger zooplankton such as copepods, leads to a high export ratio (the ratio of exported material to primary production) as fast sinking faecal pellets are produced. In oligotrophic environments, the larger grazers are much less abundant and all but a small fraction of the grazing is associated with the microzooplankton. In these areas, the export ratio is much lower as more material is recycled in the upper layers via the microbial loop. The number of compartments required to effectively simulate the microbial loop, in addition to the linear food chain, remains an open question. Although the argument for minimizing the number of model compartments is strong, it is important that the model remains sufficiently flexible to be able to represent the foodweb mediated variability in the export ratio.

Flexibility in specific models is achieved by means of free parameters controlling the flows of material between compartments. The values of these parameters are estimated by fitting the model to observations. For a model to be applicable on global or basin scales, the most relevant observations are those with good spatial and temporal coverage. The main source is satellite ocean colour data from which we have useful estimates of surface chlorophyll concentration in the open ocean. *In situ* nutrient data are also available with moderately good coverage. Ideally the model would have a single parameter set throughout its domain. However, it may prove necessary to calibrate the model separately for different regions. These could be biogeochemical provinces such as those of Longhurst (1998) based on observed annual cycles in remotely sensed chlorophyll and knowledge of the relevant physical features of ocean regions. Alternatively, a method has recently been developed by Hemmings et al. (in press) for dividing a domain into separate calibration provinces in such a way as to allow the model to achieve a best fit to independent validation data distributed over the domain.

A useful model must firstly be able to give an adequate representation of the observations used in its calibration. A second, more stringent test is for it to have some predictive skill with respect to independent observations. The first test requires the uncalibrated model to be flexible, while the second requires the calibrated model to be well constrained, with the caviat that a poorly constrained model is preferable to a well constrained model which gives biased estimates of the quantities of interest. In a poorly constrained model, a range of estimates is given by values of the free parameters which are equally probable, given the calibration data.

A 15 compartment model developed by Anderson and Pondaven (2003) for examining carbon and nitrogen cycling in the Sargasso Sea performs well at the Bermuda Atlantic Time-series Study site when embedded in a 1D physical model. In particular, it is able to accurately simulate the summer drawdown of dissolved inorganic carbon (DIC) in surface waters which has been observed to occur in the absence of detectable nitrate. A similar 11 compartment model in a 3 layer physical model has been used successfully to simulate the annual cycle in dissolved organic carbon (DOC) observed at a station in the English Channel (Anderson and Williams, 1998). In both models, the microbial loop is represented by bacteria and 4 dissolved organic matter (DOM) compartments. Labile and semi-labile DOM are modelled separately and the carbon:nitrogen (C:N) ratio of each of these forms is allowed to vary. In the Anderson and Pondaven (2003) model the C:N ratio of detritus is also allowed to vary and there are separate detrital compartments for material originating from *Trichodesmium* production. These models have been shown to be flexible enough to adequately represent the action of the microbial loop at specific locations, although their predictive skill for other locations has yet to be tested. Nevertheless, on the strength of these results, the representation of the microbial loop in the models is considered plausible.

The possibility of emulating the behavior of an 11 compartment variant of the above models with a 4 compartment model is investigated in the following experiments. Results for a model with a basic parameterization of the microbial loop are compared with those for a model in which the microbial loop has no explicit representation.

2 Method

The experiments described take the form of non-identical twin experiments in which a synthetic 'truth' is defined by the 11 compartment model. The two alternative 4 compartment models were derived by simplifying the 11 compartment model, termed the 'parent model'. Each was then fit to the true chlorophyll and nutrient trajectories, provided by the parent model, by optimizing their free parameters.

2.1 Parent model

The parent model (Figure 1) differs from the model of Anderson and Pondaven (2003) as follows.

- The parent model runs in zero-dimensional mode, simulating mixed layer concentrations only.
- *Trichodesmium* production is excluded.
- Photosynthesis is driven by a non-spectral light model.

DIC and alkalinity are also excluded but this has no effect on the dynamics.

The model is forced by time series of photosynthetically available radiation (PAR), mixed layer depth and temperature representative of 3 different latitudes along the 20°W meridian. PAR was determined from cloudiness data (Bishop *et al.*, 1994) by applying the Evans and Parslow (1985) transmission model, calibrated as in Hemmings *et al.* (in press). Mixed layer depth and temperature were supplied by an integration of the Miami Isopycnic Co-ordinate Ocean Model (MICOM, Bleck *et al.*, 1992). Details of the run are as described in Hemmings *et al.* (in press). Nitrate at the base of the mixed layer was determined from World Ocean Atlas annual mean profiles (Conkright *et al.*, 1998). All other concentrations are zero at this boundary.

Parameter values are the same as those used by Anderson and Pondaven (2003), with the exception of the half-saturation constant for zooplankton grazing which is increased to damp out oscillatory behavior. No attempt has been made to tune the model to give realistic responses to the forcing data. Production at 50°N and 60°N is very high compared with observational estimates and nutrient is used up too quickly. The present focus is on emulating the model behavior under a range of different conditions. It is desirable that a simpler model should be able to emulate the 'true' model over a wide range of inputs (parameter values and forcing data) including the present parameter values.

2.2 Reduced models

The reduced complexity models were derived by removing the carbon compartments and reducing the number of nitrogen compartments to 4.

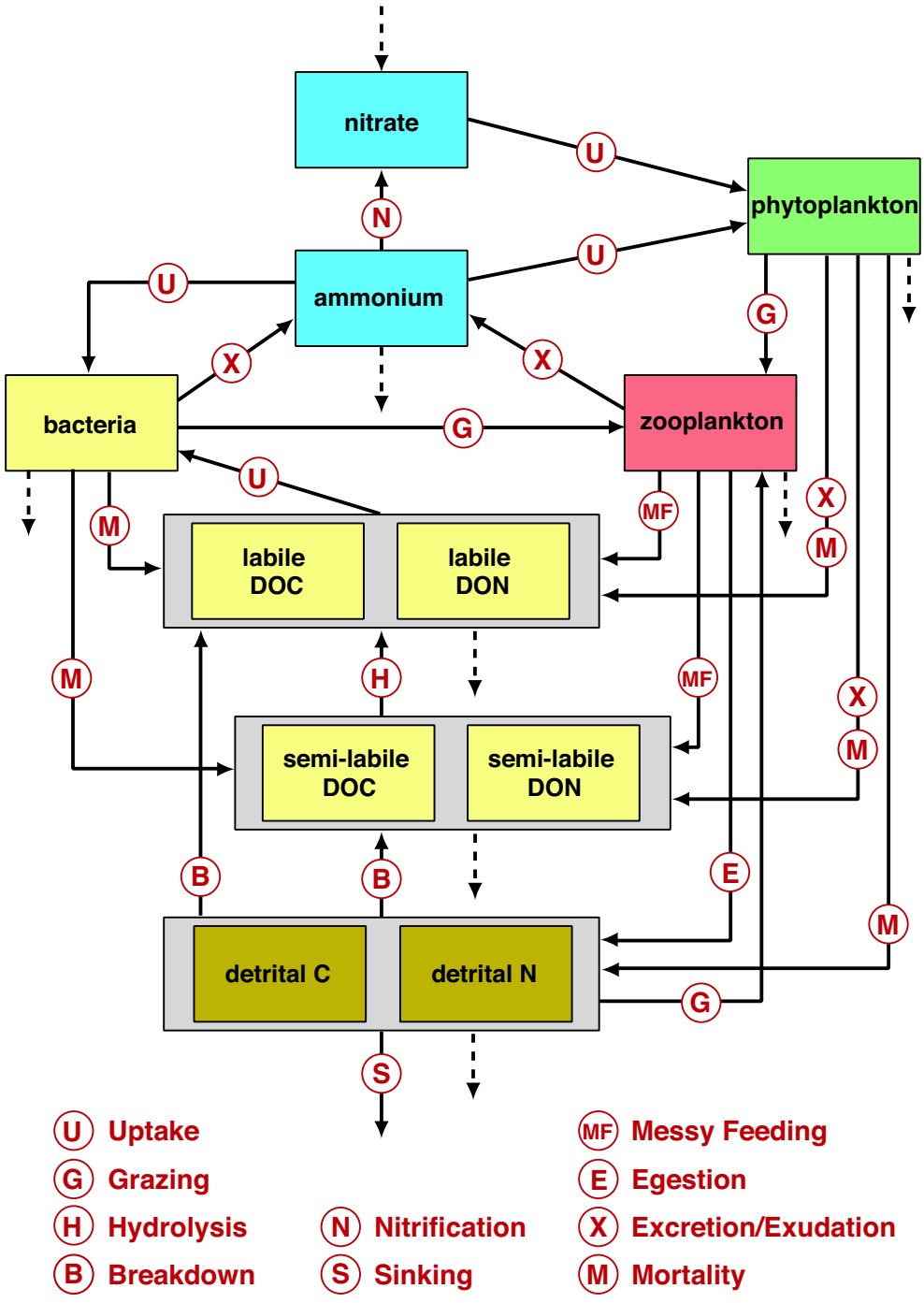

Figure 1: Parent model compartments and fluxes.

In the first model, the 'NPHD' model (Figure 2), the compartments are dissolved inorganic nutrients (N), phytoplankton (P), a heterotrophic recycling pool (H) and detritus (D). The new heterotrophic recycling compartment includes the zooplankton, bacteria, labile and semi-labile dissolved organic nitrogen (DON) pools which are represented as separate compartments in the parent model. The fluxes for the new compartment are determined by adding the fluxes for its individual components, treating each as a constant but unknown fraction of the total nitrogen in the pool. (Messy feeding fluxes to DON are ignored in the present study.) The model thus incorporates a very basic parameterization of the microbial loop.

The second model is a more traditional 'NPZD' model (Figure 3) In this model, all fluxes to and from the bacteria and DON pools were ignored. The heterotrophic recycling compartment is thus replaced by a zooplankton only compartment (Z) and the microbial loop is not represented. The two models are described in more detail in the appendix (Section A).

2.3 Parameter optimization

The 4 compartment models' free parameters were each allowed to vary over a prescribed range. Optimal values were estimated by minimizing a cost function given by the squared r.m.s. error over all simulated daily observations. (Chlorophyll and nutrient errors are weighted such that their numerical values in mg m^{-3} and mmol m^{-3} are equivalent). The optimization procedure, Powell's conjugate direction set method (Press *et al.*, 1992), gives results which are sensitive to an initial guess for the values in the parameter set. Robust results were obtained from an ensemble optimization, using 100 different initial guess parameter vectors drawn randomly from a 'top hat' joint probability distribution with zero parameter covariances. In this prior probability distribution, all parameter values have equal probability within the prescribed ranges and zero probability outside. In each optimization experiment, a number of ensemble members produced parameter estimates for which the cost was only slightly different from the minimum found. In each case, these estimates are interpreted as a sample of the posterior probability distribution, which contains information on the extent to which the parameters are constrained by the observations.

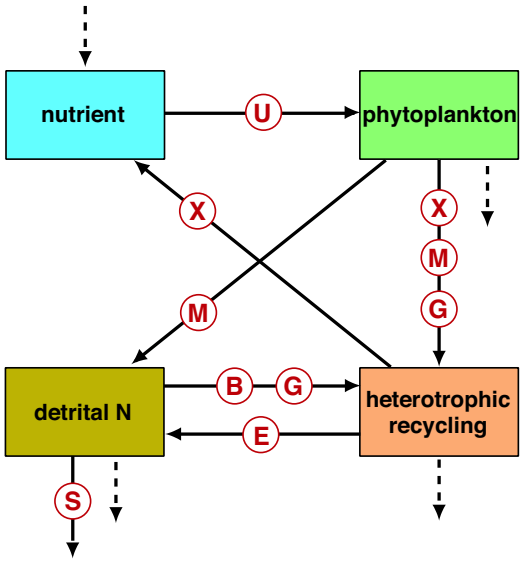

Figure 2: NPHD model compartments and fluxes. For key to fluxes see Figure 1.

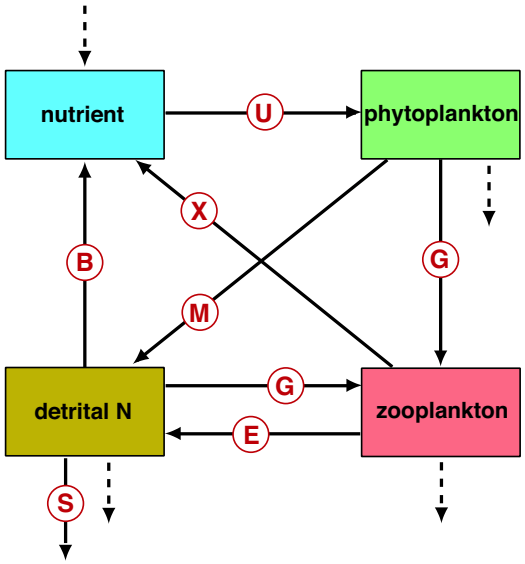

Figure 3: NPZD model compartments and fluxes. For key to fluxes see Figure 1.

2.4 Evaluation

The models are evaluated according to the following criteria in order of importance.

- The model should have sufficient flexibility to fit chlorophyll and nutrient cycles output by the parent model.
- The calibrated model should produce unbiased estimates of production and export.
- The calibrated model should produce precise estimates of production and export.

Although export from the mixed layer in the parent model is dominated by fluxes due to spring detrainment much of this material would be re-entrained when the mixed layer deepens. Only the export due to sinking particles is considered here on the assumption that it is the major factor controlling export to deep water.

With respect to the first criterion, similar performance was achieved for both models by varying the number of free parameters before comparing the models' performance with respect to the other criteria. The NPHD model has 7 free parameters (Table 2). These are parameters which are not defined by the parent model. In the NPZD model, only 2 parameters are undefined (the feeding preference for phytoplankton and the detrital C:N ratio). However, optimizing with 2 free parameters gives an r.m.s. error about twice that for the NPHD model. To make the results more comparable a further 3 parameters were allowed to vary, the additional flexibility compensating for the absence of an explicit microbial loop. Table 3 gives the full list of free parameters.

3 Results

3.1 Posterior parameter distributions

The cost minimum found was 0.51 for both 4 compartment models (equivalent to an r.m.s. error of 0.71 units). Samples representing the posterior parameter distributions for each model are formed from the optimization ensemble members with costs differing from that for the best fit by less than 0.1 (a difference of approximately 20% for both models).

Histograms for the NPHD model and the NPZD model are shown in Figures 4 and 5 respectively. In both cases, it is clear that the free parameters are not well constrained by the synthetic observations. Only univariate distributions have been examined here. Parameter interactions may contribute to the problem. However, the extent of any such contribution is unclear without further analysis of parameter covariances.

3.2 Model output

Figure 6 shows that the structure and/or fixed parameters of both NPHD and NPZD models impose similar constraints which lead to rather poor simulation of the chlorophyll and nutrient cycles. This has implications for primary production. Separate cycles are plotted for each parameter set in the sample representing the posterior parameter distribution, although there is very little variation in the trajectories for each model.

The total annual primary production and export for all three models are given in Table 1 and the annual cycles for each of the 4 compartment models are compared with those for the parent model in Figure 7. Again, separate cycles are shown for each parameter set, indicating the post calibration uncertainty. The uncertainty is much greater in these cycles, which are not directly constrained by the synthetic observations. The tabulated annual values for the 4 compartment models are means over all of the parameter sets ($\pm$ standard error).

Both models show high biases in export fluxes at all 3 locations, contrasting with low biases in primary production. This leads to very high biases in the export ratio. The low production biases are greater in the NPHD model than in the NPZD model but the export biases are smaller. The net result is a slightly smaller bias in the export ratio at all locations, most evident at 40°N where the best fits to chlorophyll and nutrient are obtained. The reduced bias in the export ratio for the NPHD model, shows that even very basic parameterizations of the microbial loop have some potential for improving export estimates.

A slightly less serious problem is that the chosen parameter sets in both models are poorly constrained, leading to imprecise estimates of export. This might be alleviated to some extent by running simulations over a wider range of environmental conditions, as represented by the forcing data. However, it may be the case that chlorophyll and nutrient observations alone cannot provide adequate constraints.

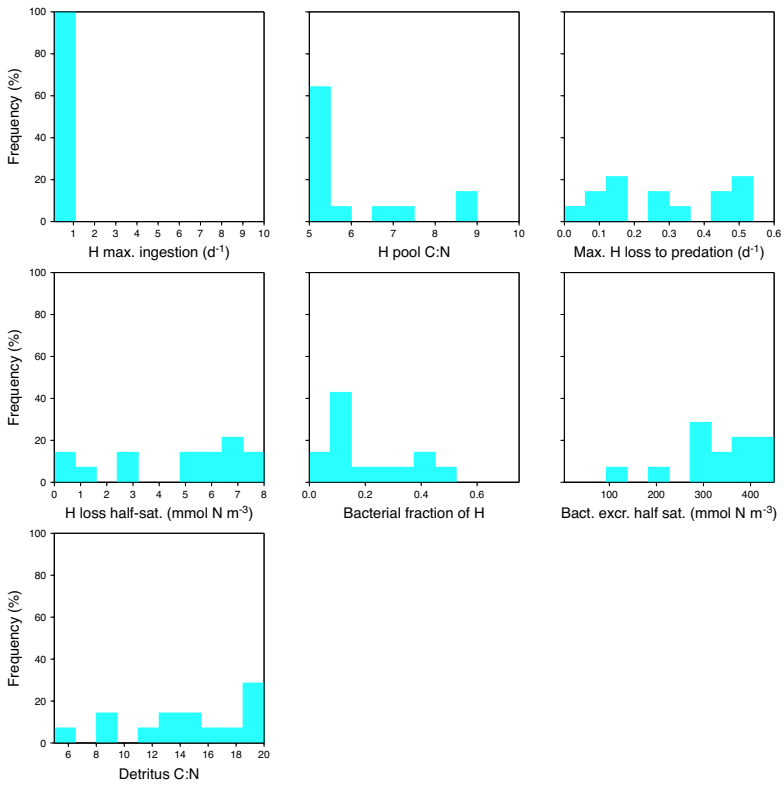

Figure 4: Univariate posterior parameter distribution estimates for the NPHD model

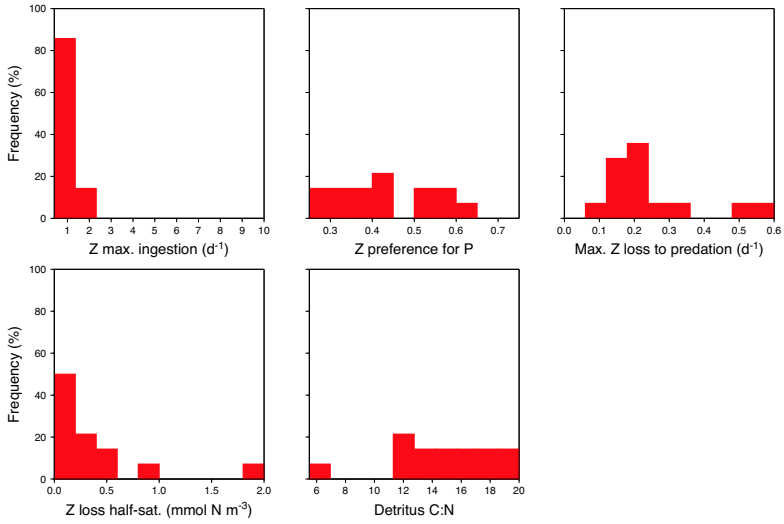

Figure 5: Univariate posterior parameter distribution estimates for the NPZD model

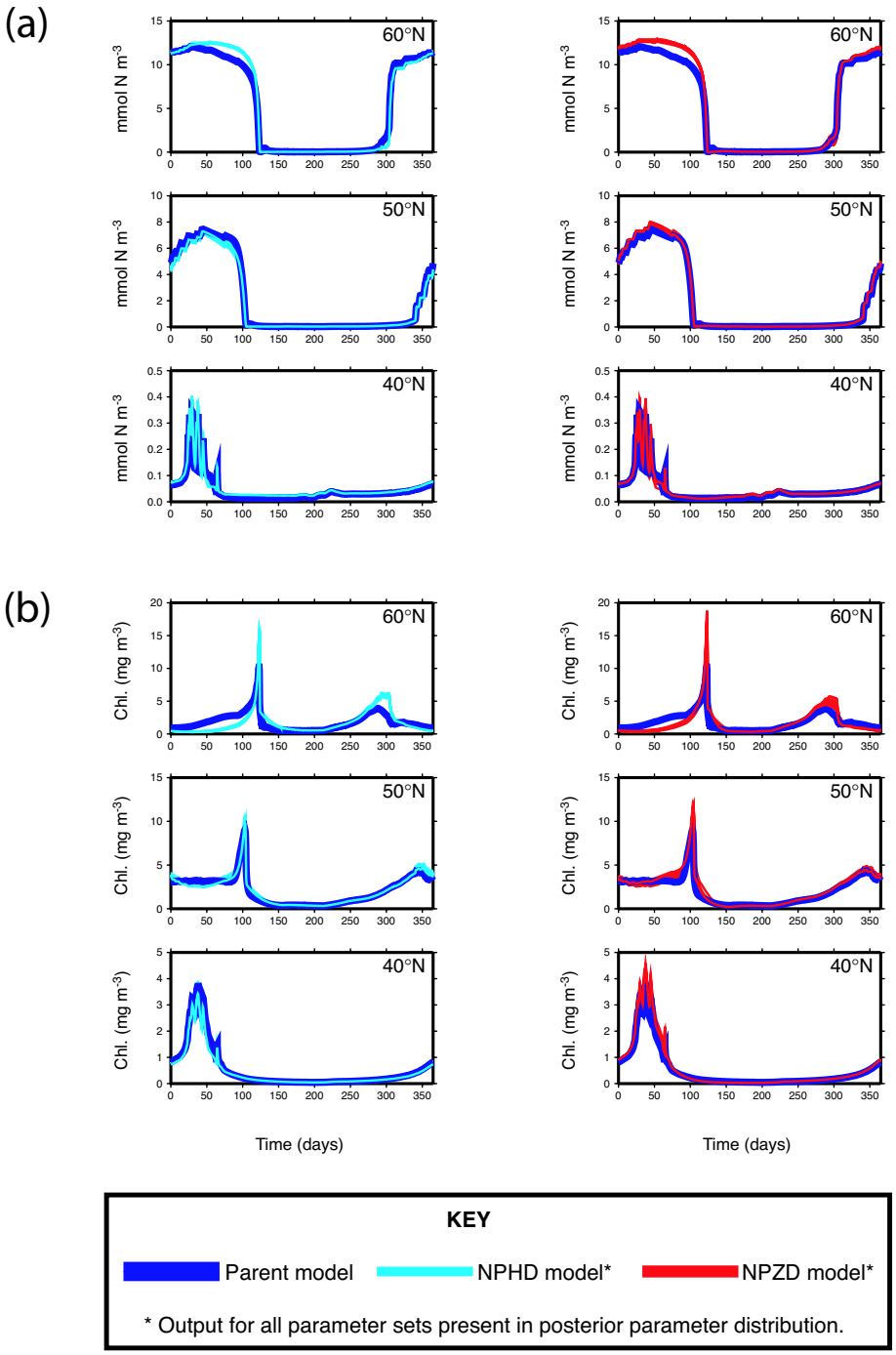

Figure 6: Annual cycles of (a) nutrient and (b) chlorophyll from the 4 compartment models compared with those from the parent model.

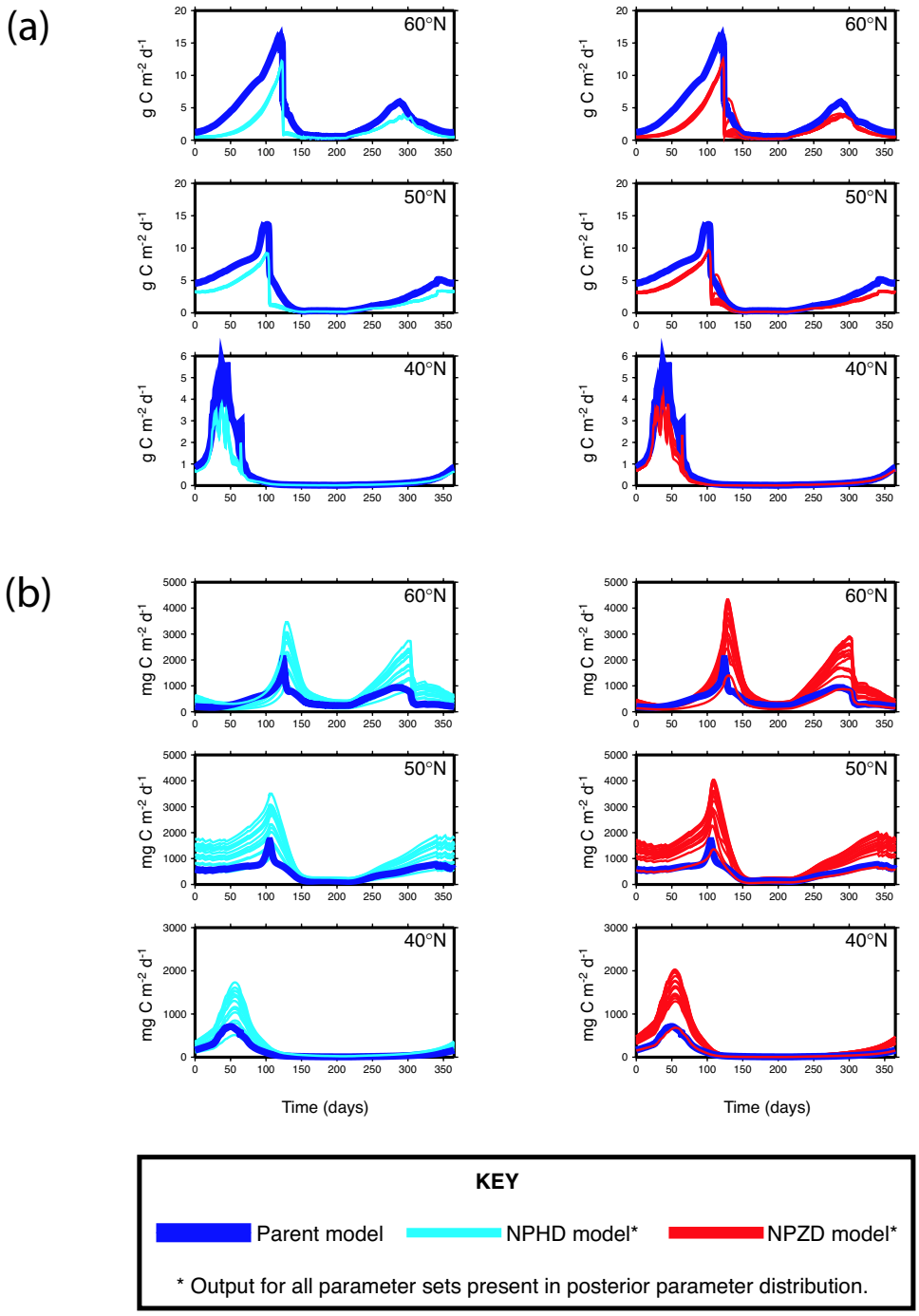

Figure 7: Annual cycles of (a) primary production and (b) export due to sinking particles from the 4 compartment models compared with those from the parent model.

Table 1: Annual production and export

Latitude (°N)	Model	Primary prod. (gC m^{-2} y^{-1})	Export (gC m^{-2} y^{-1})	Export ratio (% production)
60	parent	1360	174	13%
	NPHD	674 ± 4	276 ± 21	$41 \pm 3\%$
	NPZD	740 ± 12	318 ± 20	$43 \pm 3\%$
50	parent	1280	183	14%
	NPHD	809 ± 2	343 ± 26	$42 \pm 3\%$
	NPZD	852 ± 9	387 ± 24	$45 \pm 3\%$
40	parent	230	48	21%
	NPHD	152 ± 1	85 ± 6	$56 \pm 4\%$
	NPZD	166 ± 2	109 ± 7	$66 \pm 4\%$

In summary, neither of the 4 compartment models perform well against any of the evaluation criteria, although the NPHD model performs slightly better than the NPZD model with regard to the bias in the export ratio.

4 Conclusions and recommendations for future research

Production and export estimates given by an NPZD model with no explicit representation of the microbial loop are prone to serious biases in regions where the action of the microbial loop is significant. A basic parameterization of the microbial loop, as implemented in the NPHD model, shows some promise in addressing this problem but a more sophisticated parameterization is required to produce reliable estimates.

Invalid constraints must be removed from the NPHD model to allow a better fit to the chlorophyll and nutrient cycles to be obtained. Constraints could potentially be relaxed by choosing different free parameters but the remaining parameters are already defined by the parent model and any change in their values would imply a change in their interpretation. It seems preferable to try to remove constraints by improving the parameterization. The fixed composition of the heteroptrophic recycling compartment is a major constraint to be addressed. This compartment represents larger zooplankton grazers as well as the microzooplankton and bacteria which drive the microbial loop and the nutrients on which the bacteria feed. In the parent model, as in the real ocean, the ratios between components of the

heterotrophic recycling pool vary and it is this variation we need to model if the balance between a linear food chain and a microbial loop is to be properly represented. One promising approach, based on suggestions by Steele (1998), is to make the zooplankton fraction of the heterotrophic recycling pool dependent on other model variables in such a way as to be relatively large under eutrophic conditions, reflecting the expected abundance of larger plankton, but to decline as oligotrophic conditions develop. Relationships between variables in the parent model should be analyzed in detail to suggest different parameterizations.

In future work, a range of alternative 'true' models should be used. In particular, models including size-structure in phytoplankton and zooplankton (e.g. Ducklow and Fasham, 1992) should be considered as the present model does not explicitly represent the microzooplankton contribution to the microbial loop. It is desirable that the merits of the 'true' models be properly established by validation against independent observations (i.e. observations not used in their tuning or calibration). This would allow much greater emphasis to be given to conclusions arising from the non-identical twin experiments.

These types of non-identical twin experiments have an important role in helping us to understand the different constraints imposed by different model structures and fixed parameters. Testing reduced models with regard to their ability to emulate a range of more complex models, each representing possible truths, should enable the simpler models to be designed with fewer invalid constraints. It should then be possible to focus on determining what types of observations might provide the valid constraints needed to reduce uncertainty in the model output. Finally, although such experiments can provide valuable insight they should be regarded primarily as development tools. Like any other model, the reduced models too should be validated against independent real-world data before they are considered for an application.

Acknowledgments

Thanks are due to Tom Anderson for advice on modelling the microbial loop and setting up the parent model. This work has been supported under the NERC Data Assimilation Thematic Programme award number NER/T/S/1999/00104.

A Model equations

The two 4 compartment models are described below. Both are derived from the 11 compartment parent model.

A.1 Parent model

The parent model has the following compartments.

- Nitrate (N_{n})
- Ammonium (A)
- Phytoplankton (P)
- Zooplankton (Z)
- Bacteria (B)
- Labile DON (L_{N})
- Labile DOC (L_{C})
- Semi-labile DON (S_{N})
- Semi-labile DOC (S_{C})
- Detrital nitrogen (D_{N})
- Detrital carbon (D_{C})

With the exception of the light limitation of photosynthesis and the changes in concentration due to physical processes, the dynamics of each of these pools is as defined in Anderson and Pondaven (2003), hereafter referred to as A&P. The same values are used for all parameters with the exception of the half saturation constant for zooplankton nitrogen uptake k_{g} for which a higher value (3 mmol N m^{-3}) is used here to damp out oscillatory behavior.

The light limitation model is a simple non-spectral model taken from Fasham *et al.* (1990). As in A&P, phytoplankton production is given by

$$F_{\mathrm{P}} = JQ\mu_{\mathrm{P}}\theta_{\mathrm{chl}}P, \tag{1}$$

where J and Q are dimensionless light and nutrient limitation factors respectively, μ_{P} is the maximum biomass specific phytoplankton growth rate expressed in g C (g Chl)$^{-1}$ d^{-1} and θ_{chl} is the variable phytoplankton chlorophyll:C ratio (g Chl (g C)$^{-1}$). Here, the light limitation factor is given by

$$J = \frac{\alpha I_{\mathrm{z}}}{\sqrt{\mu_{\mathrm{P}}^2 + \alpha^2 I_{\mathrm{z}}^2}} \tag{2}$$

where α is the initial slope of the photosynthesis versus irradiance (P-I) curve and I_{z} is the underwater light field. The light field is modelled in terms of the PAR directly below the sea surface I_0, the attenuation of PAR due to water k_{w} (0.04 m^{-1}) and the specific attenuation of PAR due to chlorophyll k_{chl} (taken to be 0.02 m^2 (mg Chl)$^{-1}$):

$$I_{\mathrm{z}} = I_0 \exp\{-(k_{\mathrm{w}} + \theta_{\mathrm{chl}} w_{\mathrm{C}} \theta_{\mathrm{P}} P k_{\mathrm{chl}})z\} \tag{3}$$

where θ_{P} is the phytoplankton C:N ratio (mol C (mol N)$^{-1}$) and w_{C} is the atomic mass of carbon.

The change in concentration of any pool X due to physical processes is modelled as a function of the difference in concentration across the boundary at the base of the mixed layer $X - X_{\mathrm{base}}$, as in Fasham *et al.* (1990):

$$D(X - X_{\mathrm{base}}) = -\frac{m + h^+}{M}(X - X_{\mathrm{base}}), \tag{4}$$

where m is a diffusive mixing rate ($m = 0.1$ m d^{-1}) and h^+ is the rate of mixed layer deepening. With the exception of nitrate, all concentrations are taken to be zero below the mixed layer (i.e. $X_{\mathrm{base}} = 0$).

A.2 NPHD model

This model has 4 nitrogen compartments:

- Nutrient (N)

- Phytoplankton (P)
- Heterotrophic recycling (H)
- Detritus (D_{N}).

It is constructed from the parent model by the following procedure.

- Merge nitrate and ammonium pools into the single nutrient compartment N with uptake kinetics as for nitrate.
- Combine zooplankton, bacteria, labile and semi-labile DON pools into the single heterotrophic recycling compartment H. The fluxes for each component are added (ignoring messy feeding fluxes to DON in the present study). Dependencies of fluxes on the nitrogen content of the individual components are handled by treating each component as a constant but unknown fraction of H. A constant but unknown C:N ratio is assumed for the material pool represented by the new compartment.
- Remove the detrital carbon compartment and assume a constant but unknown C:N ratio for detritus grazed or exported.

With the exception of the fractions controlling the fate of zooplankton mortality, values for all parameters present in the parent model are the same as in that model. The zooplankton mortality fractions are adjusted to compensate for the absence of the messy feeding flux to DON. In the NPHD model, 53% of the flux goes to nutrient and 47% to detritus. These parameters are derived by assuming, as in A&P, that the zooplankton loss term is distributed between the sinks according to an infinite series of higher predators. The remaining parameters (Table 2) are treated as free parameters.

Phytoplankton

$$\frac{\mathrm{d}P}{\mathrm{d}t} = (1-\gamma_1)F_{\mathrm{P}} - G_{\mathrm{P}} - m_{\mathrm{P}}P + D(P), \tag{5}$$

where γ_1 is the fraction of phytoplankton production exuded as DON, G_{P} is the phytoplankton loss due to grazing, m_{P} is the biomass specific natural mortality rate for phytoplankton and $D(P)$ is the change in phytoplankton concentration due to

Table 2: Free parameters in the NPHD model

Parameter	Symbol	Unit	Lower bound	Upper bound
Maximum specific ingestion rate by H due to zooplankton grazing[1]	g'	d^{-1}	0.1	10
Maximum specific loss rate from H due to predation on zooplankton by unmodelled predators[2]	m'_{Z}	d^{-1}	0	0.6
Half saturation constant for H loss[3]	k'_{Z}	mmol N m^{-3}	0	8
Bacterial fraction of H pool	b		0	0.75
Half saturation constant for bacterial excretion (in terms of H concentration)[4]	k'_{L}	mmol N m^{-3}	4.5	450
Heterotroph and DOM C:N ratio	θ_{H}	mol C (mol N)$^{-1}$	5	10
Detritus C:N ratio	θ_{D}	mol C (mol N)$^{-1}$	5	20

[1] $g' = gq$, where q is the zooplankton fraction of H and g is the maximum zooplankton grazing rate in the parent model.

[2] $m'_{\mathrm{Z}} = m_{\mathrm{Z}}q$, where m_{Z} is the maximum zooplankton loss rate in the parent model.

[3] $k'_{\mathrm{Z}} = \frac{k_{\mathrm{Z}}}{q}$, where k_{Z} is the half saturation constant for zooplankton loss in the parent model.

[4] $k'_{\mathrm{L}} = \frac{k_{\mathrm{L}}}{\delta_{\mathrm{L}}\theta_{\mathrm{H}}}$, where k_{L} is the half saturation constant for labile DOC uptake in the parent model and δ_{L} is the labile DON fraction of H.

physical processes. This equation is identical to that in the parent model although there are some differences in the way the production and grazing terms are defined.

In the parent model, the nutrient limitation factor Q in the production term (see Equation 1) is a function of two nutrients: nitrate and ammonium. In the NPHD model, it is redefined for a single nutrient:

$$Q = \frac{N}{k_{\mathrm{N}} + N}, \tag{6}$$

where k_{N} is the half saturation constant for nutrient uptake. (The value for nitrate uptake in the parent model is used.)

The grazing term is a function of the concentrations of zooplankton, phytoplankton, bacteria and detritus. In the NPHD model, constant fractions q and b of H are substituted for the missing Z and B values giving

$$G_{\mathrm{P}} = g'H \frac{p_1 P^2}{k_{\mathrm{g}}(p_1 P + p_2 bH + p_3 D_{\mathrm{N}}) + p_1 P^2 + p_2 (bH)^2 + p_3 D_{\mathrm{N}}^2}. \tag{7}$$

g' is a modified maximum specific grazing rate ($g' = gq$, where q is the zooplankton fraction of H and g is the maximum grazing rate in the parent model, which is specific to zooplankton concentration). p_1, p_2 and p_3 are the grazing preferences for phytoplankton, bacteria and detritus respectively.

Heterotrophic Recycling

$$\frac{\mathrm{d}H}{\mathrm{d}t} = F_{\mathrm{Z}} - G_{\mathrm{B}} - M_{\mathrm{Z}} - E_{\mathrm{B}} + \gamma_1 F_{\mathrm{P}} + \epsilon m_{\mathrm{P}} P + m_{\mathrm{D}} D_{\mathrm{N}} + D(H) \tag{8}$$

The first three terms are zooplankton production, zooplankton grazing on bacteria and zooplankton mortality. Production is dependent on the total grazing on all food sources and the zooplankton physiological parameters as defined in A&P. (The messy feeding losses in the present study are set to zero.) Again, to derive the NPHD model terms from those in the parent model, constant fractions q and b of H are substituted for Z and B. θ_{H} replaces the bacterial C:N ratio for determining carbon ingestion.

G_{B} is of the same form as G_{P} with bH replacing P in the numerator and zooplankton mortality is given by

$$M_{\mathrm{Z}} = \frac{m_{\mathrm{Z}}(qH)^2}{k_{\mathrm{Z}} + qH} \tag{9}$$

The next term in Equation 8, E_{B}, is bacterial excretion which is also modelled after A&P, as in the parent model, but simplifies to

$$E_{\mathrm{B}} = (1 - \omega_{\mathrm{B}})\mu_{\mathrm{B}} \frac{bH}{k'_{\mathrm{H}} + H} \tag{10}$$

where ω_{B} is the bacterial gross growth efficiency and μ_{B} is the max specific DOC uptake rate. Excretion is proportional to the realized uptake of labile DOC. The simplification occurs as a consequence of DOM and bacteria sharing the same C:N ratio θ_{H}. The flux E_{B} is always positive, implying no ammonium uptake for supplementing nitrogen demand. The next three terms in Equation 8 are the DON source terms from the parent model. These represent the sum of the DON source terms in A&P, less the messy feeding terms. ϵ is the DOM fraction of phytoplankton mortality and m_{D} is the detrital breakdown rate.

Detritus

$$\begin{aligned} \frac{\mathrm{d}D_{\mathrm{N}}}{\mathrm{d}t} &= (1 - \beta_{\mathrm{N}})(G_{\mathrm{P}} + G_{\mathrm{B}} + G_{\mathrm{D}}) - G_{\mathrm{D}} + (1 - \epsilon)m_{\mathrm{P}}P + \Omega_{\mathrm{D}}M_{\mathrm{Z}} - \\ &\quad m_{\mathrm{D}}D_{\mathrm{N}} + S(D_{\mathrm{N}}) + D(D_{\mathrm{N}}), \end{aligned} \tag{11}$$

where β_{N} is the nitrogen assimilation efficiency for zooplankton, G_{D} is the zooplankton grazing on detritus (which takes the same form as the grazing terms for other food sources), Ω_{D} is the detrital fraction of zooplankton mortality and $S(D_{\mathrm{N}})$ is the loss due to detritus sinking out of the mixed layer. This is identical to the parent model equation, with the grazing and zooplankton mortality terms being rewritten in terms of H.

Nutrient

$$\frac{\mathrm{d}N}{\mathrm{d}t} = E_{\mathrm{Z}} + E_{\mathrm{B}} + \Omega_{\mathrm{N}} M_{\mathrm{Z}} - F_{\mathrm{P}} + D(N - N_{\mathrm{base}}), \tag{12}$$

where E_{Z} is zooplankton excretion as defined in A&P, Ω_{N} is the nutrient fraction of zooplankton mortality and N_{base} is the nutrient concentration immediately below the base of the mixed layer, taken to be the same as the nitrate value interpolated to this depth from World Ocean Atlas annual mean nitrate profiles (Conkright *et al.*, 1998).

A.3 NPZD model

This model also has 4 nitrogen compartments:

- Nutrient (N)
- Phytoplankton (P)
- Zooplankton (Z)
- Detritus (D_{N}).

It is constructed in the same way as the NPHD model except that fluxes to and from the bacteria and DON pools are ignored. The heterotrophic recycling compartment is thus replaced by a zooplankton only compartment. Detrital breakdown is redirected to the nutrient pool. The free parameters are shown in Table 3. With the exception of the zooplankton mortality fractions Ω_{D} and Ω_{N} (see Section A.2), all other parameter values are the same as in the parent model.

Phytoplankton

$$\frac{\mathrm{d}P}{\mathrm{d}t} = F_{\mathrm{P}} - G'_{\mathrm{P}} - m_{\mathrm{P}} P + D(P), \tag{13}$$

where G'_{P} is the analog of the A&P equation for zooplankton grazing on phytoplankton where there are only two alternative food sources, phytoplankton and detritus (i.e. no bacteria).

Table 3: Free parameters in the NPZD model

Parameter	Symbol	Unit	Lower bound	Upper bound
Zooplankton maximum specific ingestion rate	g	d^{-1}	0.4	10
Zooplankton feeding preference for phytoplankton	p'_1		0.25	0.75
Zooplankton maximum specific loss rate due to predation by unmodelled predators	m_Z	d^{-1}	0	0.6
Half-saturation constant for zooplankton loss	k_Z	mmol N m^{-3}	0	2
Detritus C:N ratio	θ_D	mol C (mol N)$^{-1}$	5.5	20

Zooplankton

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = F_\mathrm{Z} - M_\mathrm{Z} + D(Z). \tag{14}$$

Detritus

$$\begin{aligned}\frac{\mathrm{d}D_\mathrm{N}}{\mathrm{d}t} &= (1-\beta_\mathrm{N})(G'_\mathrm{P} + G'_\mathrm{D}) - G'_\mathrm{D} + m_\mathrm{P}P + \Omega_\mathrm{D}M_\mathrm{Z} - m_\mathrm{D}D + \\ &\quad S(D_\mathrm{N}) + D(D_\mathrm{N}),\end{aligned} \tag{15}$$

where G'_D is the two food source analog of the A&P equation for grazing on detritus.

Nutrient

$$\frac{\mathrm{d}N}{\mathrm{d}t} = E_\mathrm{Z} + \Omega_\mathrm{N}M_\mathrm{Z} + m_\mathrm{D}D_\mathrm{N} - F_\mathrm{P} + D(N - N_\mathrm{base}). \tag{16}$$

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