

Enhancing ocean biogeochemical model performance and generality with phytoplankton variable composition

Prima Anugerahanti¹, Onur Kerimoglu², and S. Lan Smith³

¹Japan Agency for Marine-Earth Science and Technology

²Institute for Coastal Research, Helmholtz Zentrum Geesthacht

³Frontier Research System for Global Chan

November 26, 2022

Abstract

Chlorophyll (Chl) is widely taken as a proxy for phytoplankton biomass, despite well known variations in Chl:biomass ratios as an acclimative response to changing environmental conditions. For the sake of simplicity and computational efficiency, many large scale biogeochemical models ignore this flexibility, compromising their ability to capture phytoplankton dynamics. Here we evaluate modelling approaches of differing complexity for phytoplankton growth response: fixed stoichiometry, classical variable-composition with photo-acclimation, and Instantaneous Acclimation with optimal resource allocation. We compare the performance of these models against biogeochemical observations from time-series sites BATS and ALOHA, where phytoplankton composition varies substantially. Models including photo-acclimation capture the observations better with minimal parameter tuning and are more portable. Compared to the classical variable composition approach, instantaneous acclimation yields similar performance and portability, while requiring fewer state variables. Further assessments using objective optimisation and more contrasting stations are suggested.

Enhancing ocean biogeochemical model performance and generality with phytoplankton variable composition

Prima Anugerahanti ¹, Onur Kerimoglu ², and S. Lan Smith ¹

¹Earth SURFACE System Research Center, Research Institute for Global Change, JAMSTEC, Yokosuka,
Japan

²Institute for Chemistry and Biology of the Marine Environment, University of Oldenburg, Germany

Key Points:

- We evaluate different approaches for modelling phytoplankton growth response and related biogeochemistry
- Models including variable composition agree better with observations from two oligotrophic sites
- Instantaneous acclimation model requires fewer state variables but maintains skill and portability

Corresponding author: P. Anugerahanti, panu09@jamstec.go.jp

Abstract

Chlorophyll (Chl) is widely taken as a proxy for phytoplankton biomass, despite well known variations in Chl:biomass ratios as an acclimative response to changing environmental conditions. For the sake of simplicity and computational efficiency, many large scale biogeochemical models ignore this flexibility, compromising their ability to capture phytoplankton dynamics. Here we evaluate modelling approaches of differing complexity for phytoplankton growth response: fixed stoichiometry, classical variable-composition with photo-acclimation, and Instantaneous Acclimation with optimal resource allocation. We compare the performance of these models against biogeochemical observations from time-series sites BATS and ALOHA, where phytoplankton composition varies substantially. Models including photo-acclimation capture the observations better with minimal parameter tuning and are more portable. Compared to the classical variable composition approach, instantaneous acclimation yields similar performance and portability, while requiring fewer state variables. Further assessments using objective optimisation and more contrasting stations are suggested.

Plain Language Summary

Phytoplankton (tiny floating algae) play major roles in the ocean; as the base of the food web and in exporting carbon from the surface to depth. They sustain growth by actively altering their composition in terms of nutrients and especially chlorophyll, which can be easily observed. However, for the sake of simplicity and fast calculations, many global models ignore this flexibility, which yields inaccurate estimates of phytoplankton and associated carbon export. We assess the performance and general applicability of model formulations of differing complexity. Our findings suggest that, compared to simplistic fixed-composition models: 1) variable composition enhances model performance and general applicability (portability) at the cost of more calculations, whereas 2) an efficient Instantaneous Acclimation approach enhances performance and portability without substantially increasing computational requirements.

1 Introduction

Although phytoplankton largely drive the oceanic carbon cycle, including the export of carbon (C) from the surface to depth, direct observations of their carbon biomass are rare. The most widely observed metric of phytoplankton is chlorophyll (Chl), because

of its distinctive optical properties (Macintyre et al., 2000), but Chl:C:nutrient ratios vary widely in response to fluctuations in ambient light and nutrient levels (Geider & La Roche, 2002; Mongin et al., 2006; Martiny et al., 2013). Inaccurate estimates of phytoplankton C biomass limit our ability to quantify C export, and therefore our understanding of how climate change is affecting marine ecosystems (Polovina et al., 2008; Arteaga et al., 2016). Nonetheless, for the sake of computational efficiency and simplicity, many large scale marine biogeochemical (MBGC) models use a simplistic Monod (1949) type formulation for phytoplankton growth, assuming constant composition (Bopp et al., 2013; Totterdell, 2019; Le Quere et al., 2005). That assumption may not be problematic in some regions, such as the Mediterranean Sea (Faugeras et al., 2003) or the North Atlantic (Ward et al., 2013). However, variable composition is central to the complex biogeochemistry of the vast oligotrophic ocean (Ayata et al., 2013; Mongin et al., 2006; Steinberg et al., 2001).

Compared to models assuming constant composition, those accounting for acclimation processes (individual-level physiologic response and associated variations in Chl:C:nutrient ratios) reproduce better observations at oligotrophic time-series sites (Schartau et al., 2001; Ayata et al., 2013). However, including flexible composition can be computationally expensive; the dynamics of C and nutrients bound to phytoplankton (i.e., internal stores) are typically described using the Droop 'quota' model (Caperon, 1968; Droop, 1968), which requires a separate state variable for each element or nutrient resolved (Ward, 2017; Chen & Smith, 2018). Apart from computational cost, added complexity also increases the number of uncertain parameters (Kwiatkowski et al., 2014; Ward, 2017) and can make models less portable (Friedrichs et al., 2007). Recently, a computationally efficient 'Instantaneous Acclimation' (IA) model was shown to capture phytoplankton seasonality, including variable composition, at two contrasting stations in a 0-D setup (Smith et al., 2016). Further tests suggested that it may be suitable for application in large-scale MBGC models (Ward, 2017).

For global scale studies, particularly Earth system climate modelling, MBGC models pose the formidable challenge of capturing a wide range of oceanic regions with computational efficiency and minimal parameter tuning. Here, we evaluate different formulations for the flexible composition and acclimative response of phytoplankton, in terms of model performance in a 1-D setup. We apply the IA-based FlexPFT model (Smith et al., 2016) and two controls: a droop-quota model, which captures variable composition by calculating phytoplankton C and nitrogen (N) separately (and is therefore less

computationally efficient), and a typical Monod-type fixed stoichiometry model. Each phytoplankton model is incorporated into an otherwise identical Nutrient Phytoplankton Detritus (NPD) model. We compare the performance of the three model variants at two oligotrophic sites, where phytoplankton composition is known to deviate from the average 'Redfield ratio' (Ayata et al., 2013; Mongin et al., 2006; Steinberg et al., 2001) typically assumed in fixed stoichiometry models. The two sites differ in physical conditions; ALOHA (A Long term Oligotrophic Habitat Assessment, 22.75°N, 158°W), with permanent stratification (Kavanaugh et al., 2018) and BATS (Bermuda Atlantic Time Series, 31.67°N, 64.167°W) with its seasonal cycle of deep mixing (Dave & Lozier, 2010). We then conduct cross-validation experiments to test each model's ability to capture the dynamics at these two challenging sites.

2 Methods

The IA, monod-type (hereafter FS), and droop quota (hereafter DQ) model variants are all implemented within the NFlexPD model (Kerimoglu et al., submitted) with one phytoplankton type and one limiting nutrient (nitrogen), written in the Framework for Aquatic Biogeochemical Models (FABM, (Bruggeman & Bolding, 2014)). This allows switching between different formulations to describe phytoplankton growth and uptake in a common modelling framework. In the FS model phytoplankton growth rate is limited by the ambient nutrient, following the Monod formulation. The DQ and IA models assume that phytoplankton growth rate depends on the the internal cellular quota (molar N:C ratio) and photoacclimation (C:Chl ratio of the chloroplast). In the IA model, these internal ratios as well as physiological allocation factors acclimate instantly to optimize net growth rate (Smith et al., 2016). However, the DQ model, which lacks such physiological allocations, calculates phytoplankton C and N separately. Despite different assumptions, all model variants follow a similar set of differential equations for the dynamics of the state variables: dissolved inorganic nitrogen (DIN), C and N bound to phytoplankton (P_C and P_N), Detritus (D_C and D_N), Dissolved Organic Nitrogen (DON), and Dissolved Organic Carbon (DOC). The DQ variant is described in detail in the supplementary material section 1 and Fig S1. Kerimoglu et al. (submitted) describe the IA and FS variants in detail.

2.1 Simulations

We simulate two oligotrophic stations with extensive time-series observations: ALOHA and BATS. In order to simulate realistic conditions with a 1-D setup, we use the General Ocean Turbulence Model (GOTM, (Burchard et al., 2006)). As the initial conditions for the hydrodynamical model, we use in situ temperature and salinity profiles (obtained from <https://hahana.soest.hawaii.edu/hot/hot-dogs/cextraction.html> and <https://bios.edu/BATS/ctd/> for ALOHA and BATS, respectively). Meteorological forcing, from the European Centre for Medium-Range Weather Forecasts (ECMWF), ERA-5 hourly reanalysis, with horizontal resolution of $0.25^\circ \times 0.25^\circ$ (<https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-single-levels?tab=overview>), include: wind speed, air pressure, air temperature, humidity, cloud cover, shortwave radiation, and precipitation, each calculated using the Fairall et al. (1996) method. The model domain, split into 100 levels with surface zooming, extends to 500m for ALOHA and 450m for BATS, where some temperature and salinity profiles are limited to 450m. To describe the background turbidity, we assume Jerlov type IA for ALOHA, based on field measurements in the North Pacific (Paulson & Simpson, 1977), and Jerlov type I for the very clear water at BATS (Kullenberg, 1984).

All model variants are run for eight years, from 1st January 2008 - 31st December 2016. The first three years, as spinup period, are forced using repeating climatology of the meteorology, temperature, and salinity. The last five years of model output is compared with observations of Chl, DIN and primary production (PP), which can be obtained from <http://batsftp.bios.edu/BATS/bottle/> and <https://hahana.soest.hawaii.edu/hot/hot-dogs/bextraction.html>, for BATS and ALOHA, respectively.

In order to thoroughly assess how well each model variant captures the observations, and its portability (i.e., applicability to different sites without re-tuning parameter values), we perform three experiments: (i) the reference simulations of each station with individually tuned parameter sets (model runs labelled IA, FS, and DQ); (ii) cross-validation, where phytoplankton-related parameters tuned for station ALOHA are applied at station BATS and vice versa, (model runs labelled IA-X, FS-X, and DQ-X); and (iii) simultaneous runs using a common parameter set for phytoplankton-related processes at both stations, (labelled IA-S, FS-S, and DQ-S). For experiments (ii) and (iii) initial conditions and some abiotic parameters, such as sinking speed and detrital degradation

rate, are kept the same as experiment (i) for each station. We quantify model performance in terms of correlation, bias, RMSE, and a weighted cost function for overall mismatch between models and observations. However, as we did not conduct data assimilation, we omit the ψ_k term from the cost function (equation (1) in Friedrichs et al. (2007)). Thus, the individual (variable specific) and total cost functions, J_m and J , respectively becomes:

$$J_m = \frac{W_m^2}{N_m} \sum_{j=1}^{N_m} (a_{jm} - \hat{a}_{jm})^2 \quad (1a)$$

$$J = \frac{1}{M} \sum_{m=1}^M J_m \quad (1b)$$

Where M is the number of variable types ($M=3$; Chl, DIN, and PP), N_m is the number of observations of type m , and a_{jm} and $\hat{a}_{jm}$ are the modelled and observed values, respectively. The weight, W_m , is proportional to the reciprocal of the standard deviation (σ) for each observation type ($W_m = \frac{C_m}{\sigma}$, where $C_m = 3.5$, for Chl and DIN and $C_m = 5$ for PP, since it has larger variance). We quantify model portability in terms of the portability index (PI , Friedrichs et al. (2007)) which is the ratio of total costs (equation 1) from simultaneous experiment and the cross-validation experiment:

$$PI = J^s / J^x \quad (2)$$

PI values approaching unity indicate increasing portability. For all experiments, parameters for the IA and FS variants were manually tuned within the literature values (i.e. Sommer, 1991; Edwards et al., 2012; Kane et al., 2011; Yool et al., 2013; Pahlow et al., 2013; Smith et al., 2016; Robson et al., 2018), described in supporting information Table S1. In order to isolate the effect of instantaneous acclimation from that of parameter sensitivity, we apply similar parameter sets for the IA and DQ variants. For the FS and DQ variants, the fixed allocation factors (fractional allocation towards nutrient uptake and Chl:C ratio of chloroplast) are set to their biomass-weighted mean values from the IA runs. We compare the model outputs with observed Chl, DIN, and PP.

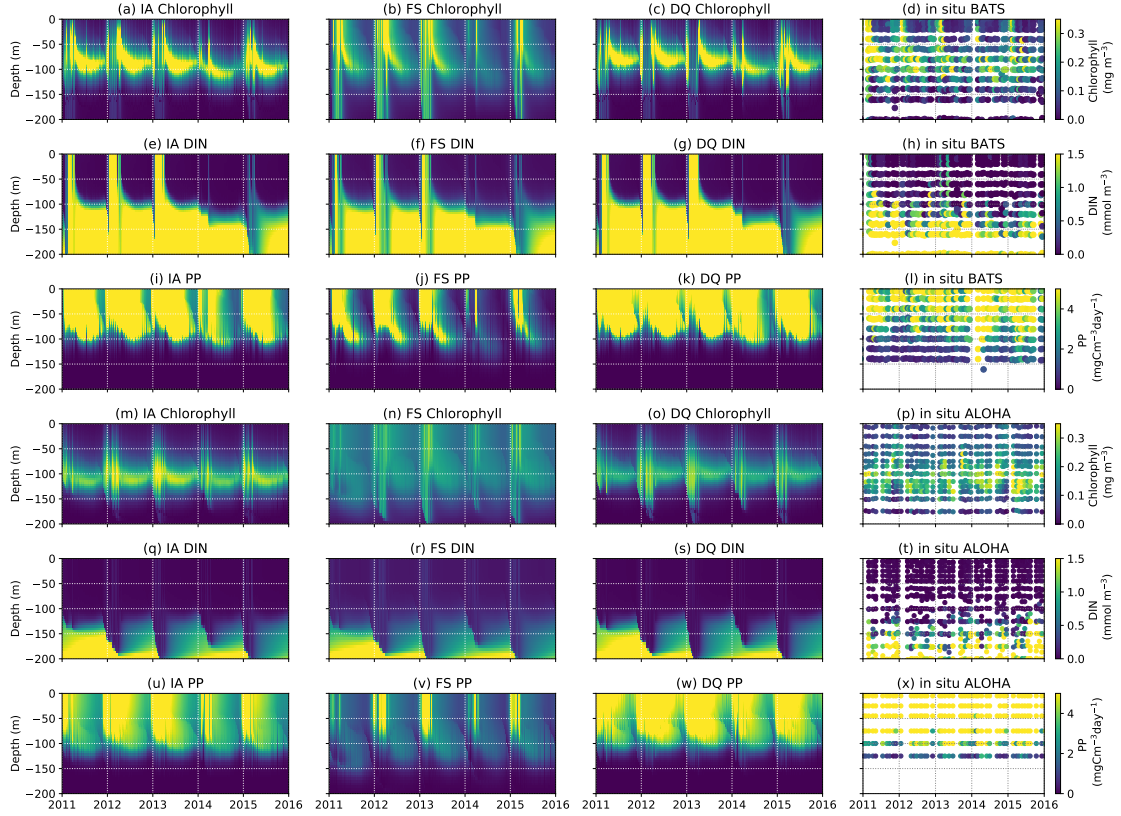


Figure 1. Contour plots of Chl, DIN, and PP at stations BATS (a-l) and ALOHA (m-x) from 1st of January 2011 to 31st December 2015.

3 Results

3.1 Performance of the three variants

In oligotrophic regions, summertime nutrient concentrations are typically < 0.01 mmol m^{-3} within the euphotic zone (Anderson & Pondaven, 2003; Dave & Lozier, 2010; Steinberg et al., 2001), with vertical stratification that is destroyed by deep mixing during winter and spring (Dave & Lozier, 2010). All model variants capture these characteristics well, as seen in the DIN distributions (Fig 1e-g, Fig. 2d-f, and Fig. 3c and d). At station BATS, winter mixing typically increases DIN from ~ 0.05 to 0.5 mmol m^{-3} (Fig 1h), as captured by all model variants, but exaggerated by the IA and DQ (Fig 1e and g). The FS variant overestimates average summertime DIN within the upper 50m (Fig 3 c-d). However, at 75-125m between summer and fall the three variants are more similar, with the DQ variant producing slightly higher DIN than the FS variant (Fig 3g-h). The IA variant consistently produces the lowest DIN concentrations. Although all

169 model variants realistically capture DIN seasonality in the upper 50m, none captures the
 170 sporadic spikes of DIN that occur at both stations (Fig 3g-h).

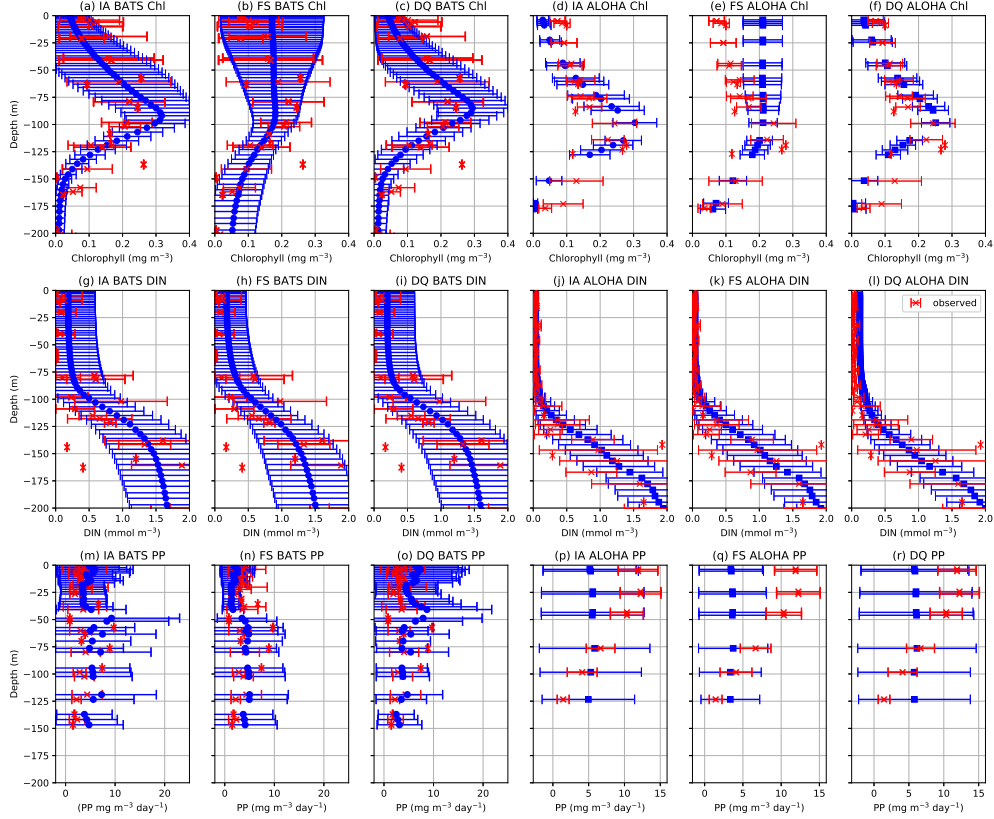


Figure 2. Vertically averaged values of modeled (blue) and observed (red) Chl, DIN, and PP from 1st January 2011 to 31st December 2015. Profiles for station BATS are shown in a-c, g-i, and m-o, for Chl, DIN, and PP respectively. For station ALOHA, profiles are shown in d-f, j-l, and p-r, for Chl, DIN, and PP respectively.

171 Similar to DIN, Chl in the oligotrophic region is typically scarce in the euphotic
 172 zone due to nutrient limitation. At depths between 50-200m where nutrients are more
 173 abundant, subsurface Chl maxima (SCM) occur during summer (Dave & Lozier, 2010;
 174 Mignot et al., 2014). All variants capture these characteristics qualitatively well, both
 175 seasonally and vertically at BATS (Fig 1a-c). However, at ALOHA the FS variant is un-
 176 able to simulate low Chl in the upper 100m, nor distinct summertime SCM profiles (Fig 1n,
 177 and Fig 2h). All model variants capture typical Chl concentrations and seasonality for
 178 the SCMs that usually occur between 75-125m at both stations (Fig 2a-c and Fig 3e).
 179 However, when averaged vertically, the IA variant tends to overestimate Chl concentra-

tions compared to other variants (Fig 2a). This result differs from Ayata et al. (2013), where all models underestimated SCM concentrations, except during blooms. Although the IA and DQ variants are qualitatively similar at BATS, generally the latter simulates slightly lower Chl and shallower SCMs at both stations, compared to the IA variant (Fig 1a, c). This agrees with the IA variant's generally lower C:N and higher Chl:C ratios, compared to the DQ (see supplementary material Fig. S2). Comparing all model variants, from 75 to 125m, the FS variant produces the lowest Chl because it lacks flexible quota, but from June through November, it produces higher Chl than DQ. Despite capturing the DIN concentration in the upper 50m, neither the DQ nor IA variant captures the summer Chl at ALOHA (Fig 3b and d).

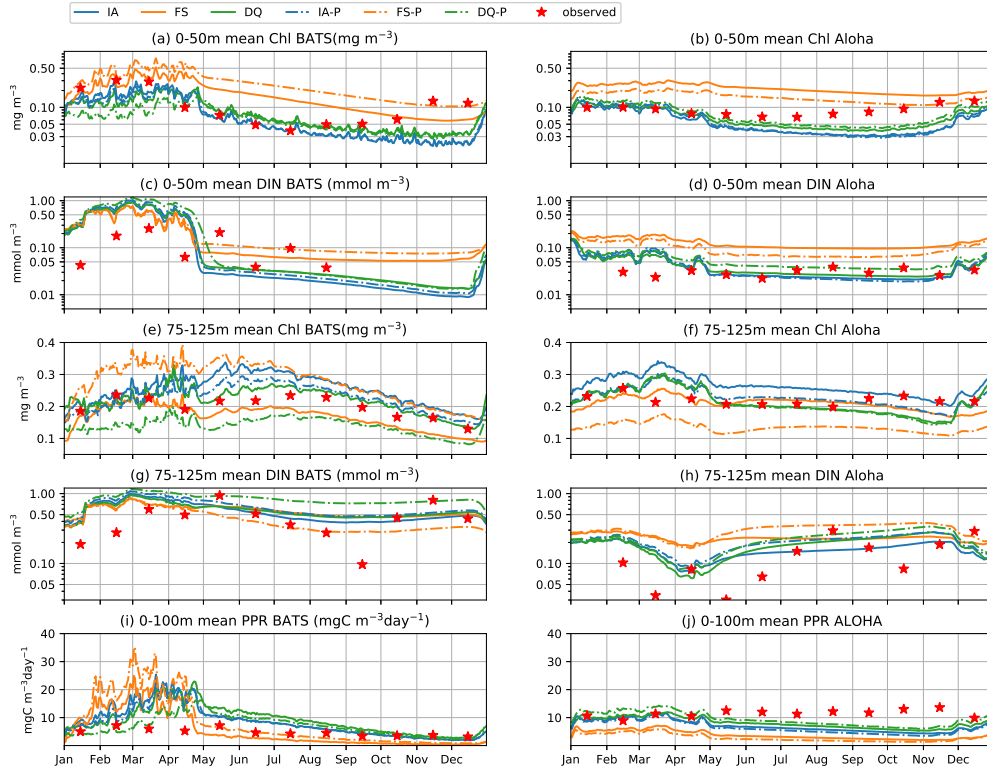


Figure 3. Depth averaged (upper 50m, and between 75-125m) Chl, DIN, and PP for the period of 1st January 2011 to 31st December 2015, for the IA (blue), FS (orange), and DQ (green) model variants respectively. Solid lines: individually tuned runs; dash-dot lines: cross-validation experiments; red stars: monthly averaged *in situ* DIN, Chl, and PP measurements. The upper 50m is most consistently stratified, and the nutricline and SCM usually occur from 75 to 125m. PP was averaged over the upper 100m, where PP is $> 3 \text{ mgC m}^{-3} \text{ day}^{-1}$.

Unlike Chl and DIN, PP in oligotrophic regions usually occurs within the upper $\sim 120\text{m}$ (Dave & Lozier, 2010). All variants capture the PP depth and its decline during summer at BATS, but with higher PP and later peaks than observed (Fig 1i-j and Fig 3i). The FS variant produces the most distinct pattern with brief spikes of higher PP ($>20 \text{ mgC m}^{-3} \text{ day}^{-1}$) compared to the observations and other variants. When averaged horizontally, the photo-acclimative variants generally capture well observed PP, but the FS underestimates PP in the top 50m because of its low summertime PP (Fig 1i). The IA and DQ variants simulate a slight increase in PP at $\sim 50\text{m}$, but in the observations, it occurs at $\sim 60\text{m}$ (Fig 2m and o). Unlike BATS, PP at ALOHA peaks in the summer, and declines in spring (Dave & Lozier, 2010), with the highest rate recorded in the upper 50m, decreasing with depth (Fig 2p-r). None of the variants capture these patterns, especially the FS variant which consistently underestimates PP in the upper 50m (Fig 3j and 2q), but the IA and DQ do capture winter and spring PP rates. The DQ variant produces generally the highest PP, as well as the highest C:N ratio within the upper 50m (supplementary material Fig S2), and therefore agrees best with the observations at ALOHA (Fig 3j).

The target diagrams (Jolliff et al., 2009) and cost values (J_m , J) quantify differences between the model variants, which perform similarly for DIN, but differ more for Chl and PP (Figs. 4 and S3). In terms of overall performance, the IA produced the lowest cost and bias, and the highest correlation for Chl. The DQ variant produces better statistical metrics and the lowest J for PP, but slightly lower correlations, and higher RMSD and cost for DIN and Chl, compared to IA. At BATS J for DQ is lower than for IA (Fig. S3). The FS variant performed the worst in terms of Chl and PP, and consequently, produced the largest overall costs (see Table S2 in the supporting material). In terms of DIN the FS variant produced the lowest cost and bias, and slightly higher correlation compared to the other variants (e.g. DIN correlations for FS, DQ, and IA are 0.74, 0.73, and 0.72, respectively at ALOHA). For DIN the IA and DQ variants produce higher bias and RMSD, compared to the FS, especially at BATS, which is also reflected in the J_{DIN} .

3.2 Model portability

The cross-validation experiment tests a model's ability to reproduce observations from different regions without tuning, and therefore its predictive ability (Friedrichs et

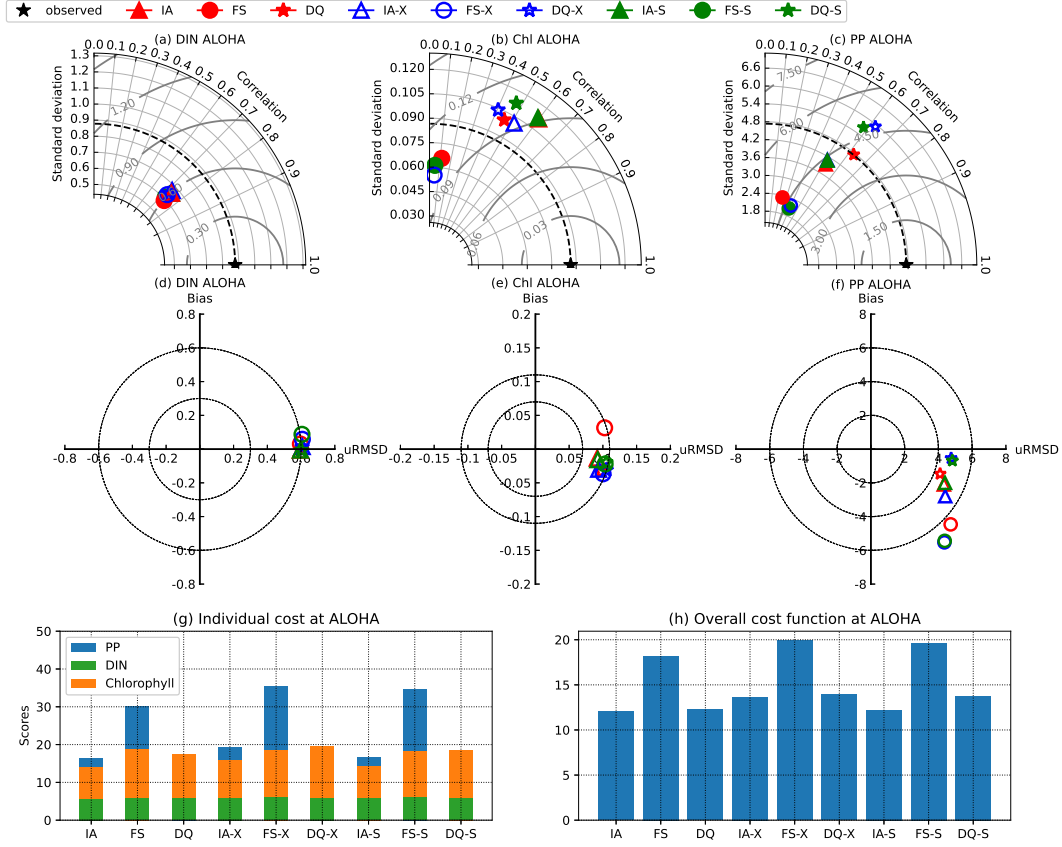


Figure 4. Taylor (a-c), target (d-f) diagrams (μ RMSD is normalised RMSD), and costs (g-h) for Chl, DIN, and PP at station ALOHA for the IA (triangles), FS (circles), and DQ (stars) variants, each tuned individually to the observations (red), cross-validated (blue), and simulating both stations with a common parameter set (green). The cost functions J_m (g) and J (h) were calculated for the individually tuned runs, cross validation experiment (-X suffix) and the simultaneous experiment using a common parameter set (-S suffix), for each model. The figure for BATS is shown in supporting information Fig. S3. Values for J_m , J and PI are provided in supporting information Table S2.

al., 2006). In this experiment, all model variants differ only slightly in their statistical metrics for DIN, compared to the individual tuning. However, for Chl and PP, using the parameter set tuned for a different station generally increases RMSD, bias, and reduces correlation for all variants (Fig 4a-c, supporting Fig. S3a-c). In the cross-validation experiment the FS variant's performance suffers most, and also differs most compared to the individual tuning, notably between 75-125m (dot-dashed and solid lines in Fig 3e and f). For the IA and DQ variants, the cross validation and individually tuned results differ only slightly from the observations within the upper 50m, especially during summer. However, at 75-125m, the cross validations from IA and DQ often overestimate and underestimate observed Chl at BATS and ALOHA, respectively (Fig 3e and f). Overall between cross-validation and individual tuning, the DQ variant differs least in terms of J and bias followed by IA, and FS (Fig 4d-h). However, in terms of correlations and RMSD, the IA differs least.

The simultaneous experiment evaluates the potential applicability of each model variant at multiple stations with a common parameter set, as in a typical global biogeochemical model (Friedrichs et al., 2007). Individual and simultaneous tuning yield relatively similar J values and statistical metrics. As discussed in (Friedrichs et al., 2007), the ideal model would have a $PI \sim 1$ (equation 2), indicating good performance at multiple sites without being tuned individually for each, while also having a low cost. Fig 4 and Fig S3 reveals that the models with photoacclimation have lower cost, as well as greater portability; i.e. including variable internal composition enhances portability, at least between these oligotrophic sites. Overall the DQ variant produces slightly better cost than IA (average costs over all experiments for IA and DQ are 27.3 and 26.9, respectively) and in terms of portability the IA variant is nominally closer to 1, indicating similar portability and skill for these two model variants.

4 Discussion

Phytoplankton acclimate, i.e. regulate their physiology and composition, in order to sustain growth under changing conditions (Smith et al., 2011; Moreno & Martiny, 2018). For example, as light becomes limiting Chl:C ratio increases (Laws & Bannister, 1980; Geider et al., 1998), and as nutrients increase C:N ratio decreases (Mongin et al., 2006). However, large-scale MBGC models often assume constant elemental and pigmentary composition for phytoplankton (Laufkotter et al., 2015; Bopp et al., 2013), similar to the

FS approach herein. Others represent these flexibilities in elemental composition, typically using a Droop quota model, but seldom with a more consistent allocation framework in large-scale MBGC models (Kerimoglu et al., 2017; Kwiatkowski et al., 2018; Pahlow et al., 2020). These approaches typically require additional state variables and calculations. To overcome these problems, Smith et al. (2016) proposed the IA approach, which optimizes Chl:C:nutrient ratios instantaneously for local conditions, so that variable composition can be tracked via a single state variable (biomass). We have recently demonstrated that the IA approach behaves similar to the fully dynamic version in a spatially explicit 1D setup (Kerimoglu et al., submitted). Here we assess the performance, against *in-situ* observations at two oceanic stations with differing physics, of three different models for phytoplankton growth: FS, DQ, and IA, with varying degrees of flexible composition and computational efficiency. Specifically, we test whether variable elemental and pigment compositions are sufficient for model generality and portability (DQ vs. FS) and whether physiological acclimation provides further benefits (IA vs. DQ).

4.1 Model performance with individual tuning

With parameters tuned individually for each station, compared to the FS variant, the photo-acclimative variants capture better common features in the oligotrophic ocean, such as the depletion of DIN and Chl in the summer, near-surface primary production, and deep SCM (Mignot et al., 2014; Ayata et al., 2013; Kavanaugh et al., 2018). Because the FS variant cannot adjust its internal composition, i.e decrease its Chl:C and N:C during the stratified summer, it often overestimates near-surface Chl and DIN, underestimates SCM concentrations, and produces brief bursts of intense PP. The three variants differ most in terms of Chl between 75-125m, where the optimal physiological acclimation in the IA variant sustains growth and hence higher biomass and Chl (Fig S2, supporting information), and higher C:N ratio than the DQ during summertime nutrient depletion (Fig 3e and f). Despite its lack of optimal resource allocation, the DQ variant, which relies on a fixed parameterization for variable C:N ratios and acclimation of chloroplast-specific chlorophyll density, captures PP better, as reflected in its highest correlation and lowest overall cost, J . However, this is also because PP has a higher weight than other observables, and a larger sum of squared differences $((a_{jm} - \hat{a}_{jm})^2)$. Furthermore, *in situ* PP is measured using ^{14}C incubation at both stations (Letelier et al., 1996; Steinberg et al., 2001). It is known that this procedure can result in inaccurate PP val-

ues, including over-estimates in the presence of slow-growing species (Pei & Laws, 2013, 2014), and it is unclear whether they measure net or gross PP (Marra, 2009; Kavanaugh et al., 2018).

Although the IA and DQ variants realistically simulate near-surface DIN (Fig 3d), they do not capture the summer phytoplankton blooms (Dore et al., 2008) and increase in PP (Dave & Lozier, 2010) that usually occurs in the North Pacific Subtropical Gyre. This discrepancy may be due to the absence of nitrogen fixers in NFlexPD (Dore et al., 2008; Church et al., 2009; Böttjer et al., 2017), or the lack of sporadic mixing, which lifts the thin layer of Chl in the subsurface (Dore et al., 2008) and other processes, such as anticyclonic eddies or effects of El-Nino (Church et al., 2009; Kavanaugh et al., 2018) that are not well simulated by the 1D physical model. At BATS, DIN concentrations during winter mixing are often overestimated by the IA and DQ variants. This may be due to the lower mortality rate (0.75 d^{-1}) applied herein for the FS variant, compared to the IA and DQ variants (2.5 d^{-1}). Additionally, nutrient and light limitation in FS are multiplicative, compared to the interactive effects of multi-resource limitation in the IA variant (see Fig. 3 of Smith et al. (2011)). Hence, as either nutrient or light becomes depleted, growth is more severely limited in the FS variant, compared to the IA.

4.2 Model Portability

The physiological acclimation, which aims to optimize growth rate in the IA and DQ variants, is similar to dynamic optimization of parameter values (e.g. Mattern et al., 2012), which is typically applied to capture complex adaptive behaviours in response to environmental changes (Arhonditsis & Brett, 2004), e.g. physiological plasticity or succession of plankton groups (Follows & Dutkiewicz, 2011). It is therefore expected that the IA variant, which continually re-allocates resources to optimize growth, would capture better DIN and Chl dynamics at both stations in the cross-validation and simultaneous experiments. Although earlier studies (Friedrichs et al., 2007; Kriest et al., 2012; Ward et al., 2013) found that increasing model complexity does not necessarily improve misfits or predictive capability, here we find that the acclimative models overall perform better compared to the simpler FS variant. Comparing the FS with the DQ and IA variants, including flexible composition increases portability, based on the statistical metrics, J , and PI . When compared to DQ, optimal acclimation as formulated in the IA variant does not massively enhance portability; however, IA has fewer state variables and

produces better statistical metrics for Chl and DIN. Thus, when applied to a 3D regional MBGC model for oligotrophic regions, the IA variant can be expected to more realistically capture phytoplankton growth, nutrient uptake, and chlorophyll concentrations, with fewer state variables.

4.3 Future outlook

This study has shown that adding photoacclimation and variable phytoplankton composition can improve model portability and performance. The portability experiment could be extended by applying data assimilation to fit each model variant to the observations as done previously in a 0-D setup (Smith et al., 2016) and by performing cross validation experiments between more contrasting (e.g., subpolar and subtropical) regions. Behrenfeld et al. (2016) showed that across most of the ocean variations in Chl, the most widely observed metric of phytoplankton, result more from physiological acclimation than from variations in their biomass. Models that account for photoacclimation can help to disentangle the mechanisms underlying observed Chl variations. Although both the IA and DQ variants capture Chl, PP, and DIN concentrations well, the idealized models presented herein are too simplistic to fully capture oligotrophic ecosystem dynamics. Multiple plankton types inhabit oligotrophic regions, including zooplankton (Dave et al., 2015) and N-fixers (Dore et al., 2008; Karl et al., 2012) as well as other nutrients, such as phosphate (Steinberg et al., 2001; Karl et al., 2012); but our models only represent one type of phytoplankton and nutrient. Other physical processes such as mesoscale eddies and inter-annual variations driven by El-Nino/La-Nina events, cannot be captured by the 1-D setup. For comprehensive MBGC model applications, it is essential to trace C, O₂, and alkalinity (Kwiatkowski et al., 2014).

5 Conclusions

We test an NPD-type model with three different variants differing with respect to phytoplankton flexible composition and acclimative response: A Monod-type variant with fixed stoichiometry (FS), another one with Droop quota (DQ) with photoacclimation, and finally the Instantaneous Acclimation (IA) variant. We assess whether adding variable composition and acclimation can enhance generality and portability at two oligotrophic stations BATS and ALOHA. We find that the DQ and IA variants with variable C:N and Chl:C ratios capture better the observations at both stations compared to the FS

variant. Flexible composition also enhances portability and hence potential applicability at large scales. Optimal acclimation only slightly enhances portability, but does improve realism for DIN and Chl as quantified by statistical metrics. However, these experiments are done without parameter optimisation and limited to oligotrophic sites. Further studies using objective optimisation (data assimilation) and including more contrasting regions would provide a more comprehensive and thorough assessment.

Acknowledgments

PA, SLS, and OK are funded jointly by the Japan Society for the Promotion of Science, JSPS (P.I: SLS) and German Research Foundation DFG (grant no. KE 1970/2-1, P.I.: OK). The NFlexPD model is described in Kerimoglu et al. (submitted) and available in the ‘fabm-nflexpd’ branch of the git repository: <https://github.com/OnurKerimoglu/fabm-nflexpd>. Target diagrams are plotted using ‘SkillMetrics’ python package (<https://github.com/PeterRochford/SkillMetrics/wiki>), and Taylor diagrams plots are done using the python code provided by Yannick Copin (<https://gist.github.com/ycopin/3342888>). This publication is based upon Hawaii Ocean Time-series observations supported by the U.S. National Science Foundation under Award #1756517. All authors designed the study, PA performed the model runs, analysed the outputs, and prepared the figures. All authors contributed equally to the writing of the manuscript.

References

- Anderson, T. R., & Pondaven, P. (2003). Non-redfield carbon and nitrogen cycling in the Sargasso Sea: Pelagic imbalances and export flux. *Deep-Sea Research Part I: Oceanographic Research Papers*, 50(5), 573–591. doi: 10.1016/S0967-0637(03)00034-7
- Arhonditsis, G. B., & Brett, M. T. (2004). Evaluation of the current state of mechanistic aquatic biogeochemical modeling. *Marine Ecology Progress Series*, 271(21), 13–26. doi: 10.3354/meps271013
- Arteaga, L., Pahlow, M., & Oschlies, A. (2016). Modeled Chl:C ratio and derived estimates of phytoplankton carbon biomass and its contribution to total particulate organic carbon in the global surface ocean. *Global Biogeochemical Cycles*, 30(12), 1791–1810. doi: 10.1002/2016GB005458
- Ayata, S. D., Lévy, M., Aumont, O., Sciandra, A., Sainte-Marie, J., Tagliabue, A., &

- 380 Bernard, O. (2013). Phytoplankton growth formulation in marine ecosystem
381 models: Should we take into account photo-acclimation and variable stoichiometry
382 in oligotrophic areas? *Journal of Marine Systems*, 125, 29–40. doi:
383 10.1016/j.jmarsys.2012.12.010
- 384 Behrenfeld, M. J., O'Malley, R. T., Boss, E. S., Westberry, T. K., Graff, J. R.,
385 Halsey, K. H., ... Brown, M. B. (2016). Revaluating ocean warming im-
386 pacts on global phytoplankton. *Nature Climate Change*, 6(3), 323–330. doi:
387 10.1038/nclimate2838
- 388 Bopp, L., Resplandy, L., Orr, J. C., Doney, S. C., Dunne, J. P., Gehlen, M., ...
389 Vichi, M. (2013). Multiple stressors of ocean ecosystems in the 21st century:
390 Projections with CMIP5 models. *Biogeosciences*, 10(10), 6225–6245. doi:
391 10.5194/bg-10-6225-2013
- 392 Bruggeman, J., & Bolding, K. (2014). A general framework for aquatic biogeochemi-
393 cal models. *Environmental Modelling and Software*, 61, 249–265. doi: 10.1016/
394 j.envsoft.2014.04.002
- 395 Burchard, H., Bolding, K., Kühn, W., Meister, A., Neumann, T., & Umlauf, L.
396 (2006, jul). Description of a flexible and extendable physical-biogeochemical
397 model system for the water column. *Journal of Marine Systems*, 61(3-4),
398 180–211. doi: 10.1016/j.jmarsys.2005.04.011
- 399 Böttjer, D., Dore, J. E., Karl, D. M., Letelier, R. M., Mahaffey, C., Wilson, S. T.,
400 ... Church, M. J. (2017). Temporal variability of nitrogen fixation and par-
401 ticulate nitrogen export at station aloha. *Limnology and Oceanography*, 62(1),
402 200–216. doi: <https://doi.org/10.1002/lno.10386>
- 403 Caperon, J. (1968). Population growth response of *Isochrysis Galbana* to nitrate
404 variation at limiting concentrations. *Ecology*, 49(5), 866–872.
- 405 Chen, B., & Smith, S. L. (2018). Optimality-based approach for computation-
406 ally efficient modeling of phytoplankton growth, chlorophyll-to-carbon, and
407 nitrogen-to-carbon ratios. *Ecological Modelling*, 385(August), 197–212. doi:
408 10.1016/j.ecolmodel.2018.08.001
- 409 Church, M. J., Mahaffey, C., Letelier, R. M., Lukas, R., Zehr, J. P., & Karl, D. M.
410 (2009). Physical forcing of nitrogen fixation and diazotroph community struc-
411 ture in the North Pacific subtropical gyre. *Global Biogeochemical Cycles*,
412 23(2). doi: 10.1029/2008GB003418

- 413 Dave, A. C., Barton, A. D., Lozier, M. S., & McKinley, G. A. (2015). What drives
414 seasonal change in oligotrophic area in the subtropical North Atlantic? *Journal*
415 *of Geophysical Research: Oceans*(120), 3958–3969. doi: 10.1002/jgrc.20224
- 416 Dave, A. C., & Lozier, M. S. (2010). Local stratification control of marine productiv-
417 ity in the subtropical North Pacific. *Journal of Geophysical Research: Oceans*,
418 *115*(12), 1–16. doi: 10.1029/2010JC006507
- 419 Dore, J. E., Letelier, R. M., Church, M. J., Lukas, R., & Karl, D. M. (2008, jan).
420 Summer phytoplankton blooms in the oligotrophic North Pacific Subtropical
421 Gyre: Historical perspective and recent observations. *Progress in Oceanogra-*
422 *phy*, *76*(1), 2–38. doi: 10.1016/j.pocean.2007.10.002
- 423 Droop, M. R. (1968, oct). Vitamin B 12 and Marine Ecology. IV. The Kinetics of
424 Uptake, Growth and Inhibition in *Monochrysis Lutheri*. *Journal of the Marine*
425 *Biological Association of the United Kingdom*, *48*(3), 689–733. doi: 10.1017/
426 S0025315400019238
- 427 Edwards, K. F., Thomas, M. K., Klausmeier, C. A., & Litchman, E. (2012). Al-
428 lometric scaling and taxonomic variation in nutrient utilization traits and
429 maximum growth rate of phytoplankton. *Limnology and Oceanography*, *57*(2),
430 554–566. doi: 10.4319/lo.2012.57.2.0554
- 431 Fairall, C. W., Bradley, E. F., Rogers, D. P., Edson, J. B., & Young, G. S. (1996).
432 Bulk parameterization of air-sea fluxes for tropical ocean-global atmosphere
433 coupled-ocean atmosphere response experiment. *Journal of Geophysical Re-*
434 *search: Oceans*, *101*(C2), 3747–3764. doi: 10.1029/95JC03205
- 435 Faugeras, B., Lévy, M., Mémer, L., Verron, J., Blum, J., & Charpentier, I. (2003).
436 Can biogeochemical fluxes be recovered from nitrate and chlorophyll data? A
437 case study assimilating data in the Northwestern Mediterranean Sea at the
438 JGOFS-DYFAMED station. *Journal of Marine Systems*, *40-41*, 99–125. doi:
439 10.1016/S0924-7963(03)00015-0
- 440 Follows, M. J., & Dutkiewicz, S. (2011). Modeling diverse communities of marine
441 microbes. *Annual review of marine science*, *3*, 427–451. doi: 10.1146/annurev-
442 -marine-120709-142848
- 443 Friedrichs, M. A. M., Dusenberry, J. A., Anderson, L. A., Armstrong, R. A., Chai,
444 F., Christian, J. R., ... Wiggert, J. D. (2007). Assessment of skill and
445 portability in regional marine biogeochemical models: Role of multiple plank-

- 446 tonic groups. *Journal of Geophysical Research: Oceans*, 112(8), 1–22. doi:
447 10.1029/2006JC003852
- 448 Friedrichs, M. A. M., Hood, R. R., & Wiggert, J. D. (2006). Ecosystem model
449 complexity versus physical forcing: Quantification of their relative impact with
450 assimilated Arabian Sea data. *Deep-Sea Research Part II: Topical Studies in*
451 *Oceanography*, 53(5-7), 576–600. doi: 10.1016/j.dsr2.2006.01.026
- 452 Geider, R. J., & La Roche, J. (2002). Redfield revisited: Variability of C:N:P in
453 marine microalgae and its biochemical basis. *European Journal of Phycology*,
454 37(1), 1–17. doi: 10.1017/S0967026201003456
- 455 Geider, R. J., MacIntyre, H. L., & Kana, T. M. (1998). A dynamic regulatory model
456 of phytoplanktonic acclimation to light, nutrients, and temperature. *Limnology*
457 *and Oceanography*, 43(4), 679–694. doi: 10.4319/lo.1998.43.4.0679
- 458 Jolliff, J. K., Kindle, J. C., Shulman, I., Penta, B., Friedrichs, M. A., Helber, R.,
459 & Arnone, R. A. (2009). Summary diagrams for coupled hydrodynamic-
460 ecosystem model skill assessment. *Journal of Marine Systems*, 76(1-2), 64–82.
461 doi: 10.1016/j.jmarsys.2008.05.014
- 462 Kane, A., Moulin, C., Thiria, S., Bopp, L., Berrada, M., Tagliabue, A., ... Badran,
463 F. (2011). Improving the parameters of a global ocean biogeochemical model
464 via variational assimilation of in situ data at five time series stations. *Journal*
465 *of Geophysical Research: Oceans*, 116(6), 1–14. doi: 10.1029/2009JC006005
- 466 Karl, D. M., Church, M. J., Dore, J. E., Letelier, R. M., & Mahaffey, C. (2012).
467 Predictable and efficient carbon sequestration in the north pacific ocean sup-
468 ported by symbiotic nitrogen fixation. *Proceedings of the National Academy of*
469 *Sciences*, 109(6), 1842–1849. doi: 10.1073/pnas.1120312109
- 470 Kavanaugh, M. T., Church, M. J., Davis, C. O., Karl, D. M., Letelier, R. M., &
471 Doney, S. C. (2018). ALOHA from the edge: Reconciling three decades
472 of in situ eulerian observations and geographic variability in the North Pa-
473 cific subtropical Gyre. *Frontiers in Marine Science*, 5(APR), 1–14. doi:
474 10.3389/fmars.2018.00130
- 475 Kerimoglu, O., Anugerahanti, P., & Smith, S. L. (submitted). FABM-NflexPD 1.0:
476 Assessing an Instantaneous Acclimation Approach for Modelling Phytoplank-
477 ton Growth. *Geoscientific Model Development Discussions*.
- 478 Kerimoglu, O., Hofmeister, R., Maerz, J., Riethmüller, R., & Wirtz, K. W. (2017).

- 479 The acclimative biogeochemical model of the southern North Sea. *Biogeo-*
 480 *sciences*, 14(19), 4499–4531. doi: 10.5194/bg-14-4499-2017
- 481 Kriest, I., Oeschles, A., & Khatiwala, S. (2012). Sensitivity analysis of simple global
 482 marine biogeochemical models. *Global Biogeochemical Cycles*, 26(2), 1–15. doi:
 483 10.1029/2011GB004072
- 484 Kullenberg, G. (1984). Observations of light scattering functions in two oceanic ar-
 485 eas. *Deep Sea Research Part A. Oceanographic Research Papers*, 31(3), 295 -
 486 316. doi: [https://doi.org/10.1016/0198-0149\(84\)90106-7](https://doi.org/10.1016/0198-0149(84)90106-7)
- 487 Kwiatkowski, L., Aumont, O., Bopp, L., & Ciais, P. (2018). The Impact of Variable
 488 Phytoplankton Stoichiometry on Projections of Primary Production, Food
 489 Quality, and Carbon Uptake in the Global Ocean. *Global Biogeochemical*
 490 *Cycles*, 32. doi: 10.1002/2017GB005799
- 491 Kwiatkowski, L., Yool, A., Allen, J. I., Anderson, T. R., Barciela, R., Buitenhuis,
 492 E. T., ... Cox, P. M. (2014). IMarNet: An ocean biogeochemistry model
 493 intercomparison project within a common physical ocean modelling framework.
 494 *Biogeosciences*, 11(24), 7291–7304. doi: 10.5194/bg-11-7291-2014
- 495 Laufkotter, C., Vogt, M., Gruber, N., Aita-Noguchi, M., Aumont, O., Bopp, L., ...
 496 Volker, C. (2015). Drivers and uncertainties of future global marine primary
 497 production in marine ecosystem models. *Biogeosciences*, 12(23), 6955–6984.
 498 doi: 10.5194/bg-12-6955-2015
- 499 Laws, E. A., & Bannister, T. T. (1980). Nutrient- and light-limited growth of Tha-
 500 lassiosira fluviatilis in continuous culture, with implications for phytoplankton
 501 growth in the ocean. *Limnology and Oceanography*, 25(3), 457–473. doi:
 502 10.4319/lo.1980.25.3.0457
- 503 Le Quere, C., Harrison, S. P., Prentice, I. C., Buitenhuis, E. T., Aumont, O., Bopp,
 504 L., ... Wolf-Gladrow, D. (2005). Ecosystem dynamics based on plankton
 505 functional types for global ocean biogeochemistry models. *Global Change in*
 506 *Biology*, 11(11), 2016–2040. doi: 10.1111/j.1365-2486.2005.01004.x
- 507 Letelier, R., Dore, J., Winn, C., & Karl, D. (1996). Seasonal and interannual varia-
 508 tions in photosynthetic carbon assimilation at station. *Deep Sea Research Part*
 509 *II: Topical Studies in Oceanography*, 43(2), 467 - 490. doi: [https://doi.org/10](https://doi.org/10.1016/0967-0645(96)00006-9)
 510 [.1016/0967-0645\(96\)00006-9](https://doi.org/10.1016/0967-0645(96)00006-9)
- 511 Macintyre, H. L., Kana, T. M., & Geider, R. J. (2000). The effect of water mo-

- tion on short-term rates of photosynthesis by marine phytoplankton. *Trends in Plant Science*, 5(1), 12–17. doi: 10.1016/S1360-1385(99)01504-6
- Marra, J. (2009). Net and gross productivity: Weighing in with ^{14}C . *Aquatic Microbial Ecology*, 56(2-3), 123–131. doi: 10.3354/ame01306
- Martiny, A. C., Pham, C. T., Primeau, F. W., Vrugt, J. A., Moore, J. K., Levin, S. A., & Lomas, M. W. (2013). Strong latitudinal patterns in the elemental ratios of marine plankton and organic matter. *Nature Geoscience*, 6(4), 279–283. doi: 10.1038/ngeo1757
- Mattern, J. P., Fennel, K., & Dowd, M. (2012). Estimating time-dependent parameters for a biological ocean model using an emulator approach. *Journal of Marine Systems*, 96-97, 32–47. doi: 10.1016/j.jmarsys.2012.01.015
- Mignot, A., Claustre, H., Uitz, J., Poteau, A., Ortenzio, F. D., & Xing, X. (2014). Understanding the seasonal dynamics and the deep chlorophyll maximum in oligotrophic. *AGU. global biogeochemical cycles*(1), 856–876. doi: 10.1002/2013GB004781.Received
- Mongin, M., Nelson, D. M., Pondaven, P., & Treguer, P. (2006). Simulation of upper-ocean biogeochemistry with a flexible-composition phytoplankton model: C, N and Si cycling and Fe limitation in the Southern Ocean. *Deep-Sea Research Part I*, 53(5-7), 601–619. doi: 10.1016/j.dsr2.2006.01.021
- Monod, J. (1949). The Growth of Bacterial Cultures. *Annual Review of Microbiology*, 3(1), 371–394. doi: 10.1146/annurev.mi.03.100149.002103
- Moreno, A. R., & Martiny, A. C. (2018). Ecological stoichiometry of ocean plankton. *Annual Review of Marine Science*, 10, 43–69. doi: 10.1146/annurev-marine-121916-063126
- Pahlow, M., Chien, C.-T., Arteaga, L. A., & Oschlies, A. (2020). Optimality-based non-Redfield plankton–ecosystem model (OPEM v1.1) in UVic-ESCM 2.9 – Part 1: Implementation and model behaviour. *Geoscientific Model Development*, 13(10), 4663–4690. doi: 10.5194/gmd-13-4663-2020
- Pahlow, M., Dietze, H., & Oschlies, A. (2013). Optimality-based model of phytoplankton growth and diazotrophy. *Marine Ecology Progress Series*, 489, 1–16. doi: 10.3354/meps10449
- Paulson, C. A., & Simpson, J. J. (1977, 11). Irradiance Measurements in the Upper Ocean. *Journal of Physical Oceanography*, 7(6), 952–956. doi: 10.1175/1520

- 545 -0485(1977)007(0952:IMITUO)2.0.CO;2
- 546 Pei, S., & Laws, E. A. (2013). Does the 14c method estimate net photosynthesis?
547 implications from batch and continuous culture studies of marine phytoplank-
548 ton. *Deep Sea Research Part I: Oceanographic Research Papers*, 82, 1 - 9. doi:
549 <https://doi.org/10.1016/j.dsr.2013.07.011>
- 550 Pei, S., & Laws, E. A. (2014). Does the 14c method estimate net photosynthesis?
551 ii. implications from cyclostat studies of marine phytoplankton. *Deep Sea Re-*
552 *search Part I: Oceanographic Research Papers*, 91, 94 - 100. doi: [https://doi](https://doi.org/10.1016/j.dsr.2014.05.015)
553 [.org/10.1016/j.dsr.2014.05.015](https://doi.org/10.1016/j.dsr.2014.05.015)
- 554 Polovina, J. J., Howell, E. A., & Abecassis, M. (2008). Ocean's least productive wa-
555 ters are expanding. *Geophysical Research Letters*, 35(3), 2–6. doi: 10.1029/
556 2007GL031745
- 557 Robson, B. J., Arhonditsis, G. B., Baird, M. E., Brebion, J., Edwards, K. F., Ge-
558 offroy, L., . . . Steven, A. (2018). Towards evidence-based parameter values
559 and priors for aquatic ecosystem modelling. *Environmental Modelling and*
560 *Software*, 100, 74–81. doi: 10.1016/j.envsoft.2017.11.018
- 561 Schartau, M., Oschlies, A., & Willebrand, J. (2001). Parameter estimates of a zero-
562 dimensional ecosystem model applying the adjoint method. *Deep-Sea Research*
563 *Part II: Topical Studies in Oceanography*, 48(8-9), 1769–1800. doi: 10.1016/
564 S0967-0645(00)00161-2
- 565 Smith, S. L., Pahlow, M., Merico, A., Acevedo-Trejos, E., Sasai, Y., Yoshikawa, C.,
566 . . . Honda, M. C. (2016). Flexible phytoplankton functional type (FlexPFT)
567 model: Size-scaling of traits and optimal growth. *Journal of Plankton Re-*
568 *search*, 38(4), 977–992. doi: 10.1093/plankt/fbv038
- 569 Smith, S. L., Pahlow, M., Merico, A., & Wirtz, K. (2011). Optimality-based mod-
570 eling of planktonic organisms. *Limnology and Oceanography*, 56(6), 2080–2094.
571 doi: 10.4319/lo.2011.56.6.2080
- 572 Sommer, U. (1991). A comparison of the droop and the monod models of nutrient
573 limited growth applied to natural populations of phytoplankton. *Functional*
574 *Ecology*, 5(4), 535–544.
- 575 Steinberg, D. K., Carlson, C. A., Bates, N. R., Johnson, R. J., Michaels, A. F., &
576 Knap, A. H. (2001). Overview of the US JGOFS Bermuda Atlantic Time-series
577 Study (BATS): a decade-scale look at ocean biology and biogeochemistry. ,

- 578 48, 1405–1447.
- 579 Totterdell, I. J. (2019). Description and evaluation of the Diat-HadOCC model v1.0:
 580 The ocean biogeochemical component of HadGEM2-ES. *Geoscientific Model*
 581 *Development*, 12(10), 4497–4549. doi: 10.5194/gmd-12-4497-2019
- 582 Ward, B. A. (2017). Assessing an efficient ”instant Acclimation” approximation
 583 of dynamic phytoplankton stoichiometry. *Journal of Plankton Research*, 39(5),
 584 803–814. doi: 10.1093/plankt/fbx040
- 585 Ward, B. A., Schartau, M., Oschlies, A., Martin, A. P., Follows, M. J., & Ander-
 586 son, T. R. (2013). When is a biogeochemical model too complex? Objective
 587 model reduction and selection for North Atlantic time-series sites. *Progress in*
 588 *Oceanography*, 116, 49–65. doi: 10.1016/j.pocean.2013.06.002
- 589 Yool, A., Popova, E. E., & Anderson, T. R. (2013). MEDUSA-2.0: An intermedi-
 590 ate complexity biogeochemical model of the marine carbon cycle for climate
 591 change and ocean acidification studies. *Geoscientific Model Development*, 6(5),
 592 1767–1811. doi: 10.5194/gmd-6-1767-2013

Supporting Information for ”Enhancing ocean biogeochemical model performance and generality with phytoplankton variable composition”

Prima Anugerahanti ¹, Onur Kerimoglu ², and S. Lan Smith ¹

¹Earth SURFACE System Research Centre, Research Institute for Global Change, JAMSTEC, Yokosuka, Japan

²Institute for Chemistry and Biology of the Marine Environment, University of Oldenburg, Germany

Contents of this file

1. Equations related to the Droop Quota Model
2. Figure S2
3. Figure S3
4. Parameter Table S1
5. Table S2

Introduction

The supporting information contains: 1) an explanation for the DQ model and how it differs from the dynamic acclimation model described in Kerimoglu, Anugerahanti, and Smith (submitted) in section 1, 2) Figure S2, which shows the seasonal averages of C:N and Chl:C ratios within the upper 50m and between 75-125m, related to Figure 2 in

the main manuscript, 3) Figure S3 which shows the statistical metrics for station BATS, related to Figure 4 in the main manuscript, 4) Parameter Table S1 for individual tuning and simultaneous experiment, and 5) Table S2, which contain the information on the cost functions, related to Figure 4 in the main manuscript and Figure S3.

1. Equations related to the Droop Quota model

The Droop Quota (DQ) model variant in this study is similar to the Dynamic Acclimation (DA) version from Kerimoglu et al. (submitted), but with the physiological allocation factors prescribed instead of dynamically calculated. The DA approach is based on the study by Pahlow and Oschlies (2013), which analytically derived the Droop quota model from an optimality-based formulation that maximizes growth rate μ , by balancing the respiration and allocation costs against the benefits in terms of nutrient uptake and carbon assimilation V .

1.1. Dynamic Acclimation with fixed allocation factor

In this section, we show that despite having the allocation factor fixed (not dynamically calculated) the ‘fixed’ DA version still retains the Droop growth relationship, whereby the cell quota will saturates as growth increases to a certain level. Assuming that a fixed amount of cellular nitrogen, N , is bound in the structural material (Q_s), the remainder is allocated between requirements for growth and nutrient uptake. N uptake rate, V is proportional the fractional allocation of intra-cellular nitrogen resources for that purpose, f_V , and C assimilation rate is proportional to the remaining resources available for that purpose, expressed as the relative size of the chloroplast, f_C . These two allocation factors

are thus related via the following assumed trade-off:

$$f_C = 1 - \frac{Q_s}{Q} - f_V$$

The cellular gross growth rate, μ depends on the potential light limited growth rate ($\hat{\mu}^I$, see equation 21 in Kerimoglu et al. (submitted)). Because this process occurs in the chloroplast, μ is scaled by the chloroplast size, f_C :

$$\mu = \hat{\mu}^I f_C \quad (1)$$

As discussed previously, the overall N acquisition rate depends on the potential uptake of ambient dissolved inorganic nitrogen (DIN), ($\hat{V}^N$, see equation 8) and the fractional allocation of cellular resources for N uptake, f_V :

$$V = f_V \hat{V}^N \quad (2)$$

Following Pahlow and Oschlies (2013) the optimal cell quota, Q can be calculated as:

$$Q = Q_s \left[1 + \sqrt{1 + \frac{1}{Q_s \left(\frac{\hat{\mu}^I}{\hat{V}^N} + \zeta_N \right)}} \right] \quad (3)$$

Thus, the optimal Q depends on the ratio of light- to nutrient-limitation ($\frac{\hat{\mu}^I}{\hat{V}^N}$). By balancing growth and uptake, $\mu Q = V$, via the balanced growth equation (Burmester, 1979), it is possible to calculate the optimal f_V (Pahlow & Oschlies, 2013):

$$f_V = \left(\frac{Q_s}{Q} \right) - \zeta_N (Q - Q_s) \quad (4)$$

where ζ_N is the cost of assimilating DIN (mol C (mol N)⁻¹). Thus f_V increases with decreasing cellular N quota, Q ; i.e., more nutrient limited cells allocate more resources towards nutrient uptake. Equations 1, 2, and 4 can all be found in equations 3, 4, and 14, respectively in Kerimoglu et al. (submitted).

According to equation 1, calculating f_V dynamically using equations 3 and 4 results in a saturating response for μ as a function of Q . That is, increasing Q to high levels yields diminishing returns in terms of growth as shown in Fig S1 (blue curve), which is the classical representation of the Droop equation. However, if we fix f_V to a constant value (in this case, the biomass weighed average as calculated by the IA model variant) and calculate μ and Q , using equations 1 and 3, respectively, the saturating relationship still holds, albeit somewhat flatter (i.e. μ saturates at a lower rate than when f_V is dynamically calculated, and growth is faster at lower Q , as shown in Fig S1). Thus, the model with fixed allocation factors retains the characteristics response of the Droop model. Compared to the DA and IA model variants, the DQ variant will produce lower Q , and therefore higher C:N ratios, at low μ .

1.2. Down-regulation term

As stated in the main manuscript, all model variants follow a similar set of differential equations. However, the DQ formulation calculates Phy_C explicitly, and its rate of change is similar to equation 1b in Kerimoglu et al. (submitted). With the assumption of fixed f_V , nutrient uptake rate for the whole cell can become unrealistically high, as DIN and hence Phy_N increase, making Q become unrealistically high. Therefore, a down-regulation term is required to limit Q values. This is done by prescribing a maximum quota $Q_{\max}$ in the Droop equation, via the following limiting quotient:

$$f_Q = \frac{Q_{\max} - Q}{Q_{\max} - \frac{Q_0}{2}} \quad (5)$$

The nutrient uptake rate, V in equation 2 then becomes:

$$V = f_V \hat{V} f_Q \quad (6)$$

which also affects the respiratory cost of nutrient uptake, R_N (equation 7 in Kerimoglu et al. (submitted)):

$$R_N = \zeta_N f_V \hat{V} f_Q \quad (7)$$

The $\hat{V}$ in the DA variant in Kerimoglu et al. (submitted) is described using the allocation factor towards nutrient affinity, f_A . Increasing f_A increases affinity ($\hat{A} = f_A \hat{A}_0$, where $\hat{A}_0$ is the potential maximum nutrient affinity), and simultaneously decreases the maximum nutrient uptake rate ($\hat{V}_{\max} = (1 - f_A) \hat{V}_0$, where $\hat{V}_0$ is the potential maximum nutrient uptake rate). Since the DQ variant here does not include any physiological acclimation, the f_A term is prescribed to its biomass weighted average as calculated by the IA model. However the equation for $\hat{V}$ remains unchanged:

$$\begin{aligned} \hat{V} &= \frac{\hat{V}_{\max} \hat{A} \text{ DIN}}{\hat{V}_{\max} + \hat{A} \text{ DIN}} \\ &= \frac{(1 - f_A) \hat{V}_0 f_A \hat{A}_0 \text{ DIN}}{(1 - f_A) \hat{V}_0 + f_A \hat{A}_0 \text{ DIN}} \end{aligned} \quad (8)$$

References

- Burmaster, D. E. (1979). The Continuous Culture of Phytoplankton: Mathematical Equivalence Among Three Steady-State Models. *The American Naturalist*, 113(1), 123–134. doi: 10.1086/283368
- Edwards, K. F., Thomas, M. K., Klausmeier, C. A., & Litchman, E. (2012). Allometric scaling and taxonomic variation in nutrient utilization traits and maximum growth rate of phytoplankton. *Limnology and Oceanography*, 57(2), 554–566. doi: 10.4319/lo.2012.57.2.0554
- Kane, A., Moulin, C., Thiria, S., Bopp, L., Berrada, M., Tagliabue, A., ... Badran, F.

- (2011). Improving the parameters of a global ocean biogeochemical model via variational assimilation of in situ data at five time series stations. *Journal of Geophysical Research: Oceans*, 116(6), 1–14. doi: 10.1029/2009JC006005
- Kerimoglu, O., Anugerahanti, P., & Smith, S. L. (submitted). FABM-NflexPD 1.0: Assessing an Instantaneous Acclimation Approach for Modelling Phytoplankton Growth. *Geoscientific Model Development Discussions*.
- Pahlow, M., Dietze, H., & Oschlies, A. (2013). Optimality-based model of phytoplankton growth and diazotrophy. *Marine Ecology Progress Series*, 489, 1–16. doi: 10.3354/meps10449
- Pahlow, M., & Oschlies, A. (2013). Optimal allocation backs droop’s cell-quota model. *Marine Ecology Progress Series*, 473(2010), 1–5. doi: 10.3354/meps10181
- Robson, B. J., Arhonditsis, G. B., Baird, M. E., Brebion, J., Edwards, K. F., Geoffroy, L., ... Steven, A. (2018). Towards evidence-based parameter values and priors for aquatic ecosystem modelling. *Environmental Modelling and Software*, 100, 74–81. doi: 10.1016/j.envsoft.2017.11.018
- Smith, S. L., Pahlow, M., Merico, A., Acevedo-Trejos, E., Sasai, Y., Yoshikawa, C., ... Honda, M. C. (2016). Flexible phytoplankton functional type (FlexPFT) model: Size-scaling of traits and optimal growth. *Journal of Plankton Research*, 38(4), 977–992. doi: 10.1093/plankt/fbv038
- Sommer, U. (1991). A comparison of the droop and the monod models of nutrient limited growth applied to natural populations of phytoplankton. *Functional Ecology*, 5(4), 535–544.

Yool, A., Popova, E. E., & Anderson, T. R. (2013). MEDUSA-2.0: An intermediate complexity biogeochemical model of the marine carbon cycle for climate change and ocean acidification studies. *Geoscientific Model Development*, 6(5), 1767–1811. doi: 10.5194/gmd-6-1767-2013

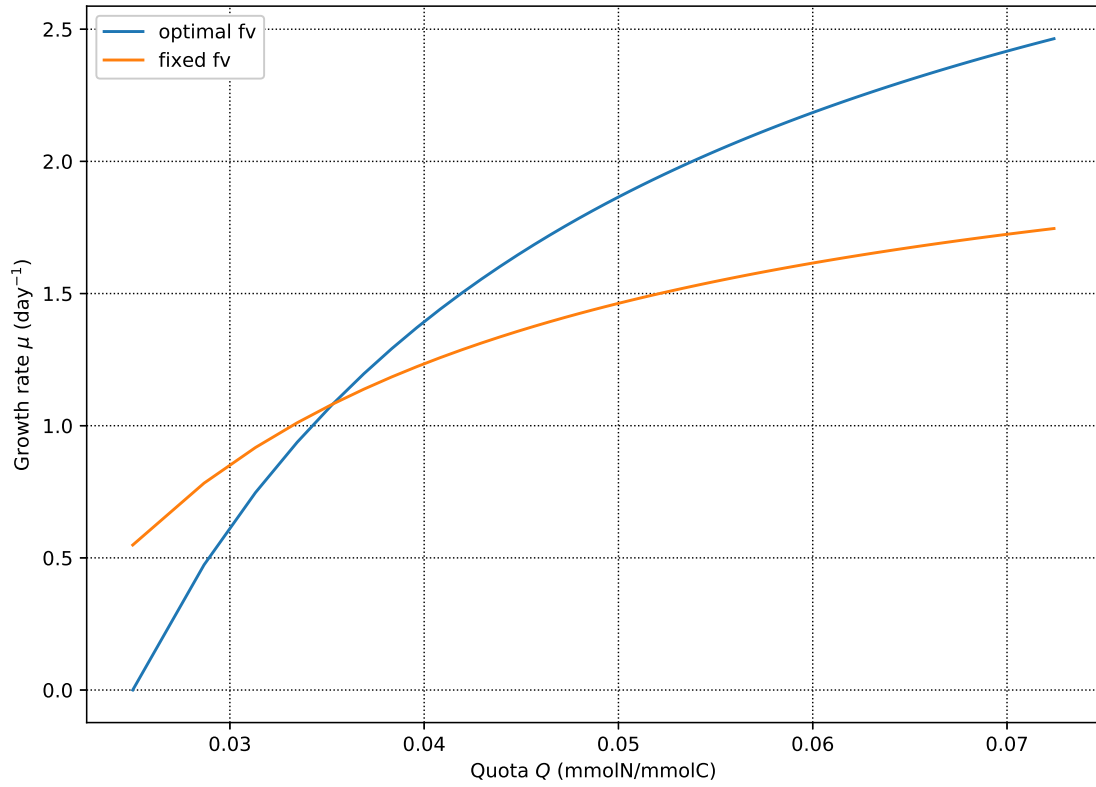


Figure S1. Growth rate against quota when f_V is dynamically calculated to its optimal value and when its prescribed (we use the value of 0.35 for f_V). Growth rate and cell quota here were calculated based on equation 3 and 10, respectively in Pahlow and Oschlies (2013). Light limited growth and nutrient uptake formulations are parameter are all the same as Kerimoglu et al. (submitted)

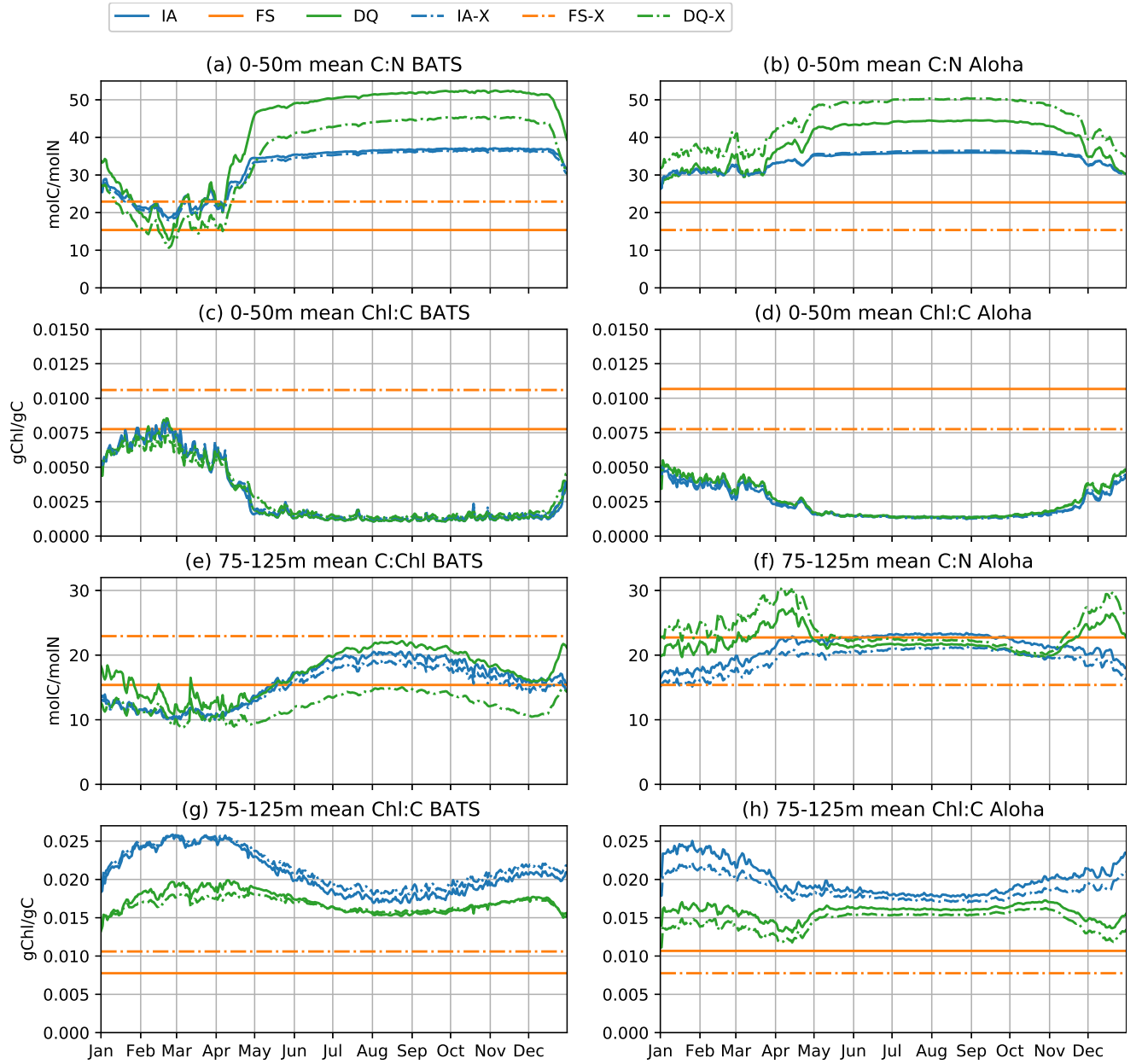


Figure S2. Seasonal average of C:N (a, b, e, and f) and Chl:C (c, d, g, and h) ratios for the three model variants at BATS and ALOHA averaged within the top 50m and between 75-125m. Line color and styles as in Fig. 2 in the main manuscript.

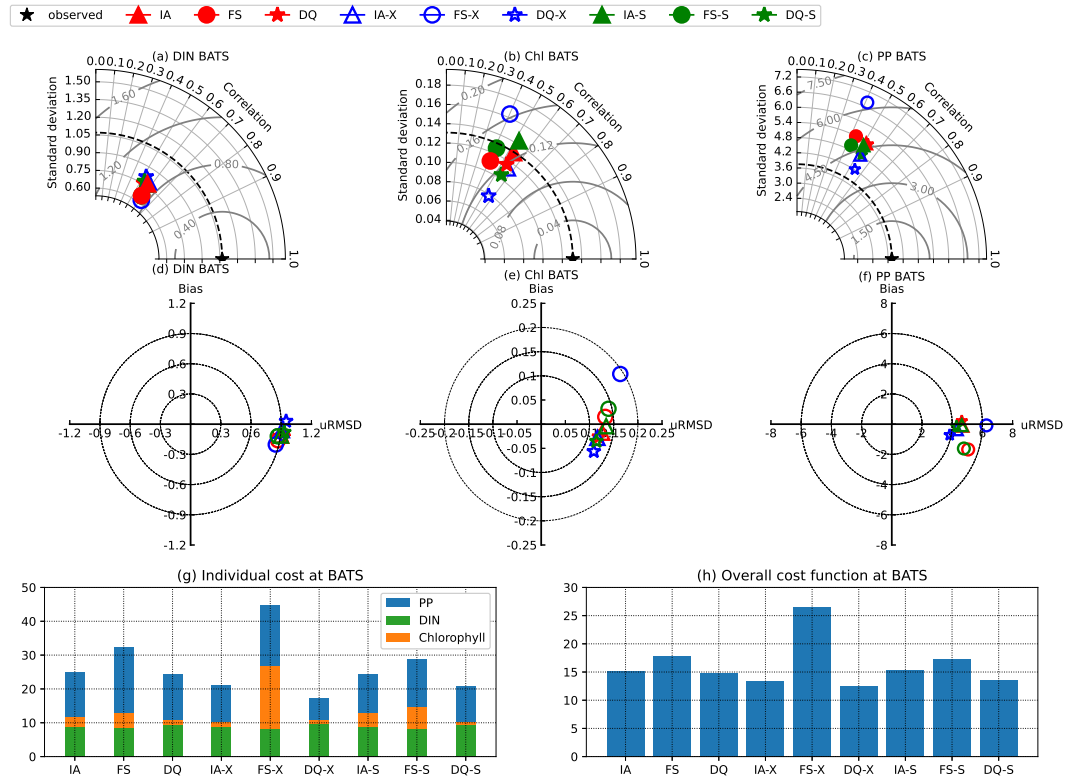


Figure S3. Similar to Fig. 4 in the main manuscript but at station BATS.

Table S1. Parameter values for simulations of stations ALOHA and BATS. The DQ variant uses the same parameter set as IA, and the same fixed values for the allocation factors as the FS variant. Initial conditions for phytoplankton carbon biomass for the DQ variants are 0.46 and 0.33 for stations BATS and ALOHA, respectively, following the Redfield ratio. For the simultaneous and cross-validation experiments, k_{cp} , w_{phy} , all abiotic parameters, and initial conditions are kept the same for each stations. The parameters are taken within Smith et al. (2016); Pahlow et al. (2013); Robson et al. (2018), apart from α^I (Kane et al., 2011), Q_0 (Sommer, 1991), $\hat{V}_0$, $\hat{A}_0$ (Edwards et al., 2012), and w_{det} (Yool et al., 2013). Mortality rates are higher than literature values to implicitly account for predation.

		Parameter	BATS		ALOHA		Simultaneous	
term	Definition	units	IA	FS	IA	FS	IA	FS
Phytoplankton								
k_{cp}	specific light extinction	$\text{m}^2 \text{mmol N}^{-1}$	0.03		0.02			
w_{phy}	vertical velocity	m d^{-1}	0		-0.02			
$\hat{R}_{chl}$	loss rate of chlorophyll	d^{-1}	0.08	0.1	0.1	0.1	0.1	0.1
$\hat{\theta}$	Chl:C ratio	gChl molC^{-1}		0.18		0.35		0.25
$\hat{\mu}_0$	maximum potential growth rate	d^{-1}	4	4	3.7	3.5	3.75	4
α^I	Chl-specific slope of the PI curve	$\text{m}^{-2} \text{E}^{-1} \text{mol C gChl}^{-1}$	3.8	3.5	3.7	5	3.75	3.5
f_A	Allocation towards affinity			0.73		0.83		0.76
f_V	Allocation towards nutrient uptake			0.26		0.35		0.3
Q_0	Subsistence cell quota	molN molC^{-1}	0.025	0.025	0.025	0.025	0.025	0.025
Q_{fixed}	Fixed cell quota	molN molC^{-1}		0.083		0.044		0.75
$\hat{V}_0$	Potential maximum uptake rate	$\text{mol N molC}^{-1} \text{d}^{-1}$	1.2	1	1.2	1	1.2	1
$\hat{A}_0$	Potential maximum nutrient affinity	$\text{m}^3 \text{mmolC}^{-1} \text{d}^{-1}$	0.7	0.5	0.7	0.3	0.6	0.7
K_N	Half saturation constant	mmolN m^{-3}		0.69		0.81		0.75
ζ_N	C-cost of N uptake	molC molN^{-1}	0.4	0.4	0.5	0.3	0.5	0.4
ζ_{Chl}	C-cost of Chl synthesis	molC gChl^{-1}	1	0.5	0.8	0.4	0.9	0.6
M_p	Quadratic mortality rate	$\text{m}^3 \text{molN}^{-1} \text{d}^{-1}$	2.5	0.75	3.1	1.5	2.5	1.2
M_{part}	Part of mortality that goes to detritus		0.4	0.6	0.4	0.5	0.4	0.6
Abiotic								
w_{det}	sinking of detritus	m d^{-1}	-2.5		-2.5			
k_c	specific light extinction	$\text{m}^2 \text{mmol}^{-1}$	0.03		0.03			
k_{det}	degradation rate of Detritus	d^{-1}	0.03		0.045			
k_{don}	remineralisation rate of DON	d^{-1}	0.03		0.02			
$\text{PAR}_0 \text{dt}_0$	daily average par at the surface on the first time step		4.5		4.5			
$k_c \text{dt}_0$	attenuation coefficient on the first time step		0.02		0.02			
Initial conditions								
Phy_N	Phytoplankton N biomass	mmol m^{-3}	0.7		0.5			
DIN	Dissolved Inorganic Nitrogen	mmol m^{-3}	0.7		0.5			
DON	Dissolved Organic Nitrogen	mmol m^{-3}	0.7		0.5			
DOC	Dissolved Organic Carbon	mmol m^{-3}	0.7		0.5			
det_N	Detritus N	mmol m^{-3}	0.7		0.5			
det_C	Detritus C	mmol m^{-3}	0.7		0.5			

Table S2. Cumulative cost functions J_m and J at stations ALOHA and BATS for each model run, and portability index PI ($=J^s/J^x$).

Model Run	J_{Chl}	J_{DIN}	J_{PP}	J	PI
IA	25.60	14.41	41.42	27.14	
FS	31.56	13.99	62.44	36.00	
DQ	28.12	15.10	38.00	27.07	
IA-X	26.02	14.68	40.64	27.11	
FS-X	45.46	14.02	80.00	46.50	
DQ-X	30.32	15.48	33.66	26.48	
IA-S	27.29	14.39	41.00	27.56	1.02
FS-S	32.83	14.12	63.61	36.85	0.79
DQ-S	28.79	15.10	37.92	27.27	1.03