Optimality-based approach for computationally efficient modeling of phytoplankton growth, chlorophyll-to-carbon, and nitrogen-to-carbon ratios

Bingzhang Chen*, S. Lan Smith

Research Center for Global Change Research, JAMSTEC (Japan Agency for Marine-Earth Science and Technology), 3173-25 Showa-machi, Kanazawa-ku, Yokohama 236-0001, Japan

*Corresponding author: bingzhang.chen@gmail.com

Keywords: Ocean model, North Pacific, light, nutrient, Metropolis-Hastings Monte Carlo

Running head: Optimal phytoplankton growth model
Abstract

To increase the efficiency of computing phytoplankton growth rate ($\mu$), chlorophyll-to-carbon ($\theta$) and nitrogen-to-carbon ratios ($Q^N$) in three-dimensional ocean circulation models, it is preferable to directly calculate $\theta$ and $Q^N$ from ambient environmental factors instead of treating them as independent tracers. Optimality-based modeling has emerged as a novel and efficient approach to fulfill this task. However, it is still unclear precisely how the response of optimality-based models differs from conventional models. We compare a recent optimality-based phytoplankton model (PAHLOW model), based on which the familiar Droop function can be derived, to a commonly used Monod-type (MONOD) model. The two models generate similar patterns of $\mu$ with some important differences. Compared to the MONOD model, the PAHLOW model predicts higher $\mu$ under light limitation. The PAHLOW model also predicts that $\theta$ decreases with decreasing light under dim light and predicts decreasing $Q^N$ with increasing light even at constant nutrient levels. Compared to the MONOD model, these features of the PAHLOW model qualitatively agree better with laboratory data. The PAHLOW model also suffers from a few shortcomings including the underestimation of $\theta$ under very low light and two times of computation time compared to the MONOD model. The two models generate striking differences of $Q^N$ and $\theta$ in a one-dimensional implementation. Validation of such patterns will require more direct in situ measurements of $\mu$, $\theta$ and $Q^N$. 
1. Introduction

Functional relationships for phytoplankton properties such as the growth rate ($\mu$), chlorophyll-to-carbon ($\theta$), and nitrogen-to-carbon ratios ($Q^N$) in terms of abiotic environmental factors such as nutrient and light are essential to any plankton model and have been studied extensively (Droop, 1974; Jassby and Platt, 1976; Cloern et al., 1995; Litchman et al., 2007; Edwards et al., 2012, 2015, 2016). A widely-adopted approach is to treat phytoplankton carbon, nitrogen, and chlorophyll as independent tracers and make $\mu$ dependent on $Q^N$ such as the Droop function (Droop, 1974) and also dependent on $\theta$ and light as in Geider et al. (1997, 1998). This approach has been implemented in some three-dimensional ocean general circulation models (GCMs) such as ERSEM (Butenschön et al., 2016) and a global size-structured plankton model (Ward et al., 2012). Although sound, this approach requires a great many calculations, particularly when a large number of phytoplankton species are included in a 3D GCM (Follows et al., 2007; Barton et al., 2010; Ward et al., 2012). Another drawback is that for tracers having spatial gradients of opposite sign (e.g., phytoplankton carbon concentrations are typically higher near the sea surface while chlorophyll concentrations are higher at depth due to photo-acclimation), their corresponding diffusive fluxes will be in opposite directions, which is unrealistic. It is therefore preferable not to have multiple tracers for components of the same phytoplankton biomass. On the other hand, fixed $\theta$ or $Q^N$ based on the Redfield ratio are unrealistic and should be avoided to the extent possible (Geider and La Roche, 2002; Flynn, 2003; Christian, 2005).

One approach to this dilemma is provided by optimality-based models, which can be viewed as intermediate between the two extremes considered above (Flynn, 2003). The principle of the optimality concept is that all organisms that face physiological
tradeoffs can be assumed to attain maximal fitness by adjusting trait values (Sutherland, 2005; Armstrong, 2006; Smith et al., 2011). Mathematically, the optimal trait value can be computed by solving the fitness gradient function by assuming instantaneous acclimation (Smith et al., 2011) and $\mu$, $\theta$, and $Q^N$ can be directly calculated based on external environmental conditions such as temperature, light, and nutrient concentrations. This speeds up computation because otherwise two or more independent tracers (phytoplankton chlorophyll and carbon) must be added to the model (Geider et al., 1998; Ward et al., 2012). Encouragingly, Ward (2017) recently showed that the instantaneous acclimation of cellular nutrient quota can accurately approximate the simulation outputs of a dynamic quota model, which requires an additional tracer for each nutrient considered, even under dynamic environmental conditions.

In this study, we focus on an optimality-based phytoplankton model developed by Pahlow and coworkers, hereafter PAHLOW model (Fig. 1; Pahlow and Oschlies, 2013; Pahlow et al., 2013; Smith et al., 2016). The success of the PAHLOW model is reflected in that it provided the first theoretical derivation of the well-known Droop quota model (Pahlow and Oschlies, 2013) and has been validated extensively against laboratory datasets (Pahlow et al., 2013) and somewhat against oceanic observations (Arteaga et al., 2014; Fernández-Castro et al., 2016; Smith et al., 2016).

Although elegant, the basic mathematical properties of the PAHLOW model and its coupling to ocean circulation models have not been thoroughly investigated (Smith et al., 2016). In particular, given that the fundamental relationships of $\mu$ versus light and nutrient appear similar to the widely used Monod-type model, it remains to be explored to what extent the simpler Monod-type model can, with suitable tuning of parameter values, reproduce the output of the PAHLOW model (Burmaster, 1979;
Another consideration is that although the optimality assumptions have simplified much of the computation, the PAHLOW model still requires more calculations compared with the computationally simpler MONOD model. If it can be shown that the two models are mathematically similar and generate similar patterns under realistic ocean conditions, then the use of the MONOD model may be justified in many cases.

Due to the mathematical complexity of the PAHLOW model, its complete algebraic manipulation, as begun by Smith et al. (2016), is beyond the scope of this study. Instead, we tuned the Monod-type models to approximate the output of the mathematically more complex PAHLOW model and compared the resulting growth responses to light and nutrient. We also embedded the two models of phytoplankton in a one-dimensional model set up at two representative time-series observation stations in the subtropical North Pacific (Fig. 2) and compared the performance of the two models against observations.

2. Methods

2.1. Optimality-based phytoplankton model (PAHLOW model)

In the PAHLOW model, phytoplankton cells are assumed to instantaneously optimize their cellular Chl a and nitrogen contents to obtain maximal net growth, which is the net outcome of CO$_2$ fixation minus the energetic costs of photosynthesis and nutrient uptake. Note that although Pahlow et al. (2013) also included phosphorus limitation and nitrogen fixation in their model, for simplicity we here consider only nitrogen as the limiting nutrient.

There are three levels of optimization in the simplified PAHLOW model. The first is the optimization of the Chl:C ratio within the chloroplast ($\hat{\theta}_0$) to maximize net photosynthesis (i.e. gross photosynthesis minus the cost of chlorophyll maintenance).
Pahlow et al. (2013) necessarily assumed that the net photosynthesis of a chloroplast is independent of nutrient levels (but the number of chloroplasts within one cell is dependent on nitrogen availability). By solving the gradient function of net photosynthesis of one chloroplast against $\theta_0$, $\theta_0$ can be solved as follows (see Pahlow et al. (2013) for details):

$$\theta_0 = \frac{1}{\chi_{chl}} + \frac{\mu_0}{\alpha_{chl}} \left( 1 - W_0 \left( 1 + \frac{R^{chl}_M}{\mu_0} \right) e^{\left( \frac{1 + \alpha_{chl}^0}{\chi_{chl}^0} \right)} \right)$$

if $I > I_0$ \hspace{1cm} (1)

$$\theta_0 = \theta_{min}$$

if $I \leq I_0$

in which $I$ is irradiance (W m$^{-2}$). $\alpha_{chl}$ is the chlorophyll-specific initial slope of photosynthesis–irradiance (P–I) curve. $\chi_{chl}$ is the cost of photosynthesis coefficient. $R^{chl}_M$ is the cost of Chl maintenance. $\mu_0$ is the phytoplankton potential carbon acquisition rate. $W_0$ is the zero branch of the Lambert-W function. $I_0 = \frac{\chi_{chl} R^{chl}_M}{\alpha_{chl}}$ is the threshold light level for chlorophyll synthesis. $\theta_{min}$ is the minimal chlorophyll-to-carbon ratio (equaling zero in Pahlow et al. (2013)). Both $R^{chl}_M$ and $\mu_0$ are temperature dependent and are assumed to have the same temperature coefficient $E_p$:

$$\mu_0 = \mu_0' e^{\frac{E_p}{k} \left( \frac{1}{T_0} - \frac{1}{T} \right)}$$

where $\mu_0'$ is the phytoplankton potential carbon acquisition at the reference temperature $T_0$ (288 K). $E_p$ is the activation energy (eV) of phytoplankton growth. $k$ is the Boltzmann constant ($8.62 \times 10^{-5}$ eV K$^{-1}$).

From Eq. 1, it is clear that light is the most important abiotic factor directly affecting $\theta_0$. (Temperature also has some indirect, less important effects.) As shown later, $\theta_0$ is a nonlinear function of light. Under high light, it is beneficial for the phytoplankton cell to slow down chlorophyll synthesis to reduce the cost of photosynthesis, because this reduces only slightly the rate of photosynthesis. If light...
level is too low (approaching or below $I_0$), however, the phytoplankton cell has negligible photosynthesis and also needs to reduce $\hat{\theta}_0$.

The second level of optimization is to balance the energy allocation between photosynthesis and nitrogen uptake. Pahlow and Oschlies (2013) assumed that the total nitrogen of the phytoplankton cell is partitioned among three pools (machineries of carbon acquisition and nitrogen uptake plus subsistence requirements). The net relative growth of the cell equals to net photosynthesis of the whole cell minus the respiratory cost of nitrogen uptake. By solving the gradient function of the net relative growth against the allocation factor ($f_V$) for nitrogen uptake, the optimal cellular nitrogen quota ($Q^N$, mol N (mol C)$^{-1}$) can be calculated as (Pahlow and Oschlies, 2013):

$$Q^N = Q^N_S \left[ 1 + \frac{1}{Q^N_S \left( \frac{\mu^l}{\nu^l} + \zeta^N \right)} \right]$$

(3)

where $Q^N_S$ is the structural nitrogen quota and equals half of the minimal nitrogen quota ($Q_{0N}$) as often reported in the literature. $\nu^N$ is the potential nutrient uptake rate. $\hat{\mu}^l$ is the light dependent growth rate after accounting for photosynthesis and chlorophyll maintenance. $\zeta^N$ represents the cost of nitrogen assimilation. $f_V$ can be calculated from $Q^N$:

$$f_V = \frac{Q^N}{Q^N_S} - \zeta^N (Q^N - 2Q^N_S)$$

(4)

The chlorophyll-to-carbon ratio ($\theta$, mol C gChl$^{-1}$) of the whole cell can be calculated as:

$$\theta = \hat{\theta}_0 \left( 1 - \frac{Q^N}{Q^N_S} - f_V \right).$$

(5)

$\hat{\mu}^l$ is calculated following eq. A2 in Pahlow et al. (2013):

$$\hat{\mu}^l = \mu_0 S^l - (\mu_0 S^l + R_M^{chl}) \zeta^{chl} \hat{\theta}_0$$

(6)
where $S^l$ is the degree of light saturation:

$$S^l = 1 - e^{-\frac{\alpha_{cl}I_0}{\mu_0}}$$  \hspace{1cm} (7)

It can be seen from Eq. 3 that since $\hat{\mu}^l$ increases with light and $\hat{V}^N$ increases with nitrogen, $Q^N$ should decrease with increasing light and increase with increasing nitrogen concentration.

The third level of optimization is with respect to the tradeoff between nutrient uptake on the cell surface and nutrient assimilation within the cell (Pahlow, 2005; Smith et al., 2009). The potential nutrient uptake rate ($\hat{V}^N$) is calculated as:

$$\hat{V}^N = \frac{V_0^N N}{\frac{V_0^N N}{A_0^N} + N}$$ \hspace{1cm} (8)

in which $V_0^N$ (d$^{-1}$) is the maximal potential nitrogen uptake rate. $A_0^N$ (m$^3$ mmol$^{-1}$ d$^{-1}$) is the maximal potential affinity. $N$ is ambient nitrogen concentration (mmol m$^{-3}$). Both $V_0^N$ and $A_0^N$ share the same temperature dependence as $R_{\chi l}$ and $\mu_0$ in Eq. 2. Eq. 8 differs from the Michaelis-Menten equation in that the apparent half-saturation ‘constant’ increases with $N$ (Smith et al., 2009).

Finally, phytoplankton net growth rate ($\mu$) is calculated as:

$$\mu = \hat{\mu}^l (1 - 2 \frac{\alpha_{cl}}{Q^N})$$ \hspace{1cm} (9)

Note that although Eq. 9 is in the same form as the Droop model (Droop, 1974) as derived by Pahlow and Oschlies (2013), the nutrient term also depends on light level, since $Q^N$ depends on light.

2.2. Monod-type model

A traditional model that relates phytoplankton growth rate with external nutrient concentration, light, and temperature is the Monod-type model:

$$\mu = \mu_m \frac{N}{N + K_N} \left(1 - e^{-\frac{\alpha_{cl}}{\hat{\mu}_m}}\right)$$ \hspace{1cm} (10)
where $K_N$ is the half-saturation constant of nitrogen for phytoplankton growth. $\alpha_c$ is the carbon-specific slope of the growth-irradiance curve. $\mu_m$ differs from the $\mu_0$ in that it already takes into account algal respiration. $\mu_m$ is also temperature dependent:

$$\mu_m = \mu_m^0 e^{\frac{E_0}{R_0 T^\frac{1}{2}}}$$ (11)

Note that because our intent was to directly calculate $\mu$ from abiotic environmental factors without introducing extra tracers such as Chl $a$ concentration, there is no $\theta$ in Eq. 10. Flynn (2003) noted that, although Eq. 10 may less faithfully describe the light dependence of growth compared to other models such as in Geider et al. (1997), its predictions differ only slightly from other models, at least when the temporal dynamics of photo-acclimation are not the central focus.

Following Flynn (2003), $\theta$ can be calculated as:

$$\theta = \theta_{\text{min}} + \frac{\mu}{\alpha_{\text{chl}}}$$ (12)

in which $\theta_{\text{min}}$ represents the minimal chlorophyll-to-carbon ratio at very high light. The maximal $\theta$ ($\theta_{\text{max}}$) can be achieved at minimal light and saturating nutrient conditions and can be derived following the L'Hôpital's Rule:

$$\theta_{\text{max}} = \theta_{\text{min}} + \lim_{I \to 0} \frac{\mu}{I \alpha_{\text{chl}}} = \theta_{\text{min}} + \frac{1}{\alpha_{\text{chl}}} \lim_{I \to 0} \frac{\mu_m(1-e^{\frac{\alpha_{\text{chl}} I}{\mu_m}})}{I} = \theta_{\text{min}} + \frac{\alpha_c}{\alpha_{\text{chl}}}(13)$$

By substituting $\alpha_{\text{chl}}$ in Eq. 13 into Eq. 12, we obtain:

$$\theta = \theta_{\text{min}} + \frac{\mu}{I \alpha_{\text{chl}}} (\theta_{\text{max}} - \theta_{\text{min}})$$ (14)

in which $\theta_{\text{max}}$ can be imported from the PAHLOW model (Eq. 5). Note that Eq. 12 always holds if phytoplankton growth is limited by light acquisition instead of Calvin cycle processes (Flynn, 2003). The nutrient effect on $\theta$ is embedded within the nutrient dependence of $\mu$. The derived patterns of $\theta$ to light and nutrients are also consistent with other models (Cloern et al., 1995; Geider et al., 1997).
Further, by equating ambient nutrient-dependent and internal quota-dependent growth rates (Morel, 1987):

\[ \mu = \mu_m \frac{N}{N+K_N} = \mu_m \frac{1-Q_{\min}}{1-Q_{\min}} \frac{Q_N}{Q_{\max}} \]  

(15)

where \( Q_{\min} \) is the minimal nitrogen quota (= 2\( Q_S^N \)) and \( Q_{\max} \) is the maximal nitrogen quota and is assumed 3 times of \( Q_{\min} \) (Litchman et al., 2007; Marañón et al., 2013), \( Q_N \) can be calculated from Eq. 15:

\[ Q_N = \frac{Q_{\min}}{1-(1-Q_{\min}) \frac{N}{N+K_N}} \]  

(16)

As such, our formulation of the MONOD model also allows to directly calculate \( \theta \) and \( Q_N \) from external environmental nitrogen, light, and temperature.

Thus, both the PAHLOW and MONOD models share similar inputs (i.e. temperature, light, inorganic nitrogen) and outputs (\( \mu, \theta, Q_N \)), being able to provide estimates of flexible \( \theta \) and \( Q_N \) assuming instantaneous acclimation without the necessity of computing the dynamics of independent tracers of cellular carbon and chlorophyll contents within phytoplankton cells (Fig. 1). To allow similar parameterizations between both models, we used an adaptive nonlinear least square regression to estimate the parameters (i.e., \( \mu_m, K_N \), and \( \alpha_c \)) of the MONOD model by fitting the growth rates of the MONOD model against the outputs of PAHLOW model under various light and nutrient conditions, after selecting the parameters of the PAHLOW model (Fig. 3a,d). This was implemented with the function ‘nls’ with the ‘port’ algorithm in R 3.3.2 (Dennis et al., 1981; R Core Team, 2016).

2.3. Analysis of laboratory data for phytoplankton chlorophyll-to-carbon and nitrogen-to-carbon ratios

From five published studies (Falkowski and Owens, 1980; Laws and Bannister, 1980; Terry et al., 1983; Falkowski et al., 1985; Strzepek and Price, 2000), we
compiled a dataset of $\theta$ and $Q^N$ of nine phytoplankton taxa under light limiting conditions to validate the outputs of the two models. We focus on $\theta$ and $Q^N$ because the predictions of $\theta$ and $Q^N$ under light limitation are the most striking contrasts between the PAHLOW and MONOD models. The data for two of the nine taxa were used in Pahlow et al. (2013). To be consistent with the 1D model, we converted all the light units to W m$^{-2}$ by calculating the total daily photon doses, assuming 1 W m$^{-2}$ = 2.5 mol photons m$^{-2}$ d$^{-1}$. The light levels ($I$) were log-transformed ($\log I$) to reach a quasi normal distribution.

To see the general trend of $\theta$ and $Q^N$ with light, we used a linear mixed-effect model to allow random deviations of both the slope and the intercept of $Q^N \sim \log I$.

Because the relationship of $\theta$ with light could be nonlinear due to the trend of decreasing $\theta$ with decreasing light under dim light (Pahlow et al., 2013; Westberry et al., 2016), we included a second-order term of $\log I$ in the general linear mixed-effect model of $\theta \sim \log I$. The linear mixed-effect model was implemented using the package ‘lme4’ in R (Bates et al., 2014). The parameters of the PAHLOW model shown in Table 1 mostly followed Pahlow et al. (2013). Some parameters, particularly $\alpha_{chl}$ and $A_{0N}$ that are the most important traits determining the light and nutrient affinity, can be species-specific. We used the parameters optimized from the one-dimensional model to calculate $\theta$ and $Q^N$, which were then contrasted with the laboratory data (Fig. 4).

2.4. One-dimensional model

To examine the performances of the two models under more realistic conditions, we embedded the two phytoplankton models within a simple one-dimensional (1D) numerical model (surface to 250 m depth) implemented for two stations (S1: 145 °E, 30 °N; ALOHA: 158 °E, 22.75 °N) in the North Pacific (Fig. 2a). This 1D model
contained four biological tracers: dissolved inorganic nitrogen, phytoplankton, zooplankton, and detritus. For simplicity, the physical variables relevant to biological processes (i.e. temperature, surface photosynthetically available radiance \((PAR_0)\), and vertical eddy diffusivity \((K_v)\)) were imported from external data products and linearly interpolated for each time step and depth level (Chen and Smith, 2018). \(PAR_0\) data were imported from SeaWIFS satellite monthly climatology products. Seasonal temperature vertical profiles were imported from World Ocean Atlas 2013 monthly climatology. The profiles of \(K_v\) were imported from the output of an eddy-permitting model for North Pacific (Hashioka et al., 2009). Light levels \((L)\) at depth \(z\) were calculated based on \(PAR_0\) and Chl \(a\) concentrations following the Beer-Lambert law:

\[
I_z = PAR_0 e^{-(zK_w + K_{chl} \int_0^z Chl(x) dx)}
\]  

(17)

in which \(K_w\) and \(K_{chl}\) are the attenuation coefficients for seawater and Chl \(a\), respectively. However, one problem with the Eulerian framework is that the time for a phytoplankton cell to mix throughout the surface mixed layer (ML) is much less than its doubling time (Franks, 2015). We therefore calculated the ambient light level for phytoplankton within the ML as the average light \((\bar{I})\) throughout the ML. The mixed layer depth (MLD) is defined as the deepest depth with \(K_v > 10^{-3}\) m\(^2\) s\(^{-1}\). Based on the equation \(\tau_L = \frac{L}{2K(z)}\) (eq. (1) in Franks (2015)), the average time \((\tau_L)\) for a phytoplankton cell to move at a distance \((L)\) of 100 m at the local diffusivity \((K(z))\) of \(10^{-3}\) m\(^2\) s\(^{-1}\) is roughly half a day. As such, we assumed that the phytoplankton cells within the ML should receive the average light throughout the ML. \(\bar{I}\) was used to calculate phytoplankton \(\mu, \theta,\) and \(Q^N\) for temporal evolution of phytoplankton biomass and also standing stocks of Chl \(a\). This might cause a sharp transition of phytoplankton properties across the bottom of the ML. However, to compare with *in situ* net primary production (NPP) estimates derived from incubation bottles that were
not mixed during incubation, phytoplankton $\mu$, $\theta$, and $Q^N$ were recalculated from $I_z$
based on the Beer-Lambert law. Thus, NPP depends directly on $I_z$ instead of $\bar{I}$ due to
the inevitable incubation problem:

$$NPP = P \frac{\mu(NJ_zT)}{Q^N(NJ_zT)}$$ (18)

Phytoplankton sinking was assumed negligible due to the dominance of small
phytoplankton at the two oligotrophic stations (Campbell et al., 1997; Fujiki et al.,
2016). Only detritus was assumed to sink at a constant rate $W_d$ (m d$^{-1}$). Zooplankton
specific ingestion rate ($g$, d$^{-1}$) of phytoplankton was described as a Holling III
function:

$$g = g_m e^{\frac{E_z}{k} \left( \frac{1}{T_0} - \frac{1}{T} \right)} \frac{p^2}{p^2 + K_p^2}$$ (19a)

in which $g_m$ is the maximal ingestion rate (d$^{-1}$), $E_z$ is the activation energy (eV) of
zooplankton grazing, $K_p$ is the grazing half-saturation constant ($\mu$mol N m$^{-3}$) of
zooplankton. We also tested Holling I and II functions in the model sensitivity
analysis. The Holling I function is:

$$g = g_m e^{\frac{E_z}{k} \left( \frac{1}{T_0} - \frac{1}{T} \right)} \min \left( \frac{p}{2K_p}, 1 \right)$$ (19b)

and the Holling II function is:

$$g = g_m e^{\frac{E_z}{k} \left( \frac{1}{T_0} - \frac{1}{T} \right)} \frac{p}{p + K_p}$$ (19c)

The total food intake of zooplankton ($Z_{inges}$) is partitioned into three parts. The
first part ($Z_{inges} \cdot NGE$) is used by zooplankton for net growth. The second part is
defecated to the detritus pool ($Z_{eges} = unass \cdot Z_{inges}$) and the last part is recycled back
to the DIN pool ($Z_{res} = Z_{inges} \cdot (1 - NGE - unass)$). Here $NGE$ is the net growth
efficiency of zooplankton and $unass$ is the fraction of unassimilated food.
Detritus is converted to nitrogen at a rate with the same activation energy with zooplankton, $E_z$. The zooplankton mortality term is assumed proportional to the square of zooplankton biomass (Steele and Henderson, 1992; Ohman and Hirche, 2001).

Hence, for both phytoplankton models (MONOD and PAHLOW) the following equations govern the dynamics of the four biological tracers (i.e. Dissolved inorganic nitrogen ($N$; including nitrate, ammonia, and nitrite), phytoplankton ($P$), zooplankton ($Z$), detritus ($D$)):

$$\frac{dN}{dt} = -P\mu + Zg(1 - NGE - unass) + e^{\frac{E_z}{k}\left(\frac{1}{T_0} - \frac{1}{T}\right)}DR_{dn} + \frac{d}{dz}\left(K_v \frac{dN}{dz}\right)$$  (20a)

$$\frac{dP}{dt} = P\mu - Zg + \frac{d}{dz}\left(K_v \frac{dP}{dz}\right)$$  (20b)

$$\frac{dZ}{dt} = Zg \cdot NGE - m_zZ^2e^{\frac{E_z}{k}\left(\frac{1}{T_0} - \frac{1}{T}\right)} + \frac{d}{dz}\left(K_v \frac{dZ}{dz}\right)$$  (20c)

$$\frac{dD}{dt} = Zg \cdot unass + e^{\frac{E_z}{k}\left(\frac{1}{T_0} - \frac{1}{T}\right)}(m_zZ^2 - DR_{dn}) - W_d \frac{dD}{dz} + \frac{d}{dz}\left(K_v \frac{dD}{dz}\right)$$  (20d)

in which $R_{dn}$ is the conversion rate ($d^{-1}$) of detritus to inorganic nitrogen at 15 °C. Zero flux Neumann boundary condition was applied to both surface and bottom interfaces of the water column to conserve total nitrogen budget. The forward Euler method with a constant time step of 5 min was used throughout to numerically solve the differential equations.

2.5. Observational data and sensitivity analysis

For stations S1, the observational data of total dissolved inorganic nitrogen (DIN), Chl a concentrations, and NPP were collected in the K2S1 project ([https://ebcrpa.jamstec.go.jp/k2s1/en/index.html](https://ebcrpa.jamstec.go.jp/k2s1/en/index.html); Fujiki et al., 2016; Honda, 2016; Matsumoto et al., 2016; Wakita et al., 2016). For station ALOHA, the observational data were downloaded from the Hawaii Ocean Time-series website ([http://hahana.soest.hawaii.edu/hot/](http://hahana.soest.hawaii.edu/hot/)). We pooled all the observational data into one
climatological year, assuming that seasonal changes of environmental conditions are the major factors determining changes in biological variables and inter-annual variations are relatively less important.

In addition, we estimated surface $\theta$ (9 km resolution) from a SeaWIFS monthly climatology (http://gdata1.sci.gsfc.nasa.gov/daac-bin/G3/gui.cgi?instance_id=ocean_month) by dividing phytoplankton carbon with Chl a. Following Behrenfeld et al. (2005), we assumed a constant ratio of 0.3 for phytoplankton carbon to total particulate organic carbon (POC). POC was provided as a product on the SeaWIFS website, calculated based on an empirical relationship between POC and blue-to-green band reflectance ratio (Stramski et al., 2008).

For quantitative evaluations of model performances, we calculated the sum of squared errors ($SSqE$) between the observational data and corresponding model predictions. Because the model started to converge to regular seasonal patterns from the second year, we ran the model for three years and used the output of the final year to compare with observational data. The model outputs were linearly interpolated to the observed depths and dates. To allow comparisons among different data types and downplay the effects of extreme values, both the model outputs and observational data were transformed to their 1/4 power and normalized between 0 and 1 to achieve a quasi-normal distribution:

$$SSqE_{k,i} = \sum_{j=1}^{n_{k,i}} \left( \frac{m_{k,i,j}^{0.25} - o_{k,i,min}^{0.25}}{o_{k,i,max}^{0.25} - o_{k,i,min}^{0.25}} - \frac{o_{k,i,j}^{0.25} - o_{k,i,min}^{0.25}}{o_{k,i,max}^{0.25} - o_{k,i,min}^{0.25}} \right)^2$$

(21)

where $SSqE_{k,i}$ is the sum of squared errors of data type $i$ at station $k$. $n_{k,i}$ is the number of observations for data type $i$ at station $k$. $o_{k,i,j}$ and $m_{k,i,j}$ are the observed and modeled $j^{th}$ values, respectively, for data type $i$ at station $k$. $o_{k,i,min}$ and $o_{k,i,max}$ are minimal and maximal observed values for data type $i$ at station $k$, respectively.
Note that we also first optimized parameters of the PAHLOW model against observational data at both stations using the algorithm of Delayed Rejection Adaptive Metropolis-Hastings Monte Carlo (Haario et al., 2006; Laine, 2008; Chen and Smith, 2018). Then we obtained the parameters of the MONOD model by fitting the growth rate outputs of PAHLOW model to achieve similar parameterizations for the two models. With this approach, we expected that the PAHLOW model should perform better than the MONOD model, albeit the difference should not be substantial. We then conducted a sensitive analysis to investigate whether the choice of certain parameter values would alter the relative performances between the two models. In particular, we tested how the type of grazing functions and the values of $a_{chl}$ and $A_{0N}$ affect the model results (Table 2). We varied the model parameters one by one, holding other parameters the same as in the default run in Table 1. We also limited the parameter values within realistic ranges noted in previous modeling studies (Fennel et al., 2006; Franks, 2009). The notation and values of model parameters are shown in Table 1. Note that, in preparation for future development of three-dimensional ocean models, we have intentionally applied the same set of parameters for the two stations. The model fortran codes, R scripts, and results are available on https://github.com/BingzhangChen/Citrate.

3. Results

3.1. Comparisons of $\mu$, $\theta$, and $Q^N$ between the PAHLOW and MONOD models

Both phytoplankton models estimate phytoplankton $\mu$, $\theta$, and $Q^N$ based on ambient environmental temperature, DIN concentrations, and light. The relationships between the growth rate and nitrogen, light, and temperature of the PAHLOW model when other resources are replete can be approximated by the MONOD model with slight departures (Fig. 3a,d,g). Although the differences are small, the PAHLOW
model predicts a somewhat flatter transition of growth rate than the MONOD model as resource levels increase because θ declines with increasing light and the half-saturation concentration for nitrogen uptake increases with increasing nutrient concentration (Smith et al., 2009). For this reason, the fitted value of $K_N$ for the MONOD model also depends on the nutrient range considered with the PAHLOW model. Considering a larger range of nutrient concentrations will yield a higher fitted value of $K_N$.

The growth rates differ most between the two models when both nutrients and light levels are limiting (Fig. 3). The PAHLOW model predicts higher growth rates at the same nutrient concentration than the MONOD model when light is limiting and also predicts higher growth rates under the same light level when nutrient is limiting. When nutrient or light is limiting, the PAHLOW model also predicts that the growth rate increases faster with temperature than the MONOD model.

The two models also predict different values of θ under low light (Fig. 3b,e,h). When the light deceases from high values, the PAHLOW model predicts an increasing θ with decreasing light and then a decreasing trend of θ when the light approaches the threshold value (Fig. 3e). This is particularly evident when light is plotted on a log scale (Fig. 4). By contrast, the MONOD model predicts that θ decreases strictly monotonically with decreasing light. The PAHLOW model also predicts that θ increases with temperature faster than the MONOD model when light is limiting.

For $Q^N$, although both models predict that $Q^N$ values increase with ambient $N$, the PAHLOW model predicts that $Q^N$ values should increase with decreasing light levels, while $Q^N$ values do not vary with light in the MONOD model (Fig. 3c,f). As such, under low light, the PAHLOW model predicts higher $Q^N$ values than the MONOD
model. The PAHLOW model also predicts that $Q_N$ values increase with temperature when light is limiting, while the MONOD model predicts that $Q_N$ is independent of temperature.

3.2. Comparisons with laboratory data

Analysis of laboratory data for phytoplankton $Q_N$ reveals a significant decreasing trend of $Q_N$ with increasing light when nutrients are replete (fixed effect $t = -3.69$, $p < 0.001$), although this trend varies among taxa (Fig. 4a). For $\theta$, the second-order term of the linear mixed-effect model is significantly negative ($t = -4.26$, $p < 0.001$), suggesting that the decreasing trend of $\theta$ with decreasing light under dim light is real (Fig. 4b). Thus, in general, the PAHLOW model shows better qualitative fits to the patterns of $Q_N$ and $\theta$ in laboratory experiments, although the PAHLOW model underestimates $\theta$ under dim light.

3.3. 1D model

Before comparing the modeled biological variables with in situ observations, we ensured the validity of the external physical forcing. The MLDs estimated from modeled profiles of $K_v$ fit well with observations at the two stations (Fig. 2). Station S1 shows the typical vertical mixing pattern in the subtropics with more vigorous mixing in the winter and stratification in the summer (Fig. 2b). The mixed layer depth reaches nearly 200 m in February and March. After April, the mixed layer rapidly shoals to around 15 m until August and then deepens again. Temperatures in the surface mixed layer vary from 18 °C in February and March to 27 °C in August and September (Fig. 2d). The surface PAR ranges from 19 to 54 mol photons $d^{-1} m^{-2}$ (equivalent to 47.5 to 135 W m$^{-2}$) (Fig. 2f).

Compared to station S1, the seasonal variation of mixing at station ALOHA is less drastic, although the winter mixing is still stronger than during summer (Fig. 2c).
The surface mixed layer exhibits weak mixing throughout the whole year. The mixing difference between S1 and ALOHA is also reflected in the vertical profiles of temperature, in which the seasonal variations of surface temperature are less pronounced at ALOHA than at S1 (Fig. 2e). The surface PAR, in general, is slightly stronger at ALOHA than at S1 (Fig. 2g).

Both models are able to simulate the general pattern of high DIN in the winter and the subsequent drawdown of nutrients in the surface mixed layer from winter to summer at S1 (Fig. 5a). However, the MONOD model overestimates the surface DIN at station ALOHA (Fig. 5b). The superiority of the PAHLOW model in modeling DIN is also indicated by its smaller SSqE (Table 2).

Both models are also able to reproduce the general seasonal patterns of Chl a concentrations and NPP in the surface mixed layer at S1 (Fig. 5). At ALOHA, however, the PAHLOW model underestimates Chl in surface waters, while the MONOD model agrees better with Chl a observations (Fig. 5d; Table 2). Both models underestimate surface NPP at ALOHA (Fig. 5f).

Examination of the seasonal vertical profiles at station S1 suggests that the modeled nutriclines are shallower than observed during summer and fall for both models (Fig. 6c,d). The two models also well reproduce the subsurface chlorophyll maximum (SCM) layer. Compared to the PAHLOW model, the MONOD model predicts higher Chl a concentrations below the SCM because of its higher predicted $\theta$ value under low light (Fig. 6f-h). The pattern of higher Chl a below SCM in the MONOD model than the PAHLOW model is also evident at station ALOHA (Fig. 7e-h). Both models generate an unrealistic subsurface peak of NPP during summer at S1 (Fig. 6k), while both models, particularly the PAHLOW model, underestimate NPP in surface waters at ALOHA (Fig. 7i-l).
Quantitative comparisons based on $SSqE$ yield mixed results for different variables (Table 2). The PAHLOW model simulates DIN better than the MONOD model at both stations, while the converse is true for Chl and NPP, particularly at ALOHA where the problem is mainly due to the PAHLOW model’s underestimation of Chl near the surface.

Sensitivity analysis suggests that changing the type of grazing functional response severely deteriorates the performance of the models, with other parameters unchanged (Table 2). Reducing $a_{chl}$ to half of its original value makes the model fits worse than the standard run for DIN and Chl at both stations. The only improvement is for NPP at S1. Conversely, if $a_{chl}$ is increased to twice its original value (i.e. making light limitation less likely), the fits of both models to DIN improve at both stations due to the increased nutrient uptake, while the fit to Chl worsens at ALOHA because the low DIN cannot support sufficient phytoplankton biomass. Compared to station ALOHA, this change of parameter value improves the fitting for both DIN and Chl at station S1 and only the fits for NPP worsen. Changing the nutrient affinity $A_{0N}$ barely affects the results of the PAHLOW model because of its dynamic acclimation response, but substantially affects the performance of the MONOD model, which lacks this acclimation response.

It is informative to directly compare $\mu$, $\theta$, and $Q^N$ from the 1D model outputs between the two models. Within the surface mixed layer of S1, the MONOD model gives slower growth rate during the winter when mixing is more intense and light is more limiting than other seasons (Fig. 8a). At station ALOHA, the PAHLOW model predicts lower growth rate due to the lower DIN concentration (Fig. 8b). The PAHLOW model predicts higher values of $\theta$ and $Q^N$ than the MONOD model during winter (Fig. 8c-f). Compared to the satellite-derived estimates of $\theta$, both models
predict higher values in winter and lower values in summer at S1, but underestimate it at ALOHA. Both models give lower $Q^N$ values compared to the observed particulate N:C ratios, particularly during summer.

We also show the comprehensive modeled patterns of $\mu$, $\theta$, and $Q^N$ at both stations (Fig. 9). One noticeable difference between the two models is that the PAHLOW model predicts higher growth rate than the MONOD model in deeper waters (and also in winter at S1), which reduces the upward nutrient diffusive flux and leads to lower Chl $a$ and NPP at the surface (Figs. 5-7).

A more prominent difference is that the PAHLOW model predicts low $\theta$ values (Fig. 9) in deep layers when light is negligible (Pahlow et al., 2013), which does not occur with the MONOD model. The PAHLOW model also predicts significantly higher $Q^N$ values than the MONOD model, exceeding the canonic Redfield N:C ratio in deep waters (Fig. 9).

A comparison of computation efficiency suggests that the PAHLOW model can cost 2 times of computation time than the MONOD model. When we used intel fortran compiler with the compiler option “-fast” on a macOS Sierra 10.12.5 (i386 processor), a single run of the PAHLOW model at station ALOHA took 0.071 min, around 2 times of the MONOD model (0.036 min).

4. Discussion

Optimality-based models, which account for organisms’ ability to acclimate to external environmental conditions, have been deemed a novel approach to faithfully represent biological mechanisms without compromising computational efficiency, with the potential to be widely applied in 3D GCMs (Follows and Dutkiewicz, 2011; Smith et al., 2011, 2014; Ward, 2017). Here we have compared the optimality-based PAHLOW model and a computationally more efficient and more widely-used
MONOD model, by examining the functional relationships between three key phytoplankton quantities ($\mu$, $Q^N$, and $\theta$) and environmental factors and testing whether both of them can well simulate the observed patterns in two subtropical stations. These comparisons not only provide deep understandings of the model performances, but also suggest new directions for future ocean observations.

We find that the relationships between $\mu$ and nutrient and light with the optimality-based PAHLOW model can be fairly well approximated by the widely-used MONOD model by parameter fitting, although the modeled growth rates differ noticeably under light-limiting conditions (Fig. 3). This concurs with previous arguments that simple models can well approximate the results of complicated photo-acclimation models (Flynn, 2003). However, here we have assessed these two models only at two contrasting subtropical stations, which provides a stringent but limited test of their performance, which can be expected to differ even more in applications over a wider range of environmental conditions, such as in 3D regional and global models.

Compared to the MONOD model, the faster growth rates of the PAHLOW model under low light allow phytoplankton to consume more nutrients at the SCM, yielding lower levels of surface nitrate and Chl. This effect may be overly strong, contributing to the PAHLOW model’s underestimates of surface DIN and Chl at station ALOHA (Fig. 5). It is noteworthy that the ubiquitous and ecologically important Prochlorococcus might have lost the capacity of photo-acclimation (Partensky et al., 1999), and if so the PAHLOW model may be unsuitable for modeling Prochlorococcus.

However, the PAHLOW model predicts qualitatively different patterns of $Q^N$ and $\theta$ compared to our modified MONOD model, which also gives dynamic estimates of these quantities. These differences cannot be eliminated simply by parameter tuning.
If it can be proven that the patterns generated by the PAHLOW model are in fact more realistic than those from the MONOD model, this would favor use of the PAHLOW model in GCMs, rather than tinkering with existing MONOD type models. Based on compilations of laboratory data for phytoplankton $Q^N$ and $\theta$ under light-limiting conditions (Fig. 4), the PAHLOW model does perform better in terms of the increasing trend of $Q^N$ with light limitation and the unimodal relationship between $\theta$ and light. These unique patterns may support the validity of its underlying biological assumption that phytoplankton cells optimize their internal resource allocation to achieve maximal fitness, constrained by the assumed tradeoff between photosynthesis and nutrient uptake. These assumptions were also similarly supported by Armstrong (2006). Interestingly, Goldman (1986) argued that light should not directly affect $Q^N$, which justifies that the extent of nutrient limitation can be quantified based on $Q^N$ alone without considering light. Our compiled data suggests that light can indeed affect $Q^N$, contradicting Goldman’s argument and suggesting that in order to evaluate the status of phytoplankton nutrient limitation, light should be taken into account. In other words, similar N:C ratios observed in phytoplankton cells under different light environments do not suggest that these cells are experiencing similar extents of nutrient limitation. At high latitudes where light may be more limiting than at low latitudes, phytoplankton cells need more nitrogen to synthesize light harvesting proteins and pigments (Klausmeier et al., 2004; Armstrong, 2006; Pahlow et al., 2013). This also implies that light should be considered when searching for patterns of nutrient-related traits for phytoplankton (Litchman et al., 2007; Edwards et al., 2012).

However, the PAHLOW model is not perfect, either. It strongly underestimates $\theta$ under very low light. As is apparent from Fig. 4b, although phytoplankton $\theta$ can have
a decreasing trend with decreasing light for PAR less than around 1 W m$^{-2}$, there are no observed $\theta$ values lower than 0.24 gChl molC$^{-1}$ (= 50 gC gChl$^{-1}$), as the PAHLOW model predicts.

The model estimates of $\theta$ and $Q^N$ are not less important than growth rate ($\mu$) because Chl and NPP involve combined calculations of all three outputs (i.e. $\mu$, $\theta$, and $Q^N$) from the phytoplankton models. It is possible that some model might be better in fitting Chl or NPP with the wrong combination of phytoplankton biomass in terms of nitrogen ($P$), $\mu$, $\theta$, and $Q^N$ (Eq. 18). The variations of $\theta$ are also critical for assessing the response of ocean primary production to environmental change from satellite observations, which offer us unprecedented spatial and temporal coverage (Behrenfeld et al., 2015; Westberry et al., 2016). The ideal approach to evaluate the phytoplankton models is to directly measure $P$, $\mu$, $\theta$, and $Q^N$ in the field. Currently, direct measurements of $\theta$ and $Q^N$ in the field are emerging but remain insufficient in both quantity and quality to distinguish between even the substantially different predictions of the two models considered herein (Graff et al., 2012, 2015). We urge that more measurements should be made, particularly in the lower euphotic layer, because such observations would be very useful for testing model performance and advancing understanding of phytoplankton physiology.

It is intriguing that the observed ratios of particulate organic nitrogen (PON) to POC at stations ALOHA and S1 are less than those predicted by the PAHLOW model and closer to the Redfield ratio (Fig. 10). If we trust the $Q^N$ predicted by the PAHLOW model, a reasonable explanation for the discrepancy between phytoplankton $Q^N$ and PON:POC ratios in surface waters might be that microzooplankton have higher N:C ratios than phytoplankton (Talmy et al., 2016). In deeper waters, however, the modeled phytoplankton N:C ratios even exceed the
measured PON:POC ratios, which can only be reconciled if the N:C ratios of other pools such as bacteria, zooplankton or detritus, are much lower than the Redfield ratio to offset the high phytoplankton N:C ratio. This hypothesis remains to be validated.

5. Conclusions

The original intent of this study was to use the classic Monod-type model to approximate the optimality-based model of Pahlow et al. (2013) to further simplify and speed up computation. Both models assume instantaneous acclimation and therefore allow direct calculations of phytoplankton growth rate, chlorophyll-to-carbon, and nitrogen-to-carbon ratios from ambient environmental nitrogen, light, and temperature, which circumvents the need to assign multiple tracers for the same phytoplankton population. While both models can reproduce the field observations to some extent, we find that, even though we tuned the parameters of the MONOD model to the outputs of the PAHLOW model, three features remain unique to the PAHLOW model. The first is that phytoplankton can achieve higher growth rates in the PAHLOW model than in the MONOD model when they are under light limitation. The second is that phytoplankton N:C ratios depend on light availability with the PAHLOW model, via its assumed tradeoff between photosynthesis and nutrient uptake. This dependence was stressed previously by Armstrong (2006) based on a single study (Laws and Bannister, 1980), and we have found further evidence for it, based on a larger dataset including data for nine taxa. The third is that with the PAHLOW model phytoplankton chlorophyll-to-carbon ratios decrease with decreasing light under dim light. This is also partially corroborated by laboratory data, although uncertainties remain, and field data are sparse. The commonly used MONOD model cannot easily reproduce all three of these observed patterns. We therefore conclude that some essential postulates of the optimality-based PAHLOW
model, such as the tradeoff between photosynthesis and nutrient uptake may be useful and even indispensable features that need to be considered in ocean biogeochemical models. However, we also identified some weakness of the PAHLOW model, such as the underestimation of $θ$ under very low light conditions, which may account for its inability to outperform the MONOD model in the 1D simulations (Table 2). Finally, we urge for more direct measurements of phytoplankton biomass in terms of carbon and nitrogen, specific growth rates, chlorophyll-to-carbon, and nitrogen-to-carbon ratios in the ocean.
Authors’ contributions

B. C.: designed the initial study, performed computer simulation, and wrote the first draft of the manuscript. S. L. S.: coded the initial version of the Metropolis-Hasting Monte-Carlo algorithm, provided feedbacks on the study design, and contributed to the results interpretation. Both authors contributed to discussions of the results and revision of the paper.

Conflict of interest

The authors declare no competing final interests.

Acknowledgments

We sincerely thank Markus Pahlow for his insightful comments on a previous version of the manuscript. This study was supported by a CREST Project (Grant Number JPMJCR12A3; P.I. SLS) funded by the Japan Science and Technology (JST) Agency and a Grants-in-Aid for Scientific Research (KAKENHI) (Grant Number JP16K21701; P.I. BC) funded by the Japan Society for the Promotion of Science (JSPS).
References


Honda, M.C., 2016. Short introduction to the K2S1 project. J. Oceanogr. 72, 341-342.


Biological organic carbon export estimated from the annual carbon budget observed in the surface waters of the western subarctic and subtropical North Pacific Ocean from 2004 to 2013. J. Oceanogr. 72, 665-685.


A size-structured food-web model for the global ocean. Limnol. Oceanogr. 57, 1877-1891.

Table 1. Parameters for the 1D model including both PAHLOW and MONOD models.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_w$</td>
<td>Light attenuation coefficient of seawater</td>
<td>0.04</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$K_{chl}$</td>
<td>Light attenuation coefficient of chlorophyll</td>
<td>0.025</td>
<td>(mg Chl a m$^{-2}$)$^{-1}$</td>
</tr>
<tr>
<td>$E_p$</td>
<td>Activation energy of phytoplankton rates</td>
<td>0.5</td>
<td>eV</td>
</tr>
<tr>
<td>$E_z$</td>
<td>Activation energy of zooplankton rates</td>
<td>0.6</td>
<td>eV</td>
</tr>
<tr>
<td>$Q_{ON}$</td>
<td>Phytoplankton minimal N:C ratio</td>
<td>0.04</td>
<td>mol: mol</td>
</tr>
<tr>
<td>$\theta_{min}$</td>
<td>Minimal chlorophyll-to-carbon ratio</td>
<td>0.02</td>
<td>gChl molC$^{-1}$</td>
</tr>
<tr>
<td>$unass$</td>
<td>Fraction of unassimilated food by zooplankton</td>
<td>0.24</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$NGE$</td>
<td>Net growth efficiency of zooplankton</td>
<td>0.3</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$g_m$</td>
<td>Maximal per capita ingestion rate of zooplankton</td>
<td>1.6</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>$K_p$</td>
<td>Grazing half-saturation constant of zooplankton</td>
<td>0.5</td>
<td>$\mu$M N</td>
</tr>
<tr>
<td>$W_d$</td>
<td>Sinking rate of detritus</td>
<td>1</td>
<td>m d$^{-1}$</td>
</tr>
<tr>
<td>$R_{dn}$</td>
<td>Conversion rate of detritus to inorganic nitrogen</td>
<td>0.1</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>$m_z$</td>
<td>Coefficient of mortality rate of zooplankton</td>
<td>0.15</td>
<td>($\mu$M N)$^{-1}$d$^{-1}$</td>
</tr>
</tbody>
</table>

Parameters of the MONOD model

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_C$</td>
<td>Carbon-specific initial slope of photosynthesis versus light</td>
<td>0.11</td>
<td>(W m$^{-2}$)$^{-1}$d$^{-1}$</td>
</tr>
<tr>
<td>$\theta_{max}$</td>
<td>Maximal chlorophyll-to-carbon ratio</td>
<td>0.61</td>
<td>gChl molC$^{-1}$</td>
</tr>
<tr>
<td>$K_N$</td>
<td>Phytoplankton growth half-saturation constant for nitrogen</td>
<td>1.33</td>
<td>$\mu$M N</td>
</tr>
<tr>
<td>$\mu_m'$</td>
<td>Phytoplankton maximal growth rate at 15 °C</td>
<td>2.44</td>
<td>d$^{-1}$</td>
</tr>
</tbody>
</table>

Parameters of the PAHLOW model

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_0'$</td>
<td>Phytoplankton potential carbon acquisition rate at 15°C</td>
<td>5</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>Parameter</td>
<td>Description</td>
<td>Value</td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>-------------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>$\alpha_{\text{chl}}$</td>
<td>Chlorophyll-specific initial slope of photosynthesis versus light</td>
<td>$0.59^g$ (W m$^{-2}$)$^{-1}$ (gChl molC)$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$V_{0N}$</td>
<td>Phytoplankton potential nitrogen acquisition rate at 15°C</td>
<td>$5^g$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$A_{ON}$</td>
<td>Phytoplankton maximal potential nitrogen affinity at 15 °C</td>
<td>$0.23^g$ m$^3$ mmol C$^{-1}$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$R_{M}$</td>
<td>Cost of chlorophyll maintenance</td>
<td>$0.1^g$ d$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\zeta_{\text{chl}}$</td>
<td>Cost of chlorophyll synthesis</td>
<td>$0.6^g$ (mol C) (g Chl)$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\zeta^N$</td>
<td>Cost of nitrogen assimilation</td>
<td>$0.8^g$ (mol C) (mol N)$^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>

---

$^a$Fennel et al. (2006); $^b$Chen and Laws (2017); $^c$Fitting to the PAHLOW model;

$^d$Flynn (2003); $^e$Buitenhuis et al. (2010); $^f$Chai et al. (2002); $^g$Pahlow et al. (2013).
Table 2. Sum of squared errors between model outputs and observational data for sensitive analysis. The standard run uses all the parameter values in Table 1 with a Holling type III functional response for zooplankton. The numbers within the brackets indicate the number of observations. All other parameters are kept constant.

<table>
<thead>
<tr>
<th></th>
<th>ALOHA</th>
<th>S1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Standard run</strong></td>
<td>DIN (3910) Chl (8180) NPP (1659) DIN (902) Chl (426) NPP (128)</td>
<td></td>
</tr>
<tr>
<td>MONOD</td>
<td>73.2</td>
<td>218</td>
</tr>
<tr>
<td>PAHLOW</td>
<td>58.2</td>
<td>690</td>
</tr>
<tr>
<td><strong>Holling type I</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MONOD</td>
<td>104.3</td>
<td>4928</td>
</tr>
<tr>
<td>PAHLOW</td>
<td>89.6</td>
<td>2659</td>
</tr>
<tr>
<td><strong>Holling type II</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MONOD</td>
<td>113.9</td>
<td>6377</td>
</tr>
<tr>
<td>PAHLOW</td>
<td>106.2</td>
<td>4499</td>
</tr>
</tbody>
</table>

- $\alpha_{ch}=0.3$ ($\alpha_C=0.06$)
  | MONOD        | 81.9           | 173           | 74.5          | 32.2          | 16            | 7.1           |
  | PAHLOW       | 65.5           | 915           | 75.2          | 26.8          | 17.6          | 9.2           |

- $\alpha_{ch}=1.2$ ($\alpha_C=0.2$)
  | MONOD        | 65.6           | 326           | 31.2          | 22.7          | 13.6          | 17.8          |
  | PAHLOW       | 49.6           | 1075          | 75.1          | 16.9          | 11.7          | 22.6          |

- $A_{ON}=0.1$ ($K_N=2.6$)
  | MONOD        | 82.7           | 293           | 65.6          | 30.7          | 12.5          | 10.1          |
  | PAHLOW       | 61.6           | 686           | 57.9          | 25.1          | 12.5          | 13.6          |

- $A_{ON}=0.5$ ($K_N=0.6$)
  | MONOD        | 65.0           | 227           | 33.6          | 24.4          | 15.8          | 13.1          |
  | PAHLOW       | 59.6           | 709           | 59.4          | 19.8          | 14.1          | 14.3          |
Figure legends

Fig. 1. Conceptual diagram of the two models compared herein. The PAHLOW model (left) calculates the intracellular resource allocation (vertical dashed line in the lower left figure) that optimizes specific growth rate, μ, subject to postulated costs and benefits of carbon and nitrogen assimilation. This gives an inter-dependent functional response to light (I), nutrient (N), and temperature (T). The simpler MONOD model (right) uses empirically based functions (depicted in the lower right figure) for the dependence of μ, θ (Chl : carbon ratio, g : mol), and $Q^N$ (cell quota, mol N: mol C). This gives simpler multiplicative dependences. Most notably, $Q^N$ depends on I, T, and N in the PAHLOW model, whereas it depends only on N in the MONOD model.

Fig. 2. (a) The locations of stations S1 and ALOHA superimposed on the annual mean Chl a concentration obtained from SeaWIFS. (b,c) Seasonal variations of vertical eddy diffusivity ($K_v$). The open white squares denote the mixed layer depth (MLD) from observed vertical profiles of temperature and salinity. The tannish thick line denotes the MLD calculated from vertical profiles of $K_v$. (d,e) Seasonal variations of temperature. (f,g) Seasonal variations of surface PAR.

Fig. 3. Comparisons of phytoplankton growth rate, chlorophyll-to-carbon (Chl:C) and nitrogen-to-carbon (N:C) ratios under different nitrogen, light, and temperature conditions between the MONOD and PAHLOW models.

Fig. 4. (a) Phytoplankton nitrogen-to-carbon (N:C) ratios and (b) chlorophyll-to-carbon (Chl:C) ratios versus log-transformed PAR levels. The thick solid black lines denote the fixed effects and the thin solid lines with colors denote the fits of each taxon. The red dashed lines indicate the predictions of the
PAHLOW model. The dashed horizontal blue lines indicate standard Redfield N:C ratio (0.15) in (a) and Chl:C ratio (0.24 gChl molC\(^{-1}\) = 50 gC gChl\(^{-1}\)) in (b). The histograms on the right side indicate the frequency distributions of N:C and Chl:C ratios.

Fig. 5. Seasonal variations of dissolved inorganic nitrogen (DIN), Chl \(a\) concentrations, and net primary production (NPP) averaged through the surface mixed layer. The black dots indicate observational data.

Fig. 6. Vertical distributions of modeled DIN, Chl \(a\) concentrations, and NPP at station S1 pooled into four seasons and comparisons with observational data (black dots) for the two models. The dashed lines represent 2.5% and 97.5% percentiles.

Fig. 7. The same as Fig. 6, but for station ALOHA.

Fig. 8. Seasonal variations of phytoplankton growth rate, chlorophyll-to-carbon ratios, and nitrogen-to-carbon ratios averaged through the surface mixed layer. The open triangles indicate observational data.

Fig. 9. Modeled vertical patterns of phytoplankton growth rates (\(\mu\)), chlorophyll-to-carbon (Chl:C), and nitrogen-to-carbon (N:C) ratios of the MONOD and PAHLOW models at two stations.

Fig. 10. The vertical patterns of nitrogen-to-carbon ratios of particulate organic matters in four seasons at the two stations. Black dots indicate observed values.