

1 **Optimality-based approach for computationally**
2 **efficient modeling of phytoplankton growth,**
3 **chlorophyll-to-carbon, and nitrogen-to-carbon**
4 **ratios**

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17 **Abstract**

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

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39 **1. Introduction**

40 Functional relationships for phytoplankton properties such as the growth rate (μ),
41 chlorophyll-to-carbon (θ), and nitrogen-to-carbon ratios (Q^N) in terms of abiotic
42 environmental factors such as nutrient and light are essential to any plankton model
43 and have been studied extensively (Droop, 1974; Jassby and Platt, 1976; Cloern et al.,
44 1995; Litchman et al., 2007; Edwards et al., 2012, 2015, 2016). A widely-adopted
45 approach is to treat phytoplankton carbon, nitrogen, and chlorophyll as independent
46 tracers and make μ dependent on Q^N such as the Droop function (Droop, 1974) and
47 also dependent on θ and light as in Geider et al. (1997, 1998). This approach has been
48 implemented in some three-dimensional ocean general circulation models (GCMs)
49 such as ERSEM (Butenschön et al., 2016) and a global size-structured plankton
50 model (Ward et al., 2012). Although sound, this approach requires a great many
51 calculations, particularly when a large number of phytoplankton species are included
52 in a 3D GCM (Follows et al., 2007; Barton et al., 2010; Ward et al., 2012). Another
53 drawback is that for tracers having spatial gradients of opposite sign (e.g.,
54 phytoplankton carbon concentrations are typically higher near the sea surface while
55 chlorophyll concentrations are higher at depth due to photo-acclimation), their
56 corresponding diffusive fluxes will be in opposite directions, which is unrealistic. It is
57 therefore preferable not to have multiple tracers for components of the same
58 phytoplankton biomass. On the other hand, fixed θ or Q^N based on the Redfield ratio
59 are unrealistic and should be avoided to the extent possible (Geider and La Roche,
60 2002; Flynn, 2003; Christian, 2005).

61 One approach to this dilemma is provided by optimality-based models, which can
62 be viewed as intermediate between the two extremes considered above (Flynn, 2003).
63 The principle of the optimality concept is that all organisms that face physiological

64 tradeoffs can be assumed to attain maximal fitness by adjusting trait values
65 (Sutherland, 2005; Armstrong, 2006; Smith et al., 2011). Mathematically, the optimal
66 trait value can be computed by solving the fitness gradient function by assuming
67 instantaneous acclimation (Smith et al., 2011) and μ , θ , and Q^N can be directly
68 calculated based on external environmental conditions such as temperature, light, and
69 nutrient concentrations. This speeds up computation because otherwise two or more
70 independent tracers (phytoplankton chlorophyll and carbon) must be added to the
71 model (Geider et al., 1998; Ward et al., 2012). Encouragingly, Ward (2017) recently
72 showed that the instantaneous acclimation of cellular nutrient quota can accurately
73 approximate the simulation outputs of a dynamic quota model, which requires an
74 additional tracer for each nutrient considered, even under dynamic environmental
75 conditions.

76 In this study, we focus on an optimality-based phytoplankton model developed
77 by Pahlow and coworkers, hereafter PAHLOW model (Fig. 1; Pahlow and Oschlies,
78 2013; Pahlow et al., 2013; Smith et al., 2016). The success of the PAHLOW model is
79 reflected in that it provided the first theoretical derivation of the well-known Droop
80 quota model (Pahlow and Oschlies, 2013) and has been validated extensively against
81 laboratory datasets (Pahlow et al., 2013) and somewhat against oceanic observations
82 (Arteaga et al., 2014; Fernández-Castro et al., 2016; Smith et al., 2016).

83 Although elegant, the basic mathematical properties of the PAHLOW model and
84 its coupling to ocean circulation models have not been thoroughly investigated (Smith
85 et al., 2016). In particular, given that the fundamental relationships of μ versus light
86 and nutrient appear similar to the widely used Monod-type model, it remains to be
87 explored to what extent the simpler Monod-type model can, with suitable tuning of
88 parameter values, reproduce the output of the PAHLOW model (Burmester, 1979;

89 Flynn, 2003). Another consideration is that although the optimality assumptions have
90 simplified much of the computation, the PAHLOW model still requires more
91 calculations compared with the computationally simpler MONOD model. If it can be
92 shown that the two models are mathematically similar and generate similar patterns
93 under realistic ocean conditions, then the use of the MONOD model may be justified
94 in many cases.

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

103 **2. Methods**

104 2.1. Optimality-based phytoplankton model (PAHLOW model)

105 In the PAHLOW model, phytoplankton cells are assumed to instantaneously
106 optimize their cellular Chl *a* and nitrogen contents to obtain maximal net growth,
107 which is the net outcome of CO₂ fixation minus the energetic costs of photosynthesis
108 and nutrient uptake. Note that although Pahlow et al. (2013) also included phosphorus
109 limitation and nitrogen fixation in their model, for simplicity we here consider only
110 nitrogen as the limiting nutrient.

111 There are three levels of optimization in the simplified PAHLOW model. The
112 first is the optimization of the Chl:C ratio within the chloroplast ($\hat{\theta}_0$) to maximize net
113 photosynthesis (i.e. gross photosynthesis minus the cost of chlorophyll maintenance).

114 Pahlow et al. (2013) necessarily assumed that the net photosynthesis of a chloroplast
 115 is independent of nutrient levels (but the number of chloroplasts within one cell is
 116 dependent on nitrogen availability). By solving the gradient function of net
 117 photosynthesis of one chloroplast against $\hat{\theta}_0$, $\hat{\theta}_0$ can be solved as follows (*see* Pahlow
 118 et al. (2013) for details):

$$119 \quad \hat{\theta}_0 = \frac{1}{\zeta^{chl}} + \frac{\mu_0}{\alpha_{chl} I} \left\{ 1 - W_0 \left[\left(1 + \frac{R_M^{chl}}{\mu_0} \right) e^{\left(1 + \frac{\alpha_{chl} I}{\zeta^{chl} \mu_0} \right)} \right] \right\} \quad \text{if } I > I_0 \quad (1)$$

$$120 \quad \hat{\theta}_0 = \theta_{min} \quad \text{if } I \leq I_0$$

121 in which I is irradiance (W m^{-2}). α_{chl} is the chlorophyll-specific initial slope of
 122 photosynthesis–irradiance (P–I) curve. ζ^{chl} is the cost of photosynthesis coefficient.
 123 R_M^{chl} is the cost of Chl maintenance. μ_0 is the phytoplankton potential carbon
 124 acquisition rate. W_0 is the zero branch of the Lambert-W function. $I_0 (= \frac{\zeta^{chl} R_M^{chl}}{\alpha_{chl}})$ is the
 125 threshold light level for chlorophyll synthesis. θ_{min} is the minimal chlorophyll-to-
 126 carbon ratio (equaling zero in Pahlow et al. (2013)). Both R_M^{chl} and μ_0 are temperature
 127 dependent and are assumed to have the same temperature coefficient E_p :

$$128 \quad \mu_0 = \mu'_0 e^{\frac{E_p}{k} \left(\frac{1}{T_0} - \frac{1}{T} \right)} \quad (2)$$

129 where μ'_0 is the phytoplankton potential carbon acquisition at the reference
 130 temperature T_0 (288 K). E_p is the activation energy (eV) of phytoplankton growth. k is
 131 the Boltzmann constant ($8.62 \times 10^{-5} \text{ eV K}^{-1}$).

132 From Eq. 1, it is clear that light is the most important abiotic factor directly
 133 affecting $\hat{\theta}_0$. (Temperature also has some indirect, less important effects.) As shown
 134 later, $\hat{\theta}_0$ is a nonlinear function of light. Under high light, it is beneficial for the
 135 phytoplankton cell to slow down chlorophyll synthesis to reduce the cost of
 136 photosynthesis, because this reduces only slightly the rate of photosynthesis. If light

137 level is too low (approaching or below I_0), however, the phytoplankton cell has
 138 negligible photosynthesis and also needs to reduce $\hat{\theta}_0$.

139 The second level of optimization is to balance the energy allocation between
 140 photosynthesis and nitrogen uptake. Pahlow and Oschlies (2013) assumed that the
 141 total nitrogen of the phytoplankton cell is partitioned among three pools (machineries
 142 of carbon acquisition and nitrogen uptake plus subsistence requirements). The net
 143 relative growth of the cell equals to net photosynthesis of the whole cell minus the
 144 respiratory cost of nitrogen uptake. By solving the gradient function of the net relative
 145 growth against the allocation factor (f_v) for nitrogen uptake, the optimal cellular
 146 nitrogen quota (Q^N , mol N (mol C)⁻¹) can be calculated as (Pahlow and Oschlies,
 147 2013):

$$148 \quad Q^N = Q_S^N \left[1 + \sqrt{1 + \frac{1}{Q_S^N \left(\frac{\hat{\mu}^I}{\hat{V}^N} + \zeta^N \right)}} \right] \quad (3)$$

149 where Q_S^N is the structural nitrogen quota and equals half of the minimal
 150 nitrogen quota (Q_{0N}) as often reported in the literature. \hat{V}^N is the potential nutrient
 151 uptake rate. $\hat{\mu}^I$ is the light dependent growth rate after accounting for photosynthesis
 152 and chlorophyll maintenance. ζ^N represents the cost of nitrogen assimilation. f_v can be
 153 calculated from Q^N :

$$154 \quad f_v = \frac{Q_S^N}{Q^N} - \zeta^N (Q^N - 2Q_S^N) \quad (4)$$

155 The chlorophyll-to-carbon ratio (θ , mol C gChl⁻¹) of the whole cell can be
 156 calculated as:

$$157 \quad \theta = \hat{\theta}_0 \left(1 - \frac{Q_S^N}{Q^N} - f_v \right). \quad (5)$$

158 $\hat{\mu}^I$ is calculated following eq. A2 in Pahlow et al. (2013):

$$159 \quad \hat{\mu}^I = \mu_0 S^I - (\mu_0 S^I + R_M^{chl}) \zeta^{chl} \hat{\theta}_0 \quad (6)$$

160 where S^I is the degree of light saturation:

$$161 \quad S^I = 1 - e^{-\frac{\alpha_{chl} \hat{\theta}_0^I}{\mu_0}} \quad (7)$$

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

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

$$168 \quad \hat{V}^N = \frac{V_0^N N}{\frac{V_0^N}{A_0^N} + 2 \sqrt{\frac{V_0^N N}{A_0^N} + N}} \quad (8)$$

169 in which V_0^N (d^{-1}) is the maximal potential nitrogen uptake rate. A_0^N ($\text{m}^3 \text{mmol}^{-1} \text{d}^{-1}$) is
 170 the maximal potential affinity. N is ambient nitrogen concentration (mmol m^{-3}). Both
 171 V_0^N and A_0^N share the same temperature dependence as R_M^{chl} and μ_0 in Eq. 2. Eq. 8
 172 differs from the Michaelis-Menten equation in that the apparent half-saturation
 173 ‘constant’ increases with N (Smith et al., 2009).

174 Finally, phytoplankton net growth rate (μ) is calculated as:

$$175 \quad \mu = \hat{\mu}^I \left(1 - 2 \frac{Q_s^N}{Q^N}\right) \quad (9)$$

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

179 2.2. Monod-type model

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

$$182 \quad \mu = \mu_m \frac{N}{N + K_N} \left(1 - e^{-\frac{\alpha_c I}{\mu_m}}\right) \quad (10)$$

183 where K_N is the half-saturation constant of nitrogen for phytoplankton growth. α_c is
 184 the carbon-specific slope of the growth-irradiance curve. μ_m differs from the μ_0 in that
 185 it already takes into account algal respiration. μ_m is also temperature dependent:

$$186 \quad \mu_m = \mu'_m e^{\frac{E_p}{k} \left(\frac{1}{T_0} - \frac{1}{T} \right)} \quad (11)$$

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

193 Following Flynn (2003), θ can be calculated as:

$$194 \quad \theta = \theta_{min} + \frac{\mu}{I\alpha_{chl}} \quad (12)$$

195 in which θ_{min} represents the minimal chlorophyll-to-carbon ratio at very high light.
 196 The maximal θ (θ_{max}) can be achieved at minimal light and saturating nutrient
 197 conditions and can be derived following the L'Hôpital's Rule:

$$198 \quad \theta_{max} = \theta_{min} + \lim_{I \rightarrow 0} \frac{\mu}{I\alpha_{chl}} = \theta_{min} + \frac{1}{\alpha_{chl}} \lim_{I \rightarrow 0} \frac{\mu_m (1 - e^{-\frac{\alpha_c I}{\mu_m}})}{I} = \theta_{min} + \frac{\alpha_c}{\alpha_{chl}} \quad (13)$$

199 By substituting α_{chl} in Eq. 13 into Eq. 12, we obtain:

$$200 \quad \theta = \theta_{min} + \frac{\mu}{I\alpha_c} (\theta_{max} - \theta_{min}) \quad (14)$$

201 in which θ_{max} can be imported from the PAHLOW model (Eq. 5). Note that Eq. 12
 202 always holds if phytoplankton growth is limited by light acquisition instead of Calvin
 203 cycle processes (Flynn, 2003). The nutrient effect on θ is embedded within the
 204 nutrient dependence of μ . The derived patterns of θ to light and nutrients are also
 205 consistent with other models (Cloern et al., 1995; Geider et al., 1997).

206 Further, by equating ambient nutrient-dependent and internal quota-dependent
 207 growth rates (Morel, 1987):

$$208 \quad \mu = \mu_m \frac{N}{N+K_N} = \mu_m \frac{1 - \frac{Q_{min}}{Q^N}}{1 - \frac{Q_{min}}{Q_{max}}} \quad (15)$$

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

$$212 \quad Q^N = \frac{Q_{min}}{1 - \left(1 - \frac{Q_{min}}{Q_{max}}\right)^{\frac{N}{N+K_N}}} \quad (16)$$

213 As such, our formulation of the MONOD model also allows to directly calculate θ
 214 and Q^N from external environmental nitrogen, light, and temperature.

215 Thus, both the PAHLOW and MONOD models share similar inputs (i.e.
 216 temperature, light, inorganic nitrogen) and outputs (μ , θ , Q^N), being able to provide
 217 estimates of flexible θ and Q^N assuming instantaneous acclimation without the
 218 necessity of computing the dynamics of independent tracers of cellular carbon and
 219 chlorophyll contents within phytoplankton cells (Fig. 1). To allow similar
 220 parameterizations between both models, we used an adaptive nonlinear least square
 221 regression to estimate the parameters (i.e., μ_m , K_N , and α_c) of the MONOD model by
 222 fitting the growth rates of the MONOD model against the outputs of PAHLOW model
 223 under various light and nutrient conditions, after selecting the parameters of the
 224 PAHLOW model (Fig. 3a,d). This was implemented with the function ‘*nls*’ with the
 225 ‘*port*’ algorithm in R 3.3.2 (Dennis et al., 1981; R Core Team, 2016).

226 2.3. Analysis of laboratory data for phytoplankton chlorophyll-to-carbon and
 227 nitrogen-to-carbon ratios

228 From five published studies (Falkowski and Owens, 1980; Laws and Bannister,
 229 1980; Terry et al., 1983; Falkowski et al., 1985; Strzepek and Price, 2000), we

230 compiled a dataset of θ and Q^N of nine phytoplankton taxa under light limiting
231 conditions to validate the outputs of the two models. We focus on θ and Q^N because
232 the predictions of θ and Q^N under light limitation are the most striking contrasts
233 between the PAHLOW and MONOD models. The data for two of the nine taxa were
234 used in Pahlow et al. (2013). To be consistent with the 1D model, we converted all the
235 light units to W m^{-2} by calculating the total daily photon doses, assuming $1 \text{ W m}^{-2} =$
236 $2.5 \text{ mol photons m}^{-2} \text{ d}^{-1}$. The light levels (I) were log-transformed ($\log I$) to reach a
237 quasi normal distribution.

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

250 2.4. One-dimensional model

251 To examine the performances of the two models under more realistic conditions,
252 we embedded the two phytoplankton models within a simple one-dimensional (1D)
253 numerical model (surface to 250 m depth) implemented for two stations (S1: 145 °E,
254 30 °N; ALOHA: 158 °E, 22.75 °N) in the North Pacific (Fig. 2a). This 1D model

255 contained four biological tracers: dissolved inorganic nitrogen, phytoplankton,
 256 zooplankton, and detritus. For simplicity, the physical variables relevant to biological
 257 processes (i.e. temperature, surface photosynthetically available radiance (PAR_0), and
 258 vertical eddy diffusivity (K_v)) were imported from external data products and linearly
 259 interpolated for each time step and depth level (Chen and Smith, 2018). PAR_0 data
 260 were imported from SeaWiFS satellite monthly climatology products. Seasonal
 261 temperature vertical profiles were imported from World Ocean Atlas 2013 monthly
 262 climatology. The profiles of K_v were imported from the output of an eddy-permitting
 263 model for North Pacific (Hashioka et al., 2009). Light levels (I_z) at depth z were
 264 calculated based on PAR_0 and Chl a concentrations following the Beer-Lambert law:

$$265 \quad I_z = PAR_0 e^{-(zK_w + K_{chl} \int_0^z Chl(x) dx)} \quad (17)$$

266 in which K_w and K_{chl} are the attenuation coefficients for seawater and Chl a ,
 267 respectively. However, one problem with the Eulerian framework is that the time for a
 268 phytoplankton cell to mix throughout the surface mixed layer (ML) is much less than
 269 its doubling time (Franks, 2015). We therefore calculated the ambient light level for
 270 phytoplankton within the ML as the average light (\bar{I}) throughout the ML. The mixed
 271 layer depth (MLD) is defined as the deepest depth with $K_v > 10^{-3} \text{ m}^2 \text{ s}^{-1}$. Based on the
 272 equation $\tau_L = \frac{L}{2K(z)}$ (eq. (1) in Franks (2015)), the average time (τ_L) for a
 273 phytoplankton cell to move at a distance (L) of 100 m at the local diffusivity ($K(z)$) of
 274 $10^{-3} \text{ m}^2 \text{ s}^{-1}$ is roughly half a day. As such, we assumed that the phytoplankton cells
 275 within the ML should receive the average light throughout the ML. \bar{I} was used to
 276 calculate phytoplankton μ , θ , and Q^N for temporal evolution of phytoplankton
 277 biomass and also standing stocks of Chl a . This might cause a sharp transition of
 278 phytoplankton properties across the bottom of the ML. However, to compare with *in*
 279 *situ* net primary production (NPP) estimates derived from incubation bottles that were

280 not mixed during incubation, phytoplankton μ , θ , and Q^N were recalculated from I_z
 281 based on the Beer-Lambert law. Thus, NPP depends directly on I_z instead of \bar{I} due to
 282 the inevitable incubation problem:

$$283 \quad NPP = P \frac{\mu(N, I_z, T)}{Q^N(N, I_z, T)} \quad (18)$$

284 Phytoplankton sinking was assumed negligible due to the dominance of small
 285 phytoplankton at the two oligotrophic stations (Campbell et al., 1997; Fujiki et al.,
 286 2016). Only detritus was assumed to sink at a constant rate W_d (m d⁻¹). Zooplankton
 287 specific ingestion rate (g , d⁻¹) of phytoplankton was described as a Holling III
 288 function:

$$289 \quad g = g_m e^{\frac{E_z}{k} \left(\frac{1}{T_0} - \frac{1}{T} \right)} \frac{P^2}{P^2 + K_p^2} \quad (19a)$$

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

$$294 \quad g = g_m e^{\frac{E_z}{k} \left(\frac{1}{T_0} - \frac{1}{T} \right)} \min \left(\frac{P}{2K_p}, 1 \right) \quad (19b)$$

295 and the Holling II function is:

$$296 \quad g = g_m e^{\frac{E_z}{k} \left(\frac{1}{T_0} - \frac{1}{T} \right)} \frac{P}{P + K_p} \quad (19c)$$

297 The total food intake of zooplankton (Z_{inges}) is partitioned into three parts. The
 298 first part ($Z_{inges} \cdot NGE$) is used by zooplankton for net growth. The second part is
 299 defecated to the detritus pool ($Z_{eges} = unass \cdot Z_{inges}$) and the last part is recycled back
 300 to the DIN pool ($Z_{res} = Z_{inges} \cdot (1 - NGE - unass)$). Here NGE is the net growth
 301 efficiency of zooplankton and $unass$ is the fraction of unassimilated food.

302 Detritus is converted to nitrogen at a rate with the same activation energy with
 303 zooplankton, E_z . The zooplankton mortality term is assumed proportional to the
 304 square of zooplankton biomass (Steele and Henderson, 1992; Ohman and Hirche,
 305 2001).

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

$$310 \quad \frac{dN}{dt} = -P\mu + Zg(1 - NGE - unass) + e^{\frac{E_z}{k}(\frac{1}{T_0} - \frac{1}{T})} DR_{dn} + \frac{d}{dz} \left(K_v \frac{dN}{dz} \right) \quad (20a)$$

$$311 \quad \frac{dP}{dt} = P\mu - Zg + \frac{d}{dz} \left(K_v \frac{dP}{dz} \right) \quad (20b)$$

$$312 \quad \frac{dZ}{dt} = Zg \cdot NGE - m_z Z^2 e^{\frac{E_z}{k}(\frac{1}{T_0} - \frac{1}{T})} + \frac{d}{dz} \left(K_v \frac{dZ}{dz} \right) \quad (20c)$$

$$313 \quad \frac{dD}{dt} = Zg \cdot unass + e^{\frac{E_z}{k}(\frac{1}{T_0} - \frac{1}{T})} (m_z Z^2 - DR_{dn}) - W_d \frac{dD}{dz} + \frac{d}{dz} \left(K_v \frac{dD}{dz} \right) \quad (20d)$$

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

319 2.5. Observational data and sensitivity analysis

320 For stations S1, the observational data of total dissolved inorganic nitrogen
 321 (DIN), Chl a concentrations, and NPP were collected in the K2S1 project
 322 (<https://ebcrpa.jamstec.go.jp/k2s1/en/index.html>; Fujiki et al., 2016; Honda, 2016;
 323 Matsumoto et al., 2016; Wakita et al., 2016). For station ALOHA, the observational
 324 data were downloaded from the Hawaii Ocean Time-series website
 325 (<http://hahana.soest.hawaii.edu/hot/>). We pooled all the observational data into one

326 climatological year, assuming that seasonal changes of environmental conditions are
 327 the major factors determining changes in biological variables and inter-annual
 328 variations are relatively less important.

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

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

$$345 \quad SSqE_{k,i} = \sum_{j=1}^{n_{k,i}} \left(\frac{m_{k,i,j}^{0.25} - o_{k,i,min}^{0.25}}{o_{k,i,max}^{0.25} - o_{k,i,min}^{0.25}} - \frac{o_{k,i,j}^{0.25} - o_{k,i,min}^{0.25}}{o_{k,i,max}^{0.25} - o_{k,i,min}^{0.25}} \right)^2 \quad (21)$$

346 where $SSqE_{k,i}$ is the sum of squared errors of data type *i* at station *k*. $n_{k,i}$ is the
 347 number of observations for data type *i* at station *k*. $o_{k,i,j}$ and $m_{k,i,j}$ are the observed and
 348 modeled j^{th} values, respectively, for data type *i* at station *k*. $o_{k,i,min}$ and $o_{k,i,max}$ are
 349 minimal and maximal observed values for data type *i* at station *k*, respectively.

350 Note that we also first optimized parameters of the PAHLOW model against
351 observational data at both stations using the algorithm of Delayed Rejection Adaptive
352 Metropolis-Hastings Monte Carlo (Haario et al., 2006; Laine, 2008; Chen and Smith,
353 2018). Then we obtained the parameters of the MONOD model by fitting the growth
354 rate outputs of PAHLOW model to achieve similar parameterizations for the two
355 models. With this approach, we expected that the PAHLOW model should perform
356 better than the MONOD model, albeit the difference should not be substantial. We
357 then conducted a sensitive analysis to investigate whether the choice of certain
358 parameter values would alter the relative performances between the two models. In
359 particular, we tested how the type of grazing functions and the values of α_{chl} and A_{ON}
360 affect the model results (Table 2). We varied the model parameters one by one,
361 holding other parameters the same as in the default run in Table 1. We also limited the
362 parameter values within realistic ranges noted in previous modeling studies (Fennel et
363 al., 2006; Franks, 2009). The notation and values of model parameters are shown in
364 Table 1. Note that, in preparation for future development of three-dimensional ocean
365 models, we have intentionally applied the same set of parameters for the two stations.
366 The model fortran codes, R scripts, and results are available on
367 <https://github.com/BingzhangChen/Citrate>.

368 **3. Results**

369 3.1. Comparisons of μ , θ , and Q^N between the PAHLOW and MONOD models

370 Both phytoplankton models estimate phytoplankton μ , θ , and Q^N based on
371 ambient environmental temperature, DIN concentrations, and light. The relationships
372 between the growth rate and nitrogen, light, and temperature of the PAHLOW model
373 when other resources are replete can be approximated by the MONOD model with
374 slight departures (Fig. 3a,d,g). Although the differences are small, the PAHLOW

375 model predicts a somewhat flatter transition of growth rate than the MONOD model
376 as resource levels increase because θ declines with increasing light and the half-
377 saturation concentration for nitrogen uptake increases with increasing nutrient
378 concentration (Smith et al., 2009). For this reason, the fitted value of K_N for the
379 MONOD model also depends on the nutrient range considered with the PAHLOW
380 model. Considering a larger range of nutrient concentrations will yield a higher fitted
381 value of K_N .

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

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

396 For Q^N , although both models predict that Q^N values increase with ambient N , the
397 PAHLOW model predicts that Q^N values should increase with decreasing light levels,
398 while Q^N values do not vary with light in the MONOD model (Fig. 3c,f). As such,
399 under low light, the PAHLOW model predicts higher Q^N values than the MONOD

400 model. The PAHLOW model also predicts that Q^N values increase with temperature
401 when light is limiting, while the MONOD model predicts that Q^N is independent of
402 temperature.

403 3.2. Comparisons with laboratory data

404 Analysis of laboratory data for phytoplankton Q^N reveals a significant decreasing
405 trend of Q^N with increasing light when nutrients are replete (fixed effect $t = -3.69$, $p <$
406 0.001), although this trend varies among taxa (Fig. 4a). For θ , the second-order term
407 of the linear mixed-effect model is significantly negative ($t = -4.26$, $p < 0.001$),
408 suggesting that the decreasing trend of θ with decreasing light under dim light is real
409 (Fig. 4b). Thus, in general, the PAHLOW model shows better qualitative fits to the
410 patterns of Q^N and θ in laboratory experiments, although the PAHLOW model
411 underestimates θ under dim light.

412 3.3. 1D model

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

423 Compared to station S1, the seasonal variation of mixing at station ALOHA is
424 less drastic, although the winter mixing is still stronger than during summer (Fig. 2c).

425 The surface mixed layer exhibits weak mixing throughout the whole year. The mixing
426 difference between S1 and ALOHA is also reflected in the vertical profiles of
427 temperature, in which the seasonal variations of surface temperature are less
428 pronounced at ALOHA than at S1 (Fig. 2e). The surface PAR, in general, is slightly
429 stronger at ALOHA than at S1 (Fig. 2g).

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

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

440 Examination of the seasonal vertical profiles at station S1 suggests that the
441 modeled nutriclines are shallower than observed during summer and fall for both
442 models (Fig. 6c,d). The two models also well reproduce the subsurface chlorophyll
443 maximum (SCM) layer. Compared to the PAHLOW model, the MONOD model
444 predicts higher Chl *a* concentrations below the SCM because of its higher predicted θ
445 value under low light (Fig. 6f-h). The pattern of higher Chl *a* below SCM in the
446 MONOD model than the PAHLOW model is also evident at station ALOHA (Fig. 7e-
447 h). Both models generate an unrealistic subsurface peak of NPP during summer at S1
448 (Fig. 6k), while both models, particularly the PAHLOW model, underestimate NPP in
449 surface waters at ALOHA (Fig. 7i-l).

450 Quantitative comparisons based on *SSqE* yield mixed results for different
451 variables (Table 2). The PAHLOW model simulates DIN better than the MONOD
452 model at both stations, while the converse is true for Chl and NPP, particularly at
453 ALOHA where the problem is mainly due to the PAHLOW model's underestimation
454 of Chl near the surface.

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

468 It is informative to directly compare μ , θ , and Q^N from the 1D model outputs
469 between the two models. Within the surface mixed layer of S1, the MONOD model
470 gives slower growth rate during the winter when mixing is more intense and light is
471 more limiting than other seasons (Fig. 8a). At station ALOHA, the PAHLOW model
472 predicts lower growth rate due to the lower DIN concentration (Fig. 8b). The
473 PAHLOW model predicts higher values of θ and Q^N than the MONOD model during
474 winter (Fig. 8c-f). Compared to the satellite-derived estimates of θ , both models

475 predict higher values in winter and lower values in summer at S1, but underestimate it
476 at ALOHA. Both models give lower Q^N values compared to the observed particulate
477 N:C ratios, particularly during summer.

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

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

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

493 **4. Discussion**

494 Optimality-based models, which account for organisms’ ability to acclimate to
495 external environmental conditions, have been deemed a novel approach to faithfully
496 represent biological mechanisms without compromising computational efficiency,
497 with the potential to be widely applied in 3D GCMs (Follows and Dutkiewicz, 2011;
498 Smith et al., 2011, 2014; Ward, 2017). Here we have compared the optimality-based
499 PAHLOW model and a computationally more efficient and more widely-used

500 MONOD model, by examining the functional relationships between three key
501 phytoplankton quantities (μ , Q^N , and θ) and environmental factors and testing whether
502 both of them can well simulate the observed patterns in two subtropical stations.
503 These comparisons not only provide deep understandings of the model performances,
504 but also suggest new directions for future ocean observations.

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

514 Compared to the MONOD model, the faster growth rates of the PAHLOW model
515 under low light allow phytoplankton to consume more nutrients at the SCM, yielding
516 lower levels of surface nitrate and Chl. This effect may be overly strong, contributing
517 to the PAHLOW model's underestimates of surface DIN and Chl at station ALOHA
518 (Fig. 5). It is noteworthy that the ubiquitous and ecologically important
519 *Prochlorococcus* might have lost the capacity of photo-acclimation (Partensky et al.,
520 1999), and if so the PAHLOW model may be unsuitable for modeling
521 *Prochlorococcus*.

522 However, the PAHLOW model predicts qualitatively different patterns of Q^N and
523 θ compared to our modified MONOD model, which also gives dynamic estimates of
524 these quantities. These differences cannot be eliminated simply by parameter tuning.

525 If it can be proven that the patterns generated by the PAHLOW model are in fact
526 more realistic than those from the MONOD model, this would favor use of the
527 PAHLOW model in GCMs, rather than tinkering with existing MONOD type models.
528 Based on compilations of laboratory data for phytoplankton Q^N and θ under light-
529 limiting conditions (Fig. 4), the PAHLOW model does perform better in terms of the
530 increasing trend of Q^N with light limitation and the unimodal relationship between θ
531 and light. These unique patterns may support the validity of its underlying biological
532 assumption that phytoplankton cells optimize their internal resource allocation to
533 achieve maximal fitness, constrained by the assumed tradeoff between photosynthesis
534 and nutrient uptake. These assumptions were also similarly supported by Armstrong
535 (2006). Interestingly, Goldman (1986) argued that light should not directly affect Q^N ,
536 which justifies that the extent of nutrient limitation can be quantified based on Q^N
537 alone without considering light. Our compiled data suggests that light can indeed
538 affect Q^N , contradicting Goldman's argument and suggesting that in order to evaluate
539 the status of phytoplankton nutrient limitation, light should be taken into account. In
540 other words, similar N:C ratios observed in phytoplankton cells under different light
541 environments do not suggest that these cells are experiencing similar extents of
542 nutrient limitation. At high latitudes where light may be more limiting than at low
543 latitudes, phytoplankton cells need more nitrogen to synthesize light harvesting
544 proteins and pigments (Klausmeier et al., 2004; Armstrong, 2006; Pahlow et al.,
545 2013). This also implies that light should be considered when searching for patterns
546 of nutrient-related traits for phytoplankton (Litchman et al., 2007; Edwards et al.,
547 2012).

548 However, the PAHLOW model is not perfect, either. It strongly underestimates θ
549 under very low light. As is apparent from Fig. 4b, although phytoplankton θ can have

550 a decreasing trend with decreasing light for PAR less than around 1 W m^{-2} , there are
551 no observed θ values lower than $0.24 \text{ gChl molC}^{-1}$ ($= 50 \text{ gC gChl}^{-1}$), as the PAHLOW
552 model predicts.

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

568 It is intriguing that the observed ratios of particulate organic nitrogen (PON) to
569 POC at stations ALOHA and S1 are less than those predicted by the PAHLOW model
570 and closer to the Redfield ratio (Fig. 10). If we trust the Q^N predicted by the
571 PAHLOW model, a reasonable explanation for the discrepancy between
572 phytoplankton Q^N and PON:POC ratios in surface waters might be that
573 microzooplankton have higher N:C ratios than phytoplankton (Talmy et al., 2016). In
574 deeper waters, however, the modeled phytoplankton N:C ratios even exceed the

575 measured PON:POC ratios, which can only be reconciled if the N:C ratios of other
576 pools such as bacteria, zooplankton or detritus, are much lower than the Redfield ratio
577 to offset the high phytoplankton N:C ratio. This hypothesis remains to be validated.

578 **5. Conclusions**

579 The original intent of this study was to use the classic Monod-type model to
580 approximate the optimality-based model of Pahlow et al. (2013) to further simplify
581 and speed up computation. Both models assume instantaneous acclimation and
582 therefore allow direct calculations of phytoplankton growth rate, chlorophyll-to-
583 carbon, and nitrogen-to-carbon ratios from ambient environmental nitrogen, light, and
584 temperature, which circumvents the need to assign multiple tracers for the same
585 phytoplankton population. While both models can reproduce the field observations to
586 some extent, we find that, even though we tuned the parameters of the MONOD
587 model to the outputs of the PAHLOW model, three features remain unique to the
588 PAHLOW model. The first is that phytoplankton can achieve higher growth rates in
589 the PAHLOW model than in the MONOD model when they are under light
590 limitation. The second is that phytoplankton N:C ratios depend on light availability
591 with the PAHLOW model, via its assumed tradeoff between photosynthesis and
592 nutrient uptake. This dependence was stressed previously by Armstrong (2006) based
593 on a single study (Laws and Bannister, 1980), and we have found further evidence for
594 it, based on a larger dataset including data for nine taxa. The third is that with the
595 PAHLOW model phytoplankton chlorophyll-to-carbon ratios decrease with
596 decreasing light under dim light. This is also partially corroborated by laboratory data,
597 although uncertainties remain, and field data are sparse. The commonly used
598 MONOD model cannot easily reproduce all three of these observed patterns. We
599 therefore conclude that some essential postulates of the optimality-based PAHLOW

600 model, such as the tradeoff between photosynthesis and nutrient uptake may be useful
601 and even indispensable features that need to be considered in ocean biogeochemical
602 models. However, we also identified some weakness of the PAHLOW model, such as
603 the underestimation of θ under very low light conditions, which may account for its
604 inability to outperform the MONOD model in the 1D simulations (Table 2). Finally,
605 we urge for more direct measurements of phytoplankton biomass in terms of carbon
606 and nitrogen, specific growth rates, chlorophyll-to-carbon, and nitrogen-to-carbon
607 ratios in the ocean.

608 Authors' contributions

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

614

615 **Conflict of interest**

616 The authors declare no competing final interests.

617

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812

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

Symbol	Description	Value	Unit
Common parameters			
K_w	Light attenuation coefficient of seawater	0.04 ^a	m^{-1}
K_{chl}	Light attenuation coefficient of chlorophyll	0.025 ^a	$(\text{mg Chl } a \text{ m}^2)^{-1}$
E_p	Activation energy of phytoplankton rates	0.5 ^b	eV
E_z	Activation energy of zooplankton rates	0.6 ^b	eV
Q_{0N}	Phytoplankton minimal N:C ratio	0.04 ^c	mol: mol
θ_{min}	Minimal chlorophyll-to-carbon ratio	0.02 ^d	gChl molC^{-1}
$unass$	Fraction of unassimilated food by zooplankton	0.24 ^e	dimensionless
NGE	Net growth efficiency of zooplankton	0.3 ^e	dimensionless
g_m	Maximal per capita ingestion rate of zooplankton	1.6 ^f	d^{-1}
K_p	Grazing half-saturation constant of zooplankton	0.5 ^f	$\mu\text{M N}$
W_d	Sinking rate of detritus	1 ^c	m d^{-1}
R_{dn}	Conversion rate of detritus to inorganic nitrogen	0.1	d^{-1}
m_z	Coefficient of mortality rate of zooplankton	0.15	$(\mu\text{M N})^{-1} \text{d}^{-1}$
Parameters of the MONOD model			
α_C	Carbon-specific initial slope of photosynthesis versus light	0.11 ^c	$(\text{W m}^{-2})^{-1} \text{d}^{-1}$
θ_{max}	Maximal chlorophyll-to-carbon ratio	0.61 ^c	gChl molC^{-1}
K_N	Phytoplankton growth half-saturation constant for nitrogen	1.33 ^c	$\mu\text{M N}$
μ'_m	Phytoplankton maximal growth rate at 15 °C	2.44 ^c	d^{-1}
Parameters of the PAHLOW model			
μ'_0	Phytoplankton potential carbon acquisition rate at 15°C	5 ^g	d^{-1}

α_{chl}	chlorophyll-specific initial slope of photosynthesis versus light	0.59 ^g	(W m ⁻²) ⁻¹ (gChl molC) ⁻¹ d ⁻¹
V_0^N	Phytoplankton potential nitrogen acquisition rate at 15°C	5 ^g	d ⁻¹
A_{0N}	Phytoplankton maximal potential nitrogen affinity at 15 °C	0.23 ^g	m ³ mmol C ⁻¹ d ⁻¹
R_M^{chl}	Cost of chlorophyll maintenance	0.1 ^g	d ⁻¹
ζ^{chl}	Cost of chlorophyll synthesis	0.6 ^g	(mol C) (g Chl) ⁻¹
ζ^N	Cost of nitrogen assimilation	0.8 ^g	(mol C) (mol N) ⁻¹

815 ^aFennel et al. (2006); ^bChen and Laws (2017); ^cFitting to the PAHLOW model;

816 ^dFlynn (2003); ^eBuitenhuis et al. (2010); ^fChai et al. (2002); ^gPahlow et al. (2013).

817

818

819 Table 2. Sum of squared errors between model outputs and observational data for
 820 sensitive analysis. The standard run uses all the parameter values in Table 1 with a
 821 Holling type III functional response for zooplankton. The numbers within the brackets
 822 indicate the number of observations. All other parameters are kept constant.

823

	ALOHA			S1		
Standard run	DIN (3910)	Chl (8180)	NPP (1659)	DIN (902)	Chl (426)	NPP (128)
MONOD	73.2	218	43.9	27.4	14.6	12.2
PAHLOW	58.2	690	57.1	21.7	13.8	14.5
Holling type I						
MONOD	104.3	4928	260.1	35.9	35.2	5.7
PAHLOW	89.6	2659	112.9	32.6	28.3	6.8
Holling type II						
MONOD	113.9	6377	368	40.7	53.7	7.7
PAHLOW	106.2	4499	226	39.7	48.0	6.5
$\alpha_{chl} = 0.3$ ($\alpha_C = 0.06$)						
MONOD	81.9	173	74.5	32.2	16	7.1
PAHLOW	65.5	915	75.2	26.8	17.6	9.2
$\alpha_{chl} = 1.2$ ($\alpha_C = 0.2$)						
MONOD	65.6	326	31.2	22.7	13.6	17.8
PAHLOW	49.6	1075	75.1	16.9	11.7	22.6
$A_{0N} = 0.1$ ($K_N = 2.6$)						
MONOD	82.7	293	65.6	30.7	12.5	10.1
PAHLOW	61.6	686	57.9	25.1	12.5	13.6
$A_{0N} = 0.5$ ($K_N = 0.6$)						
MONOD	65.0	227	33.6	24.4	15.8	13.1
PAHLOW	59.6	709	59.4	19.8	14.1	14.3

824

825 Figure legends

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

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

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

846 Fig. 4. (a) Phytoplankton nitrogen-to-carbon (N:C) ratios and (b) chlorophyll-to-
847 carbon (Chl:C) ratios versus log-transformed PAR levels. The thick solid
848 black lines denote the fixed effects and the thin solid lines with colors denote
849 the fits of each taxon. The red dashed lines indicate the predictions of the

850 PAHLOW model. The dashed horizontal blue lines indicate standard Redfield
851 N:C ratio (0.15) in (a) and Chl:C ratio ($0.24 \text{ gChl molC}^{-1} = 50 \text{ gC gChl}^{-1}$) in
852 (b). The histograms on the right side indicate the frequency distributions of
853 N:C and Chl:C ratios.

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

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

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

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

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

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

871