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Dynamic Coupling of Photoacclimation and Photoinhibition in a Model of Microalgae Growth

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Abstract

The development of mathematical models that can predict photosynthetic productivity of microalgae under transient conditions is crucial for enhancing large-scale industrial culturing systems. Particularly important in outdoor culture systems, where the light irradiance varies greatly, are the processes of photoinhibition and photoacclimation, which can affect photoproduction significantly. The former is caused by an excess of light and occurs on a fast time scale of minutes, whereas the latter results from the adjustment of the light harvesting capacity to the incoming irradiance and takes place on a slow time scale of days. In this paper, we develop a dynamic model of microalgae growth that simultaneously accounts for the processes of photoinhibition and photoacclimation, thereby spanning multiple time scales. The properties of the model are analyzed in connection to PI-response curves, under a quasi steady-state assumption for the slow processes and by neglecting the fast dynamics. For validation purposes, the model is calibrated and compared against multiple experimental data sets from the literature for several species. The results show that the model can describe the difference in photosynthetic unit acclimation strategies between *D. tertiolecta* (n-strategy) and *S. costatum* (s-strategy).

Keywords: microalgae, photosynthesis modeling, Droop model, Han model, acclimation strategy, PI curves

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13 1. Introduction

14 Microalgae are often considered a promising alternative for production of renewable en-
15 ergy [35]. Claimed advantages of this approach are a higher photosynthetic yield compared
16 to field crops, a reduction in fresh water consumption, and independence to agriculturally us-
17 able land [36]. These advantages could lead to large-scale production of algal biomass that is
18 not in direct competition with food production. Moreover, microalgae culture systems can be
19 coupled with wastewater treatment technologies [29], can produce high added-value products
20 such as cosmetics, pharmaceuticals and nutraceuticals [6], and can even contribute to CO₂
21 mitigation due to their inherent ability to fix carbon during photosynthesis [32]. Nonethe-
22 less, numerous problems need to be overcome on the path to a sustainable large-scale biofuel
23 production. Optimizing the entire production chain in order to reduce the production costs
24 as well as the environmental impact presents many challenges, and among them improv-
25 ing the algal biomass production efficiency has top priority. As well as developing a better
26 understanding of the key mechanisms underlying photosynthesis, the development of more
27 accurate mathematical models combining mass-conservation principle and phenomenological
28 knowledge holds much promise in this context [5].

29 Two key processes are involved in the way light conditions affect the photosynthetic yield.
30 *Photoinhibition* causes a loss of photosynthetic yield due to an excess of photons, which
31 damage some of the key proteins in the photosynthetic apparatus. *Photoacclimation*, the
32 process by which microalgae adjust their pigment content and composition to light intensity,
33 alters the rate of photosynthetic production. These two processes act on different time
34 scales: photoinhibition occurs on a time scale of minutes, whereas photoacclimation acts on
35 a time scale of days. In order to achieve optimal microalgae productivity, understanding the
36 processes of nutrient assimilation, photoinhibition and photoacclimation, together with their
37 interactions, is thus paramount. A number of mathematical models are available that account
38 for photoacclimation and nitrogen limitation at the slow time scale [15, 2, 16], yet they neglect
39 the dynamics of photoinhibition. Conversely, models describing photoinhibition in the fast
40 time scale have also been proposed [10, 17], but they do not account for photoacclimation.

41 The model by Camacho and coworkers [14], inspired from [37, 38], describes both photoin-
42 hibition and photoacclimation in nitrogen replete conditions. In contrast, the main objective
43 of this paper to develop a dynamic model of microalgae growth that couples photoinhibi-
44 tion and photoacclimation under nitrogen limitation. With regards to carbon and nitrogen
45 uptake, our model builds upon two well established models, which have been validated exper-
46 imentally and whose mathematical properties are well established. Nutrient assimilation is
47 described by the well-accepted and validated Droop model [8]. Photoinhibition is described
48 by the model proposed by Han [17], originating in the work of Eilers and Peeters [10] who
49 first introduced the concept of photosynthetic factories—also known as photosynthetic units.
50 A related, yet simpler, coupling between a photoinhibition model and the Droop model has
51 been studied by Hartmann et al. [19]. An extension of this coupling incorporating photoac-
52 climation processes constitutes the main novelty of the developed model. Specifically, we
53 propose a modification of the photosynthesis rate and pigment synthesis rate expressions to
54 account for photoacclimation effects, and we express both the effective cross-section and the
55 number of photosynthetic units—which are parameters in the Han model—as functions of
56 the chlorophyll content by means of empirical relations [12]. This approach leads to a simple
57 expression for the photosynthesis rate, which is readily amenable to mathematical analysis
58 under a quasi-steady-state approximation. This structure also makes the model easier to
59 calibrate, and we illustrate its prediction capabilities for three different species based on
60 literature data.

61 The remainder of this paper is organized as follows. Existing models of slow and fast
62 processes, including nutrient limited growth, photoacclimation and photoinhibition, are first
63 reviewed in Sect. 2. The dynamic model coupling these processes is described in Sect. 3, and
64 the properties of the resulting PI-response model are analyzed. A calibration of the coupled
65 model against several experimental data sets from the literature is presented in Sect. 4,
66 followed by a discussion in Sect. 5. Finally, Sect. 6 concludes the paper and draws future
67 research directions.

68 2. Modeling of Slow and Fast Processes in Microalgae

69 2.1. Nutrient-Limited Growth – The Droop Model

70 Droop [7] first observed that microalgae keep growing for some time after nutrients have
71 been depleted. Monod kinetics are unable to model this behavior and therefore are not suit-
72 able for predicting microalgae growth under nutrient limitation. A better way to represent
73 nutrient-limited growth is by separating the nutrient uptake rate, denoted by ρ hereafter,
74 from the growth rate, denoted by μ . This idea was followed by Droop [7, 8] in relating
75 the growth rate to the internal elemental nutrient quota. Since its introduction, the Droop
76 model has been widely studied [22, 3, 34] and thoroughly validated [8, 28, 4, 34]. A key
77 feature of our model in Sect. 3 is to build upon this model in order to inherit its structural
78 properties.

79 In a continuous and homogeneous microalgae culture, the mass-balance equations for
80 the nutrient (inorganic nitrogen) concentration s [$\text{g}_\text{N} \text{m}^{-3}$] in the bulk phase, the biomass
81 concentration x [$\text{g}_\text{C} \text{m}^{-3}$], and the carbon-specific nitrogen quota q [$\text{g}_\text{N} \text{g}_\text{C}^{-1}$] of the cells are
82 given by

$$\begin{aligned} \dot{s} &= D s_{\text{in}} - \rho(s, q) x - D s \\ \dot{x} &= \mu(q, \cdot) x - D x - R x \\ \dot{q} &= \rho(s, q) - \mu(q, \cdot) q, \end{aligned} \tag{1}$$

84 with D [s^{-1}] and R [s^{-1}] denoting the dilution rate and the endogenous respiration rate,
85 respectively; and s_{in} [$\text{g}_\text{N} \text{m}^{-3}$], the nutrient concentration in the feed.

86 Recently, an extension of the Droop model has been proposed by Bernard [2] accounting
87 for the effect of light conditions on the growth rate μ in the form

$$\mu(q, \cdot) = \bar{\mu} \left(1 - \frac{Q_0}{q} \right) \phi(\cdot), \tag{2}$$

89 where $\bar{\mu}$ [s^{-1}] stands for the maximal growth rate, i.e., the growth rate reached under non-
90 limiting conditions; Q_0 [$\text{g}_\text{N} \text{g}_\text{C}^{-1}$], the minimal cell quota, so that $\mu(Q_0, \cdot) = 0$ and $q \geq Q_0$;
91 and, $\phi(\cdot)$ is a saturation function. In particular, an expression of $\phi(\cdot)$ will be developed in
92 Sect. 3 that accounts for the state of the photosynthetic units (PSUs).

93 The nutrient uptake rate ρ , on the other hand, can be expressed as [16]

$$94 \quad \rho(s, q) = \bar{\rho} \frac{s}{s + k_s} \left(1 - \frac{q}{Q_l} \right), \quad (3)$$

95 where $\bar{\rho}$ [$\text{g}_\text{N} \text{g}_\text{C}^{-1} \text{s}^{-1}$] stands for the maximal nutrient uptake rate; k_s [$\text{g}_\text{N} \text{m}^{-3}$], the half-
 96 saturation constant for substrate uptake; and Q_l [$\text{g}_\text{N} \text{g}_\text{C}^{-1}$], the limit quota for the nitrogen
 97 uptake, so that $\rho(s, Q_l) = 0$ and $q \leq Q_l$, with equality corresponding to nutrient-replete
 98 conditions.

99 2.2. Pigment Content

100 Photoacclimation is the mechanism by which both the chlorophyll content and the pig-
 101 ment composition change in response to variations in the light irradiance. Such changes take
 102 place on a time scale of days, and it has been suggested that microalgae use photoacclimation
 103 as a means to optimize their growth at low irradiance as well as to minimize damage at high
 104 irradiance [12].

105 One way to describe photoacclimation is by accounting for the change in the chlorophyll
 106 content over time. Following Bernard [2], the chlorophyll concentration, c [$\text{g}_{\text{chl}} \text{m}^{-3}$], is
 107 assumed to be proportional to cellular protein concentration as a first approximation, which
 108 is itself represented by the particulate nitrogen concentration $x q$:

$$109 \quad c = \psi(I_g) x q, \quad (4)$$

110 where I_g [$\mu\text{E} \text{m}^{-2} \text{s}^{-1}$] represents the light irradiance at which the cells are acclimated,
 111 also called *growth irradiance*. Introducing the carbon-specific chlorophyll quota $\theta := c/x$
 112 [$\text{g}_{\text{chl}} \text{g}_\text{C}^{-1}$], the foregoing relation can be rewritten in the form

$$113 \quad \theta = \psi(I_g) q. \quad (5)$$

114 Here, we choose to express $\psi(\cdot)$ in the form of the hyperbolic function

$$115 \quad \psi(I_g) = \bar{\psi} \frac{k_I}{I_g + k_I}, \quad (6)$$

116 with parameters $\bar{\psi}$ [$\text{g}_{\text{chl}} \text{g}_\text{N}^{-1}$] and k_I [$\mu\text{E} \text{m}^{-2} \text{s}^{-1}$]. Moreover, the dynamic evolution of I_g is

117 related to the current light irradiance I by the following equation

$$118 \quad \dot{I}_g = \delta \mu(q, \cdot) (I - I_g), \quad (7)$$

119 thereby assuming that the acclimation rate is proportional to the irradiance difference ($I - I_g$)
 120 as well as to the current growth rate $\mu(\cdot)$, with the constant proportionality coefficient $\delta [-]$.

121 On the whole, a change in the current irradiance I affects I_g via (7), modifying the chlorophyll
 122 quota θ via (5) in turn.

123 *2.3. Photosynthetic Production and Photoinhibition – The Han Model*

124 The Han model [17], which is inspired by the model of Eilers and Peeters [9], describes
 125 the effect of light irradiance on microalgae growth. This model considers the damage of key
 126 proteins in PSUs to be the main contribution to photoinhibition. Particularly appealing
 127 in the Han model is the description of complex photosynthetic processes in terms of three
 128 possible states of the PSUs only, namely: open, A ; closed, B ; and, inhibited, C .

129 The equations giving the rates of change in the fractions of open, closed and inhibited
 130 PSUs are in order:

$$131 \quad \begin{aligned} \dot{A} &= -I \sigma A + \frac{B}{\tau} \\ \dot{B} &= I \sigma A - \frac{B}{\tau} + k_r C - k_d \sigma I B \\ \dot{C} &= -k_r C + k_d \sigma I B, \end{aligned} \quad (8)$$

132 with initial conditions such that $A(0) + B(0) + C(0) = 1$. A number of remarks are:

- 133 • Photosynthetic production is described by the transition between open state and closed
 134 state. Excitation is assumed to occur at a rate of σI , with $\sigma [\text{m}^2 \mu\text{E}^{-1}]$ the effective
 135 cross-section of the PSUs, whereas deexcitation is assumed to occur at a rate of $\frac{1}{\tau}$,
 136 with $\tau [\text{s}]$ the turnover time of the electron transport chain.
- 137 • Photoinhibition occurring at high light irradiance corresponds to the transition from
 138 closed state to inhibited state. This process is assumed to occur at a rate of $k_d \sigma I$,
 139 with $k_d [-]$ a damage constant. The reverse transition from inhibited state to closed

140 state accounts for the repair of damaged PSUs by enzymatic processes in the cell, a
141 mechanism that is assumed to occur at a constant rate k_r [s^{-1}].

142 The Han model provides the second brick in our model in Sect. 3, also with the objective
143 of keeping its structural properties. In particular, an interesting property of the Han model
144 is that the fractions of open, closed and inhibited states can be computed analytically from
145 (8) as a function of the irradiance I at steady state. For instance, the steady-state expression
146 A^∞ for the open state A is given by:

$$147 \quad A^\infty(I) = \frac{1}{1 + \tau \sigma I + K \tau \sigma^2 I^2}, \quad (9)$$

148 with $K := k_d/k_r$.

149 **3. Multi-Scale Model of Microalgae Growth Coupled with Photoinhibition and** 150 **Photoacclimation**

151 The proposed model couples three dynamic processes, namely (i) the PSU dynamics,
152 (ii) the dynamics of intracellular nitrogen content, and (iii) the dynamics of chlorophyll
153 content. These processes span four different timescales ranging from milliseconds for the
154 open-closed dynamics of the PSUs up to several days for the dynamics of intracellular nitro-
155 gen quota q .

156 *3.1. Coupling Between Growth, Photoinhibition and Photoacclimation*

157 Our model builds upon the Droop-Han model of Hartmann et al. [19] and incorpo-
158 rates photoacclimation processes via the dynamics of the chlorophyll quota θ introduced in
159 Sect. 2.2. More specifically, we account for two possible ways that the term $\phi(\cdot)$ in (2) can
160 depend on θ . The first effect is a direct linear dependency of photosynthesis efficiency on
161 the chlorophyll content, which is in agreement with the work of Faugeras et al. [13]. Since
162 the probability of a photon encountering an open state is proportional to AI , a second, in-
163 direct effect is via the dependence of the dynamics of A on θ . This latter dependency results
164 from the fact that the parameter σ introduced in the Han model (8) can itself depend on
165 the current acclimation state. Indeed, Falkowski and Raven [12] describe photoacclimation

166 as a process that can follow either one of two strategies: the *n-strategy* corresponds to a
 167 change in the density (per biomass unit) of PSUs, denoted by N subsequently; the *s-strategy*
 168 corresponds to a change in the size of the PSUs, and is thus directly related to the effective
 169 cross-section σ . In practice, chlorophyll is thus used either to build new PSUs or to increase
 170 the size of the antenna in existing PSUs. These two acclimation strategies run concurrently,
 171 and both can be described by defining $N(\cdot)$ and $\sigma(\cdot)$ as functions of the chlorophyll quota θ .
 172 Such relationships are further investigated in Sect. 3.3.

Based on the above, the growth rate μ can be modeled as:

$$\mu(q, \theta, I) = \bar{\alpha} \left(1 - \frac{Q_0}{q} \right) \theta A(I, \theta) I,$$

173 where $\bar{\alpha}$ is a constant parameter. At this point, we shall introduce the rate of carbon uptake
 174 per chlorophyll unit, $\mu_{\text{chl}} [\text{g}_C \text{g}_{\text{chl}}^{-1} \text{s}^{-1}]$, as

$$175 \mu_{\text{chl}}(q, \theta, I) = \frac{\mu(q, \cdot)}{\theta} = \bar{\alpha} \left(1 - \frac{Q_0}{q} \right) A(I, \theta) I, \quad (10)$$

176 which is also known as the chlorophyll-specific photosynthesis rate.

177 3.2. Structural Analysis of the PI Response

178 In experiments assessing photosynthetic efficiency of microalgae, the cells are photoac-
 179 climated to a given light irradiance I_g for a sufficiently long time and under nutrient replete
 180 conditions, before exposing them to various light irradiances I . The instantaneous growth
 181 rates obtained under these conditions—ideally via consideration of the carbon fixation rate,
 182 but often based on the O_2 production rate too—are measured and yield the so-called PI-
 183 response curve when plotted against I .

184 A common assumption about PI-response curve experiments is that they are fast enough
 185 for photoacclimation, substrate internalization and growth to be negligible; that is, time
 186 variations in the variables θ , q and x can all be neglected. In contrast, variations in the
 187 fractions of open, closed and inhibited states in the Han model can be considered fast in the
 188 time scale of PI-response curve experiments, and one can thus assume that the variables A ,
 189 B and C reach their steady states as in (9), without significantly impairing the PI response

190 predictions (quasi-steady-state approximation). Under nutrient-replete conditions, these ap-
 191 proximations lead to the following simplification of the chlorophyll-specific photosynthesis
 192 rate (10):

$$193 \quad \mu_{\text{chl}}^{\text{PI}}(\theta, I) = \bar{\alpha} \left(1 - \frac{Q_0}{Q_{\text{max}}(\cdot)} \right) \frac{I}{1 + \tau \sigma(\theta) I + K \tau \sigma^2(\theta) I^2}, \quad (11)$$

194 where $Q_{\text{max}}(\cdot)$ [$\text{g}_\text{N} \text{g}_\text{C}^{-1}$] denotes the maximal value of the nitrogen internal quota q under
 195 nutrient replete conditions, a value that typically depends on the growth irradiance I_g [2].
 196 A further reformulation gives

$$197 \quad \mu_{\text{chl}}^{\text{PI}}(\theta, I) = \alpha(\cdot) \frac{I}{1 + \tau \sigma(\theta) I + K \tau \sigma^2(\theta) I^2}, \quad (12)$$

198 with $\alpha(\cdot) := \bar{\alpha} \left(1 - \frac{Q_0}{Q_{\text{max}}(\cdot)} \right)$ [$\text{g}_\text{C} \text{g}_\text{chl}^{-1} \mu\text{E}^{-1} \text{m}^2$] denoting the initial slope of the PI response
 199 curve, i.e., the rate of change of μ_{chl} with respect to the light irradiance I for a vanishing
 200 irradiance.

201 Many authors concur to say that, for many microalgae species, the initial slope $\alpha(\cdot)$
 202 can be considered to be independent of the value of θ [23]. Nonetheless, we like to note
 203 that the constant initial slope assumption is still debated; see, for instance, the paper
 204 by Richardson et al. [27], where microalgae acclimation strategies are divided into six
 205 different categories based on photosynthesis-irradiance response data. We shall come
 206 back to this important point later on in Sect. 5, where it is argued that certain variations
 207 in initial slopes may as well be explained by transient effects in the fraction of inhibited PSUs.
 208

209 In the remainder of this subsection, we investigate structural properties of the PI-response
 210 curve under the foregoing assumptions of time-scale separation and constant initial slope.
 211 The optimal irradiance value I^* maximizing $\mu_{\text{chl}}^{\text{PI}}$ can be determined from (12) as

$$212 \quad I^*(\theta) := \frac{1}{\sigma(\theta) \sqrt{K\tau}}. \quad (13)$$

213 In turn, the maximal productivity rate $\mu_{\text{chl}}^{\text{PI}^*}$ can be expressed in the form

$$214 \quad \mu_{\text{chl}}^{\text{PI}^*}(\theta) := \alpha \frac{\sqrt{K\tau}}{\tau + 2\sqrt{K\tau}} I^*(\theta). \quad (14)$$

215 The following property follows readily from (14), provided that the Han model parameters
216 τ and K are independent of the acclimation state:

217 **Property 1.** *The maximal growth rate $\mu_{\text{chl}}^{\text{PI}^*}$ is proportional to the optimal irradiance I^*
218 regardless of the pre-acclimated state or the growth irradiance.*

219 Although a direct consequence of the constant initial slope assumption, this property does
220 not depend on a particular choice of the relationship between $\sigma(\cdot)$ and θ . Moreover, it is
221 readily tested using data from experimental PI curves corresponding to different acclimation
222 states—see Sect. 4.1.

223 3.3. Quantitative Analysis of the PI Response

224 In order to make quantitative predictions of the PI-response curve or, more generally, for
225 numerical simulation of the coupled model, relationships for the effective cross-section $\sigma(\cdot)$
226 and the density of PSUs $N(\cdot)$ in terms of the chlorophyll quota θ must be specified.

227 We start by noting that $\sigma(\theta)$ and $N(\theta)$ can both be related to the average size of a PSU
228 in terms of chlorophyll content per PSU, denoted by $\Gamma(\theta)$ subsequently. A simple relation
229 for $N(\theta)$ is:

$$230 \quad \Gamma(\theta) N(\theta) = \theta. \quad (15)$$

On the other hand, the relation between $\sigma(\theta)$ and $\Gamma(\theta)$ or $N(\theta)$ is highly complex. As well
as the geometric shape of the photosynthetic antennas, this relation must take into account
the packaging effect and the synthesis of other accessory pigments. Here, we choose to use
a simple relationship, whereby $\sigma(\cdot)$ is expressed as a power law of Γ :

$$\sigma(\theta) = \sigma_0 \Gamma(\theta)^\gamma,$$

231 with parameters σ_0 and γ .

232 Now, assuming a general power law relationship between σ and θ as:

$$233 \quad \sigma(\theta) = \beta \theta^\kappa, \quad (16)$$

234 and using (15), the density of PSUs is expressed as:

$$235 \quad N(\theta) = \left(\frac{\sigma_0}{\beta} \right)^{1/\gamma} \theta^{1-\kappa/\gamma}, \quad (17)$$

236 and similarly the average size of a PSU is given by:

$$237 \quad \Gamma(\theta) = \left(\frac{\beta}{\sigma_0} \right)^{1/\gamma} \theta^{\kappa/\gamma}. \quad (18)$$

238 Besides simplicity, expressions of $\sigma(\theta)$, $N(\theta)$ and $\Gamma(\theta)$ in the form of power laws are also
239 plausible from a biophysical standpoint. It is indeed expected that $\sigma(\theta)$ should be a mono-
240 tonically increasing function of θ , due to a higher probability of photons absorption. In
241 contrast, the expressions of $N(\theta)$ and $\Gamma(\theta)$ remain flexible enough with respect to θ , and
242 so the resulting acclimation model is capable of discrimination between the s-strategy and
243 n-strategy of PSU acclimation.

244 We note that Camacho and coworkers [14] have used a similar modeling approach and
245 proposed a monotonically increasing relation between the chlorophyll content θ and the
246 density of PSUs $N(\theta)$ (which are both decreasing functions of the growth irradiance I_g).
247 Our model is more flexible in the sense that it enables strategies whereby the chlorophyll
248 content increases while the density of PSUs decreases.

249 Substituting the power law (16) in the expression of I^* in (13), and log-linearizing the
250 resulting expression gives:

$$251 \quad \log I^*(\theta) = -\kappa \log \theta - \log(\beta\sqrt{K\tau}). \quad (19)$$

252 The following property follows directly from (19):

253 **Property 2.** *The exponent κ in the power laws (16) corresponds to the (negative) slope in*
254 *a log-log plot of I^* versus θ .*

255 Like Property 1, the linearity of the relationship between $\log I^*$ and $\log \theta$ can be readily
256 tested using data from experimental PI curves corresponding to different acclimation states.

257

258 To summarize, a complete expression of the model predicting the PI responses of a given
 259 microalgae at various pre-acclimated states is:

$$260 \quad \mu_{\text{chl}}^{\text{PI}}(q, \theta, I) = \bar{\alpha} \left(1 - \frac{Q_0}{Q_{\text{max}}(\cdot)} \right) \frac{I}{1 + \tau \beta \theta^\kappa I + K \tau \beta^2 \theta^{2\kappa} I^2}. \quad (20)$$

261 This expression is of the Haldane type with respect to the light intensity I , and it comprises
 262 the following parameters: K and τ from the Han model; β and κ from the acclimation
 263 model; and the initial slope $\bar{\alpha}$ together with the minimal and maximal nitrogen quotas Q_0
 264 and Q_{max} —or alternatively α in its simplified version.

265 4. Calibration and Confidence Analysis using Data Sets from the Literature

266 A calibration of the new features in the coupled model is carried out in this section, using
 267 experimental data sets from the works of Anning et al. [1] and Falkowski and Owens [11]. The
 268 focus is on the chlorophyll-specific photosynthesis rate (20), the density and size acclimation
 269 laws (17)-(18), and the saturation function ψ in the nitrogen-quota-to-chlorophyll-quota
 270 relationship (5).

271 4.1. Data for *Skeletonema costatum*

272 Experimental data by Anning et al. [1] are for the diatom *Skeletonema costatum*. They
 273 comprise two acclimation states at different growth irradiances I_g , namely $50 \mu\text{E m}^{-2} \text{s}^{-1}$
 274 (LL) and $1500 \mu\text{E m}^{-2} \text{s}^{-1}$ (HL). The LL irradiance corresponds to a chlorophyll quota of
 275 $\theta = 0.082 \text{ g}_{\text{chl}} \text{g}_{\text{C}}^{-1}$, and the HL irradiance to $\theta = 0.018 \text{ g}_{\text{chl}} \text{g}_{\text{C}}^{-1}$. Measurements of the number
 276 and size of PSUs are also available for four acclimation states in Falkowski and Owens [11].
 277 Only the number of photosystems I (PSI) is reported and we assume the number of PSUs
 278 to be proportional here.

279 *Calibration of PI-Response Curves.* We neglect variations of the term α in (20) as a first
 280 approximation, and we consider a nonlinear regression approach based on least-square mini-
 281 mization to estimate the values of parameters β , κ and α . On the other hand, we use default
 282 values for the Han model parameters k_r , k_d and τ ; these values are obtained by averaging
 283 over the parameter ranges reported in [18] and can be found in Table I.

Table I: Default parameter values in the Han model and parameter estimates in the photosynthesis rate (20) for *S. costatum*.

Param.	Value	Source
τ	5.50×10^{-3} [s]	Ref. [18]
k_r	1.40×10^{-4} [s ⁻¹]	Ref. [18]
k_d	5.00×10^{-6} [-]	Ref. [18]
α	1.60×10^{-2} [g _C g _{chl} ⁻¹ μE ⁻¹ m ²]	estimated
β	4.92×10^{-1} [μE ⁻¹ m ² g _{chl} ^{1/κ} g _C ^{-1/κ}]	estimated
κ	4.69×10^{-1} [-]	estimated

284 In order to certify global optimality of the parameter estimates, we use the global opti-
 285 mization solver BARON [33] in the GAMS modeling environment. The resulting parameter
 286 estimates are given in Table I, and the fitted PI-response curves (20) are plotted against the
 287 available experimental data in Fig. 1. The predictions are in excellent agreement with this
 288 experimental data sets at both light irradiances, also with regards to Property 1, thereby
 289 providing a first validation of the structural assumptions in (20).

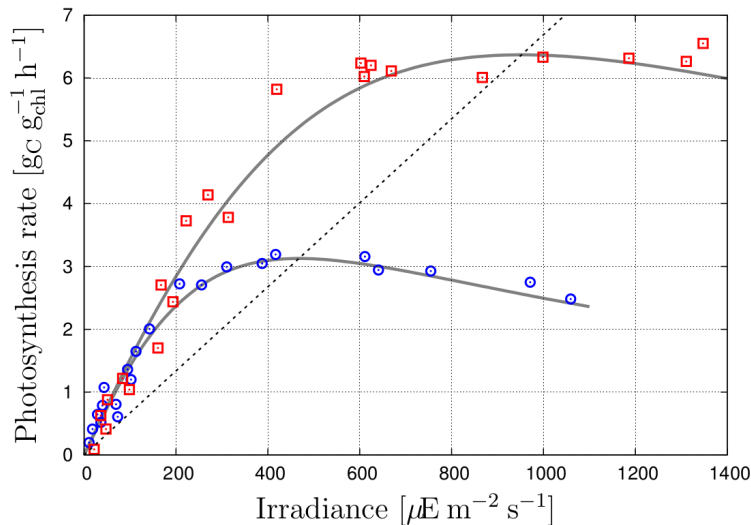


Figure 1: PI-response curves for *S. costatum* based on the data by Anning et al. [1]. The blue and red points correspond to acclimation at LL and HL, respectively. The predicted PI responses are depicted in gray solid lines. The dashed line connects the maxima of both PI curves per Property 1.

290 In order to assess the confidence of the parameter estimates in Table I, we apply set-
 291 membership parameter estimation in the bounded-error sense [21]. To conduct the analysis,
 292 we consider variations around the available photosynthesis rate measurements, here vari-

293 ations of $\pm 5\%$. A large number of scenarios is generated by sampling the resulting mea-
 294 surement ranges—using Sobol sequences and assuming no correlation between the different
 295 measurements—and globally optimal estimates for β , κ and α are then computed for every
 296 scenario. This way, we obtain the set of all possible parameter values that are consistent
 297 with the available measurements within a $\pm 5\%$ error.

298 The results obtained for the data set by Anning et al. [1] are shown in Fig. 2. Projec-
 299 tions of the confidence region onto the (β, κ) , (β, α) and (κ, α) subspaces provide parameter
 300 confidence ranges as $\beta \in [0.45, 0.54]$, $\kappa \in [0.44, 0.5]$ and $\alpha \in [0.0158, 0.0172]$. Moreover,
 301 these projections reveal the existence of a significant correlation between the parameters β
 302 and κ of the acclimation model, whereas correlations of β or κ with α are rather small. The
 303 envelopes of both PI-response curves obtained for parameter values in the confidence region
 304 are shown on the bottom-right plot of Fig. 2 as well, confirming the good agreement with
 305 the experimental data.

306 *Calibration of Density and Size Acclimation Laws.* Since experimental information is avail-
 307 able for both the density and size of PSUs at four different acclimation states, values of the
 308 acclimation parameters σ_0 and κ in the power laws (17)-(18) can be estimated for this data
 309 set too. Note that these relationships can be rewritten in the form

$$310 \quad 1/\gamma \log \left(\frac{\sigma_0}{\beta} \right) - \kappa/\gamma \log \theta = \log N - \log \theta ,$$

$$311 \quad 1/\gamma \log \left(\frac{\sigma_0}{\beta} \right) - \kappa/\gamma \log \theta = -\log \Gamma ,$$

312 thus making it possible to use a simple linear regression approach for estimating the values
 313 of $1/\gamma \log \left(\frac{\sigma_0}{\beta} \right)$ and κ/γ . Estimates for the parameters σ_0 and κ , as reported in Table II,
 314 can be obtained in turn by using the estimates for β , κ and α in Table I.

Table II: Parameter estimates in the density and size acclimation laws (17)-(18) for *S. costatum*.

Parameter	Value
σ_0	$1.63 \times 10^{-1} [\mu\text{E}^{-1} \text{m}^2 \text{g}_{\text{chl}}^{-\gamma} \text{PSU}^\gamma]$
γ	$1.18 \times 10^{-1} [-]$

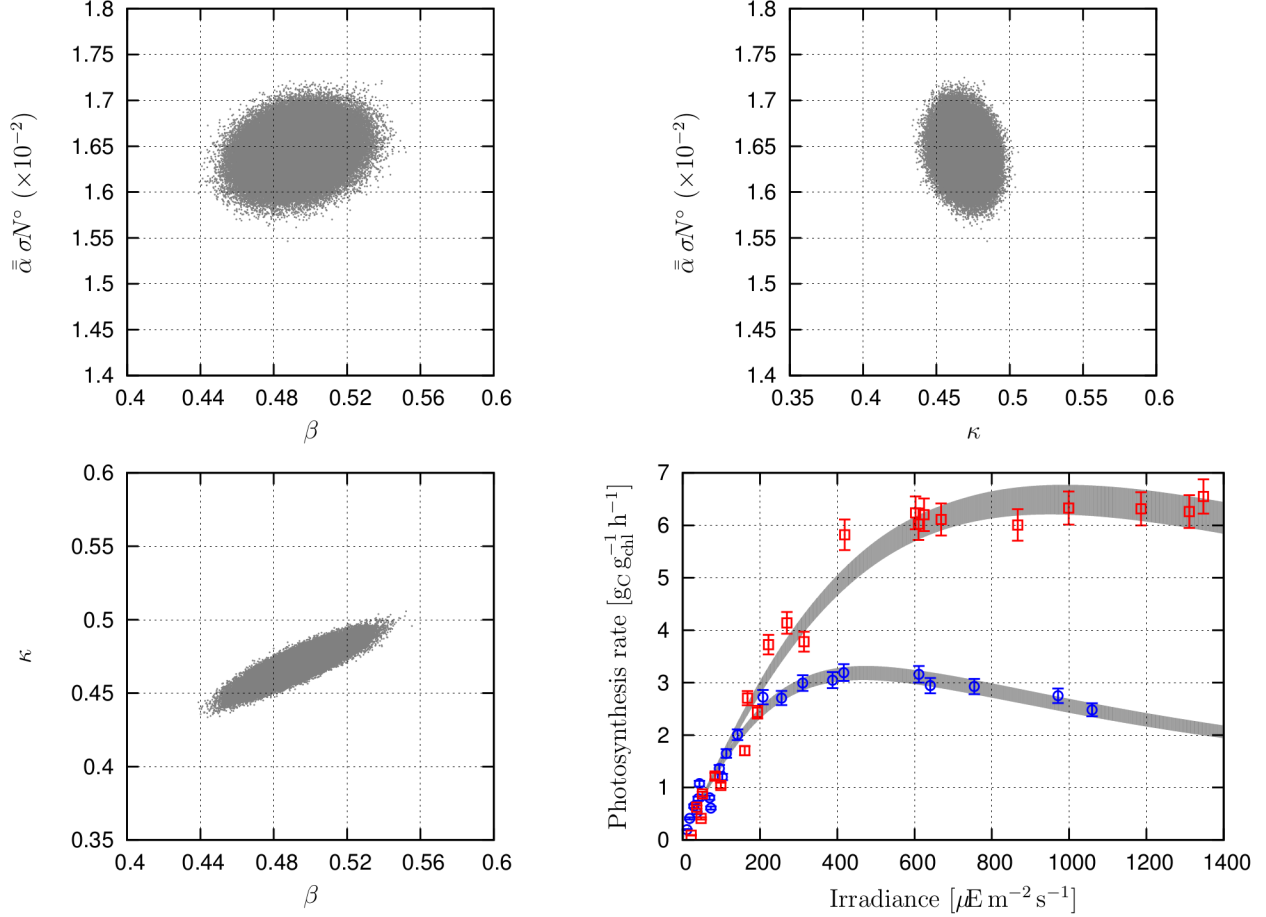


Figure 2: Confidence region of the parameter estimates β , κ and α with $\pm 5\%$ deviations and corresponding envelopes of PI curves for *S. costatum*.

315 Following a set-membership estimation approach, confidence in the foregoing parameter
 316 estimates is assessed by computing the set of all values for σ_0 and κ that are consistent
 317 with the available measurement of density and size of PSU (within variations of $\pm 5\%$), while
 318 simultaneously accounting for the uncertainty in the values of β , κ and α (Fig. 2). The
 319 resulting confidence region is shown on the left plot in Fig. 3, and the set of corresponding
 320 model fits for the experimental data on the right plot. Parameter confidence ranges are
 321 obtained as $\sigma_0 \in [0.12, 0.51]$ and $\gamma \in [0.08, 0.39]$. Despite being quite conservative, these
 322 bounds allow to confidently conclude that the parameter γ is indeed positive for *S. costatum*.
 323 This finding will be discussed further in Sect. 5.

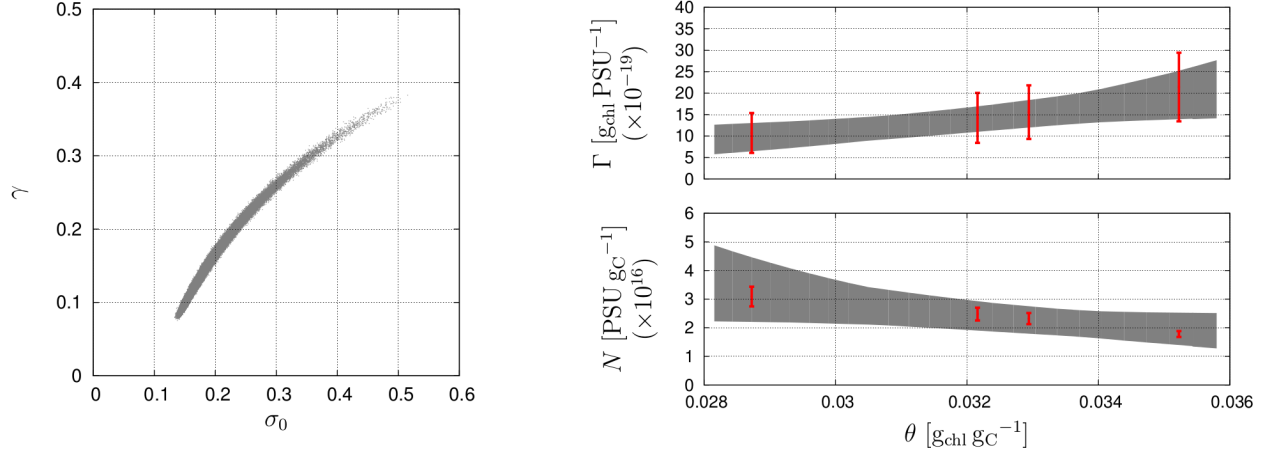


Figure 3: Confidence region of the parameter estimates γ and σ_0 for the measurement data ranges of PSU size and number (left plot) and corresponding fit envelopes (right plots) for *S. costatum*.

324 4.2. Data for *Dunaliella tertiolecta*

325 Experimental data by Falkowski and Owens [11] are for the chlorophyte *Dunaliella ter-*
 326 *tiolecta*. Amongst the available data, four PI curves are selected that were not affected by
 327 ‘bleaching’, corresponding to acclimation states at growth irradiances I_g of $60 \mu\text{E m}^{-2} \text{s}^{-1}$
 328 (L_1), $120 \mu\text{E m}^{-2} \text{s}^{-1}$ (L_2), $200 \mu\text{E m}^{-2} \text{s}^{-1}$ (L_3), and $400 \mu\text{E m}^{-2} \text{s}^{-1}$ (L_4). Measurements
 329 of carbon, nitrogen and chlorophyll content per cell for all four acclimation states make it
 330 possible to determine lower and upper ranges for both the nitrogen quota q and the chloro-
 331 phyll quota θ as well, as given in Table III. Moreover, measurements of the number and size
 332 of PSUs are also available at four acclimation states, assuming that the number of PSUs is
 333 proportional to the measured number of PSIs.

Table III: Ranges of nitrogen and chlorophyll quotas from the experimental data by Falkowski and Owens [11] at acclimation states L_1 , L_2 , L_3 and L_4 .

Growth irradiance I_g [$\mu\text{E m}^{-2} \text{s}^{-1}$]	Nitrogen quota Q_{\max} [$\text{g}_\text{N g}_\text{C}^{-1}$]	Chlorophyll quota θ [$\text{g}_\text{chl g}_\text{C}^{-1}$]
L_1 : 60	$Q_{\max} \in [0.250, 0.357]$	$\theta \in [0.0774, 0.0820]$
L_2 : 120	$Q_{\max} \in [0.222, 0.323]$	$\theta \in [0.0654, 0.0682]$
L_3 : 200	$Q_{\max} \in [0.213, 0.286]$	$\theta \in [0.0436, 0.0453]$
L_4 : 400	$Q_{\max} \in [0.172, 0.208]$	$\theta \in [0.0355, 0.0373]$

334 *Calibration of PI-Response Curves.* Since experimental information is available for the ni-
335 trogen quota q in all acclimation states, variations of the term $(1 - Q_0/Q_{\max})$ in (20) can be
336 accounted for with this data set—we consider a value of $Q_0 = 0.05 \text{ g}_N \text{ g}_C^{-1}$ for the minimal
337 nitrogen quota throughout [16, 2]. Like previously, we use a nonlinear regression approach
338 based on least-square minimization to estimate the values of parameters $\bar{\alpha}$, β and κ , and we
339 define extra variables for the nitrogen and chlorophyll quotas in the regression problem with
340 bounds as defined in Table III. As far as the Han model parameters are concerned, we use
341 the default values of τ and k_r in Table I. On the other hand, the default value for k_d is not
342 deemed suitable as photoinhibition effects are not observed on the available PI-curve data,
343 so k_d is considered an extra variable in the regression problem with bounds $[0, 10^{-7}]$ initially.
344 More data at higher light irradiance would be needed for a better calibration.

Table IV: Parameter estimates in the photosynthesis rate (20) for *D. tertiolecta*.

Param.	Value	Nitrogen quota	Chlorophyll quota
$\bar{\alpha}$	$5.50 \times 10^{-2} \text{ g}_C \text{ g}_{\text{chl}}^{-1} \mu\text{E}^{-1} \text{ m}^2$	$Q_{\max}^{60} = 0.250 \text{ g}_N \text{ g}_C^{-1}$	$\theta^{60} = 0.082 \text{ g}_{\text{chl}} \text{ g}_C^{-1}$
β	$5.48 \times 10^1 \mu\text{E}^{-1} \text{ m}^2 \text{ g}_{\text{chl}}^{1/\kappa} \text{ g}_C^{-1/\kappa}$	$Q_{\max}^{120} = 0.322 \text{ g}_N \text{ g}_C^{-1}$	$\theta^{120} = 0.065 \text{ g}_{\text{chl}} \text{ g}_C^{-1}$
κ	$1.54 \times 10^0 -$	$Q_{\max}^{200} = 0.266 \text{ g}_N \text{ g}_C^{-1}$	$\theta^{200} = 0.045 \text{ g}_{\text{chl}} \text{ g}_C^{-1}$
k_d	$1.27 \times 10^{-8} -$	$Q_{\max}^{400} = 0.208 \text{ g}_N \text{ g}_C^{-1}$	$\theta^{400} = 0.036 \text{ g}_{\text{chl}} \text{ g}_C^{-1}$

345 The solver BARON [33] in the GAMS modeling environment is again used to guarantee glob-
346 ally optimal parameter estimates. These estimates are reported in Table IV, and the fitted
347 PI-response curves (20) are plotted against the available experimental data in Fig. 4 in gray
348 solid lines. The predicted responses are generally in good agreement with the experimental
349 data, thereby confirming the ability of the model to capture the photosynthetic activity of
350 *D. tertiolecta*.

351 For sake of comparison, we also plot in gray dotted lines on Fig. 4 the fitted PI responses
352 without accounting for variations of the term $(1 - \frac{Q_0}{Q_{\max}})$ in (20); that is, the parameter α is
353 estimated in lieu of $\bar{\alpha}$. These fits, although slightly degraded, remain accurate. Moreover,
354 the corresponding parameter estimates, $\beta \approx 32.4$, $\kappa \approx 1.4$, and $\alpha \approx 0.042$, are in good
355 agreement with the values in Table IV as well as with the confidence analysis that follows.

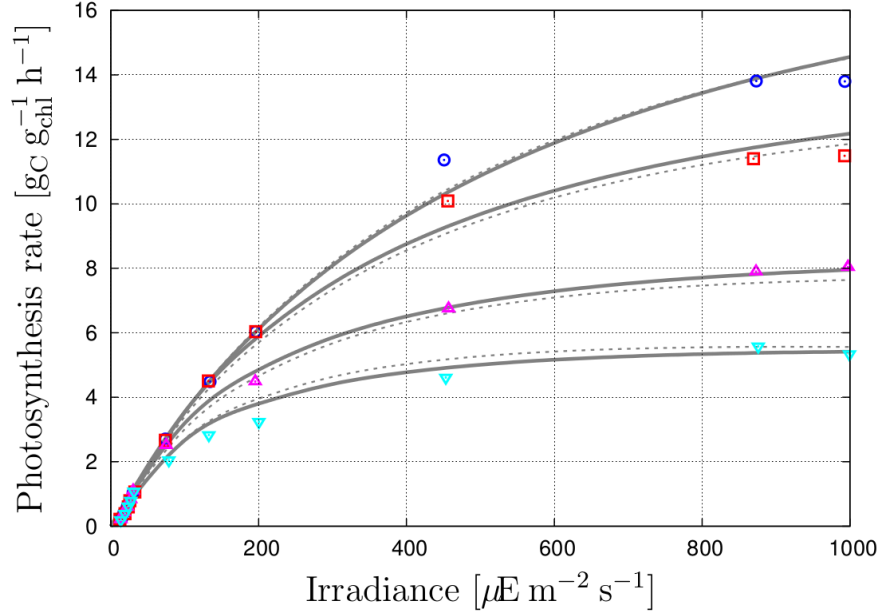


Figure 4: PI-response curves for *D. tertiolecta* based on the data by Falkowski and Owens [11]. The cyan, magenta, red, and blue points correspond to acclimation at L_1 , L_2 , L_3 and L_4 , respectively. The predicted PI responses are depicted in gray lines, with and without accounting for variations of the term $(1 - Q_0/Q_{\max})$ in solid lines and dotted lines, respectively.

356 This shows that the PI-response model (20) is robust towards uncertainty in the nitrogen
 357 maximal quota Q_{\max} .

358 As previously with *S. costatum*, we assess the confidence of the estimates obtained for
 359 the acclimation parameters $\bar{\alpha}$, β and κ in Table IV. We consider variations of $\pm 5\%$ around
 360 the available photosynthesis rate measurements and we compute the set of all possible values
 361 for $\bar{\alpha}$, β and κ that are consistent with these measurement-error ranges.

362 The results obtained for the data set by Falkowski and Owens [11] are shown in Fig. 5.
 363 Projections of the confidence region onto the (β, κ) , $(\beta, \bar{\alpha})$ and $(\kappa, \bar{\alpha})$ subspaces provide
 364 parameter confidence ranges as $\beta \in [32, 65]$, $\kappa \in [1.35, 1.6]$ and $\bar{\alpha} \in [0.052, 0.058]$. These
 365 projections also reveal the existence of a strong correlation between the parameters β and κ ,
 366 which is likely due to the absence of photoinhibition effects in this data set. In contrast, the
 367 correlations of β or κ with $\bar{\alpha}$ appear to be rather small. The envelopes of all four PI-response
 368 curves obtained for parameter values in the confidence region are shown on the bottom-right
 369 plot of Fig. 2, confirming a good agreement with the experimental data.

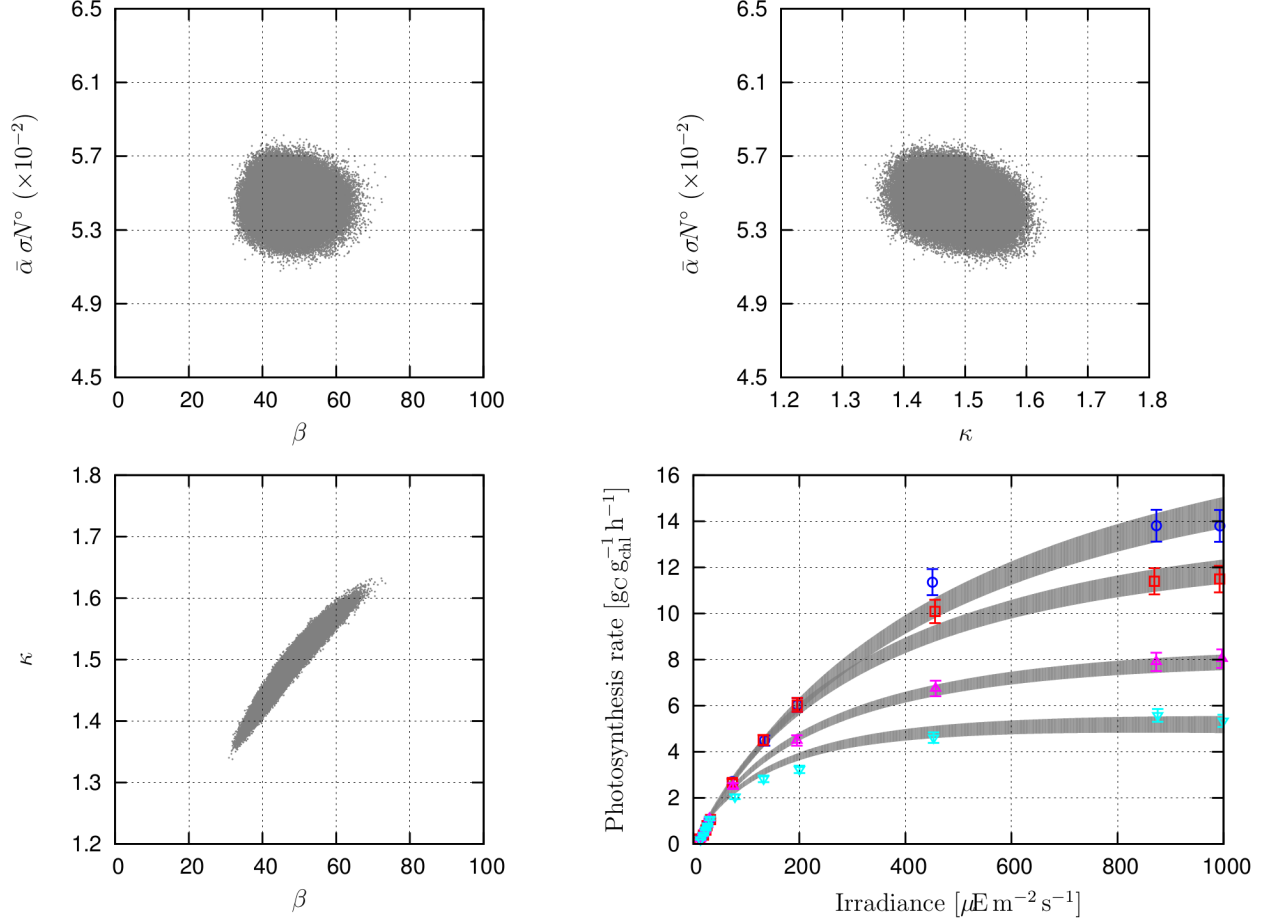


Figure 5: Confidence region of the parameter estimates $\bar{\alpha}$, β and κ with $\pm 5\%$ deviations and corresponding envelopes of PI curves for *D. tertiolecta*.

370 *Calibration of Density and Size Acclimation Laws.* Since experimental information is avail-
 371 able for both the density and size of PSUs at all four acclimation states, values of the
 372 acclimation parameters σ_0 and κ in the power laws (17)-(18) can be estimated for this data
 373 set too. We apply the same linear regression approach and confidence analysis as for *S.*
 374 *costatum* in Sect. 4.1. The estimates for the parameters σ_0 and κ in Table II are obtained
 375 by using the estimates for β , κ and α in Table IV. Then, confidence in these estimates is
 376 assessed by computing the set of all values for σ_0 and κ that are consistent with the available
 377 measurement of density and size of PSU (within variations of $\pm 5\%$), while simultaneously
 378 accounting for the uncertainty in the values of β , κ and α (Fig. 5).

379 The resulting confidence region is shown on the left plot in Fig. 6, and the set of corre-

380 sponding model fits for the experimental data on the right plot. Here, parameter confidence
 381 ranges are obtained as $\sigma_0 \in [0, \infty)$ and $\gamma \in (-\infty, -3.5]$. Clearly, the parameter σ_0 is not
 382 identifiable for this data, which is due to the fact that the size of PSU remains about constant
 383 at various acclimation states, and the range for γ is unbounded from below. Nonetheless, the
 384 upper bound for γ still allows to confidently conclude that this parameter is indeed negative
 385 for *D. tertiolecta*; see Sect. 5 for further discussion.

Table V: Parameter estimates in the density and size acclimation laws (17)-(18) for *D. tertiolecta*.

Parameter	Value
σ_0	$2.60 \times 10^{-11} [\mu\text{E}^{-1} \text{m}^2 \text{g}_{\text{chl}}^{-\gamma} \text{PSU}^{\gamma}]$
γ	$-4.64 \times 10^0 [-]$

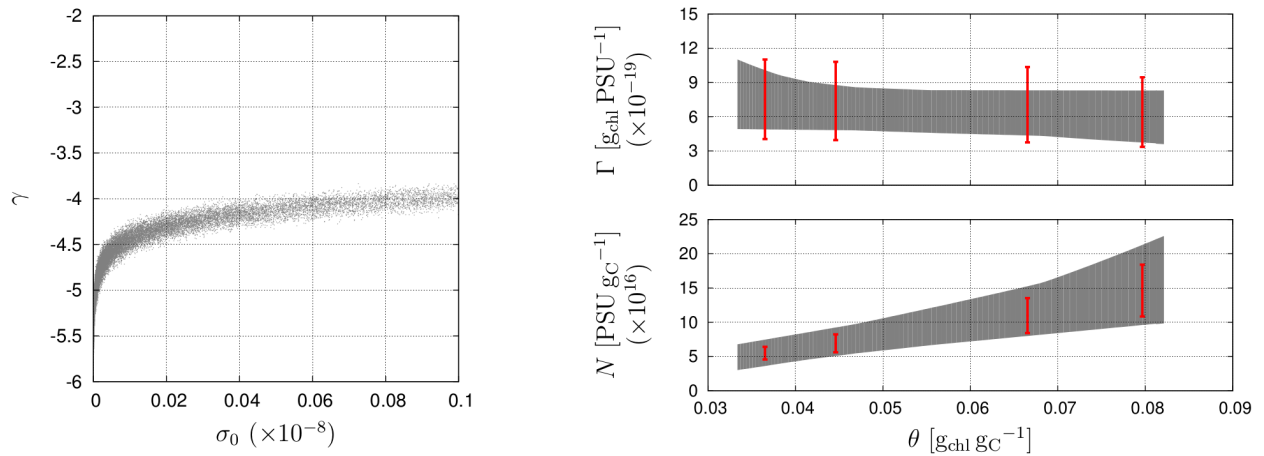


Figure 6: Confidence region of the parameter estimates γ and σ_0 for the measurement data ranges of PSU size and number (left plot) and corresponding fit envelopes (right plots) for *D. tertiolecta*.

Calibration of Nitrogen-Quota-to-Chlorophyll-Quota Relationship. Since experimental information is available for both the nitrogen quota q and the chlorophyll quota θ in all four acclimation states, values of the parameters $\bar{\psi}$ and k_I in the nitrogen-quota-to-chlorophyll-quota relationship (5)-(6) can be estimated from this data set as well. We apply a similar linear regression approach and confidence analysis as for the density and size acclimation

law, noting that the relationships (5)-(6) can be rewritten in the form:

$$\bar{\psi} \frac{q}{\theta} - \frac{1}{k_I} I_g = 1.$$

386 thus giving estimates for $\bar{\psi}$ and $\frac{1}{k_I}$, as reported in Table VI. For consistency with the previous
 387 PI-curve calibration, we use the estimated values of nitrogen and chlorophyll quotas in
 388 Table III to carry out the estimation. The nitrogen-quota-to-chlorophyll-quota predictions
 389 (black points) are plotted against the available experimental data (red circles) in Fig. 7;
 390 the gray dotted line on this plot is merely an interpolation between the predictions, since
 391 nitrogen or chlorophyll quotas are not available at intermediate irradiances. Despite some
 392 discrepancies at higher light irradiances, these results confirm the ability of the acclimation
 393 model (5)-(6) to capture the general trend of the data.

Table VI: Parameter estimates in the nitrogen-quota-to-chlorophyll-quota relationship (5)-(6) for *D. tertiolecta*.

Parameter	Value
$\bar{\psi}$	0.31 $\text{g}_{\text{chl}} \text{g}_{\text{N}}^{-1}$
k_I	440 $\mu\text{E m}^{-2} \text{s}^{-1}$

394 Finally, confidence in the foregoing parameter estimates is assessed by computing the set
 395 of all values for $\bar{\psi}$ and k_I that are consistent with the available measurement ranges of the
 396 nitrogen quota q and of the chlorophyll quota θ in all four acclimation states. The resulting
 397 confidence region is shown on the left plot in Fig. 8, providing parameter confidence ranges
 398 as $\bar{\psi} \in [0.2, 0.35]$ and $k_I \in [400, \infty)$. The bounds on $\bar{\psi}$, although wide, confirm the order
 399 of magnitude for this parameter. On the other hand, k_I can take on arbitrary large values,
 400 a result which is best understood from the upper-right plot in Fig. 8, where a horizontal
 401 line can indeed be seen to provide a good fit of the data point due to the large uncertainty
 402 in the nitrogen-quota measurements. This uncertainty is also reflected in the rather loose
 403 model-prediction envelopes on the lower-right plot.

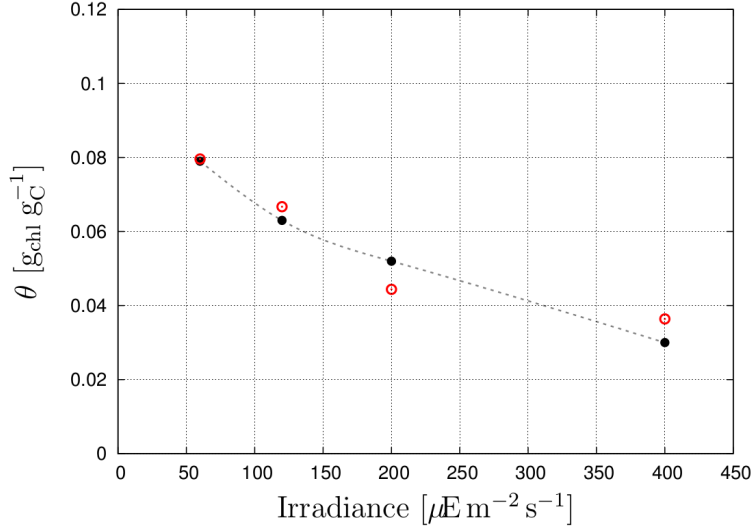


Figure 7: Relation between chlorophyll quota and growth irradiance for *D. tertiolecta*. The red circles correspond to measurements by Falkowski and Owens [11] at acclimation states L_1 , L_2 , L_3 and L_4 , respectively. The black points are computed from the calibrated nitrogen-quota-to-chlorophyll-quota relationship (5)-(6), interpolated by the gray dotted line.

404 5. Discussion

405 5.1. Model Extensions and Simplifications

406 The proposed model in Sect. 3 assumes that only the effective cross-section σ in the Han
407 model is affected by the photoacclimation processes. However, other parameters are likely
408 to vary in response to a change in θ . In particular, there is strong experimental evidence
409 supporting a variation of the parameter τ with the growth irradiance [26, 31]. A more
410 complex model encompassing adaptation of this parameter at the slow time-scale could be
411 considered, for instance by making τ a function of θ . As well as increasing complexity,
412 this extension would nonetheless introduce extra parameters, while the data available for
413 calibration are still scarce. Closer inspection of the model reveals that σ and τ always
414 appear together in (12), in the product terms $\sigma\tau$ and $\sigma\tau^2$ (the latter being more important
415 for describing photoinhibition). It is therefore likely that our modeling of σ with respect to
416 τ indirectly accounts for the variation of τ , and that the estimated parameter is effectively
417 $\sigma\tau$. This hypothesis could however reach its limit in case of strong photoinhibition, as the
418 term $\sigma\tau^2$ may become the dominant one.

419 It is also important to note that photoacclimation acts at different levels in the proposed

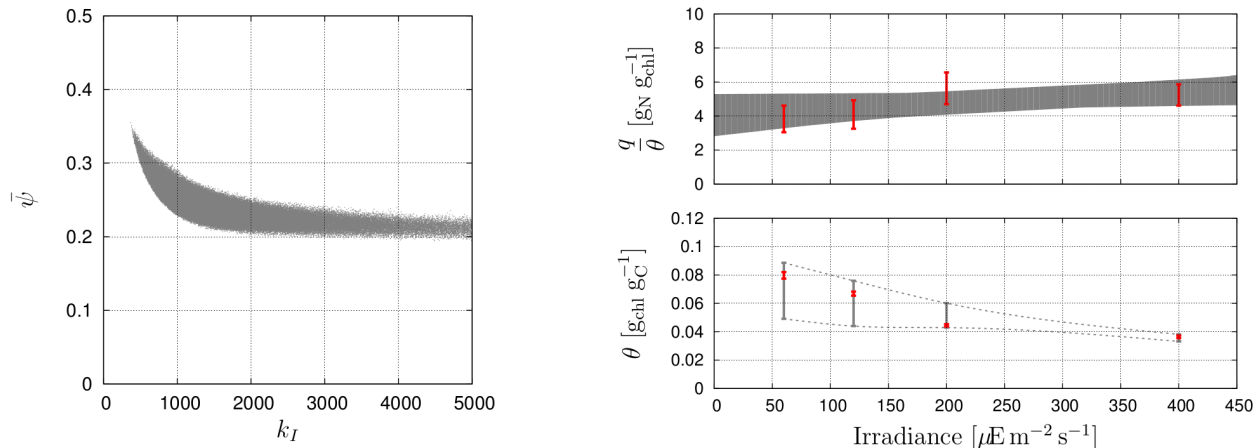


Figure 8: Confidence region of the parameter estimates $\bar{\psi}$ and k_I for the measurement data ranges of nitrogen and chlorophyll quotas given in Table III (left plot) and corresponding fit envelopes (right plots) for *D. tertiolecta*.

420 model. Direct effect of photoacclimation on growth is via the light-dependent term ϕ in
 421 (2), multiplying Droop’s classical growth rate. In doing so, we preserve the structure of
 422 the Droop model and our model inherits many of its properties. However, both terms ϕ
 423 and $(1 - Q_0/q)$ in (2) are increasing functions of the nitrogen quota. It is therefore likely
 424 that a simpler model, whereby the term $(1 - Q_0/q)$ is replaced by a constant, may also
 425 be capable of accurate predictions. Such a model would in fact be close to the model in
 426 [13], which provides a rather simple description of photosynthesis. It is the authors’ opinion
 427 however that a more structured model as the one in Sect. 3 is preferable given the amount of
 428 mathematical analysis that has been devoted to the Droop model over the past few decades.

429 5.2. Accurate Description of Acclimation Strategies and Parameters

430 The fits obtained by estimating the parameters β , κ and $\bar{\alpha}$ (or α) in the chlorophyll-
 431 specific photosynthesis rate (20) are in good agreement with the two data sets by Anning
 432 et al. [1] (Fig. 1) and Falkowski and Owens [11] (Fig. 4). Moreover, the resulting parameter
 433 estimates are found to be rather reliable in view of the confidence regions (Figs. 2 and 5),
 434 despite the presence of a significant correlation between the acclimation parameters β and
 435 κ . For both data sets, information relative to the density and size of PSUs is also available,
 436 which allows estimation of the parameters γ and σ_0 as well. Here, the confidence analysis
 437 (Figs. 3 and 6) has revealed that σ_0 may turn out to be unidentifiable when the density of

438 PSU is mainly unaffected by the chlorophyll quota, yet the range of γ can be more reliably
439 estimated. This provides a means of cross-checking the main acclimation mechanism at play,
440 namely the n-strategy versus the s-strategy:

441 • For *S. costatum* [1], the estimated value and confidence range of κ suggest that the
442 effective cross-section σ is an increasing function of θ per (16), although the rate of
443 increase σ' is slowing down with θ (concave shape); σ is therefore also a decreasing
444 function of the acclimation light I_g . Because of the low small, positive γ value, the
445 average size of PSU is fast increasing with θ , while the density of PSU is fast decreasing.
446 This behavior can thus be interpreted as a mixed n-s acclimation strategy, with
447 predominance of the s-type acclimation, in agreement with Falkowski and Owens [11].
448 Also worth noting is the fact that the effective cross-section decreases much less rapidly
449 with the acclimation light than the average PSU size, suggesting a reduced packaging
450 effect, possibly due to the relatively small size of this species [24].

451 • For *D. tertiolecta* [11], the estimated value and confidence range of κ suggest that σ is
452 increasing with θ , but the rate of increase σ' is itself increasing (convex). The average
453 size of PSU remains about constant with θ , while the density of PSU is fast increasing
454 with θ —or, equivalently, fast decreasing with the acclimation light I_g . According
455 to this analysis *D. tertiolecta* would preferentially follow the n-strategy, which is in
456 agreement with [11]. The fact that the effective cross-section is fast decreasing with
457 the acclimation light, while the average size of PSU is about constant, suggests a
458 strategy combining packaging effect and synthesis of accessory pigments in order to
459 protect the cells from high irradiance [30].

460 In sum, the model represents these two different behaviors, illustrating well its potential to
461 distinguish between competing acclimation strategies for their light harvesting capacity at
462 various irradiance levels. The fundamental differences between such strategies can in fact
463 be related to the ecological niches occupied by both species [11]: *D. tertiolecta* is primarily
464 found in shallow waters at low latitudes, and must therefore deal with high light. *S. costatum*
465 lives in deeper, cooler waters and has to deal with low light intensity.

466 Regarding the photoacclimation kinetics, the fits obtained by estimating the parameters $\bar{\psi}$
467 and k_I in the nitrogen-quota-to-chlorophyll-quota relationship (5)-(6) show a good agreement
468 with the data sets by Falkowski and Owens [11] (Fig. 7). It is worth mentioning here that the
469 estimated values of k_I and $\bar{\psi}$ (Table IV) are consistent with those reported in previous work
470 [e.g., 2]. Nonetheless, a more careful confidence analysis (Fig. 8) reveals that the nitrogen-
471 quota measurements carry too much uncertainty to determine reliable estimates, especially
472 for the parameter k_I whose confidence range happens to be unbounded. These calibration
473 results, although promising, clearly delineate the need for more accurate and richer data sets
474 in order to fully validate the proposed model.

475 5.3. Can the Dynamic Model Predict the Data of Neidhardt et al. [25]?

476 In this subsection, we consider another set of experimental data from Neidhardt et al.
477 [25] for the microalgae *Dunaliella salina*. They comprise two acclimation states at different
478 growth irradiances of $50 \mu\text{E m}^{-2} \text{s}^{-1}$ (LL) and $2000\text{--}2500 \mu\text{E m}^{-2} \text{s}^{-1}$ (HL). Estimation of
479 primary production is via the O_2 production rate by exposing the pre-acclimated microalgae
480 to a sequence of increasing light irradiances between 4.7 and $4900 \mu\text{E m}^{-2} \text{s}^{-1}$, during 150 s
481 at each irradiance level. Moreover, neither the nitrogen quotas nor the chlorophyll quotas
482 are reported.

483 As seen from Fig. 9, the initial slopes of the PI-response curves for cultures pre-acclimated
484 at LL and HL differ greatly, which is in apparent contradiction with the constant initial slope
485 assumption discussed in Sect. 3.2. Also reported on this figure (solid lines) are the results
486 of a preliminary calibration showing that such a variation in initial slope can nonetheless
487 be predicted accurately by the proposed model. More specifically, we simulated the experi-
488 mental protocol in [25], to more accurately account for the actual repair dynamics. In this
489 context, it is not assumed that a quasi steady state is reached for C . The calibration pro-
490 cedure was carried out on this basis. It is important to do so here, because each stage of
491 the PI-response protocol (150 s) may be too short for the dynamics of PSU inhibition to
492 fully equilibrate, especially for a larger chlorophyll quota (LL pre-acclimated state). The
493 initial slope expression is given by (10), with $A = 1 - C$. When microalgae are acclimated

494 at a high growth irradiance, A is smaller than one, even at very low light intensities, since
 495 a fraction of C is still not fully repaired. The lower slope is thus an index of the fraction of
 496 damaged PSU. The simulations on Fig. 9 show that, respecting the exact experimental pro-
 497 tocol, this behavior can be reproduced by the model. These results illustrate the capability
 498 of the proposed model to describe complex couplings between photoinhibition kinetics and
 499 photoacclimation.

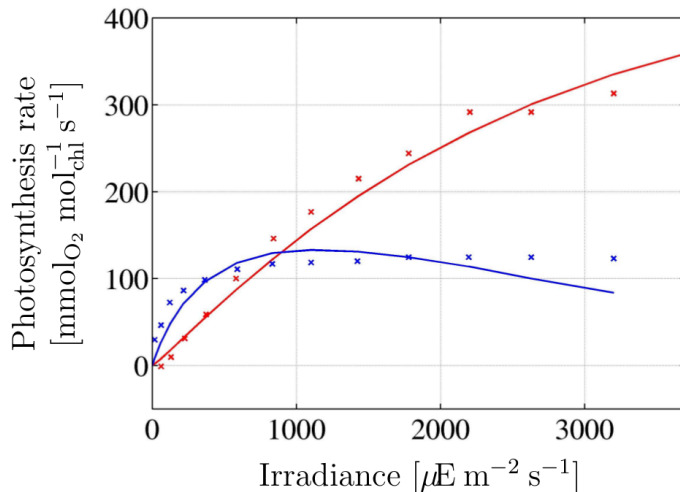


Figure 9: Dependency between growth rate and acclimation for *D. salina* [25]: blue crosses: experimental data for LL acclimation; blue curve: model simulations for LL acclimation; red crosses: experimental data for HL acclimation; red curve: model simulation for HL acclimation.

500 6. Conclusions and Future Directions

501 The dynamic model presented in this paper couples photosynthetic processes that act
 502 on different time scales. Photosynthetic production and inhibition act on fast time scales of
 503 seconds to minutes, while the dynamics of intracellular nitrogen and chlorophyll contents are
 504 bound to slow time scales of hours or days. Our model builds upon the well-accepted Droop
 505 model describing nitrogen utilization and microalgae growth, together with the Han model
 506 describing photoproduction and photoinhibition in terms of PSU states, thereby inheriting
 507 their respective properties. The main novelty lies in the use of the chlorophyll quota to
 508 relate both the acclimation and growth processes with the states of the PSUs. Combined

509 with previous (validated) models describing the dynamics of the PSUs (Han model), nitrogen
510 content (Droop model), and chlorophyll content (Geider et al. [15], Bernard [2]), our model
511 is the first of its kind to link photoinhibition, photoacclimation and nutrient-limited growth
512 all together.

513 Preliminary calibrations and confidence analyses based on PI response data from the
514 literature give encouraging results. By making the link among different PI curves, while
515 preserving a simple structure, the proposed model can serve as a tool for hypothesis testing.
516 Particularly insightful in this context is the ability to distinguish between the s-strategy
517 and the n-strategy of PSU acclimation, which sheds light on the mechanisms that underly
518 photoacclimation in various microalgae species. In order to further discriminate between the
519 n-strategy and s-strategy, more experimental data would be needed nonetheless, especially
520 data covering a wider range of acclimation states and other species. Measuring a larger
521 set of physiological variables, such as the effective cross-section [20], would also be helpful.
522 Another valuable insight from the proposed model has been that the experimental protocols
523 used for producing PI response curves may not allow enough time at each irradiance level for
524 the photoinhibition dynamics to fully develop. In practice, this may lead to overestimating
525 the actual rate of photosynthesis and could explain the variations in initial slopes that are
526 observed between PI response curves at different acclimation states in some experimental
527 studies. Finally, a mathematical analysis of the proposed model could provide valuable
528 insight into the inherent trade-offs and eventually help to identify strategies for enhancing
529 microalgae productivity in large-scale industrial systems.

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Table VII: List of symbols and acronyms.

Symbol	Description	Units
s	inorganic nitrogen concentration	$\text{g}_N \text{m}^{-3}$
s_{in}	inorganic nitrogen inlet concentration	$\text{g}_N \text{m}^{-3}$
x	biomass concentration	$\text{g}_C \text{m}^{-3}$
c	chlorophyll-a concentration	$\text{g}_{\text{chl}} \text{m}^{-3}$
q	carbon-specific nitrogen quota	$\text{g}_N \text{g}_C^{-1}$
Q_0	minimal carbon-specific nitrogen quota	$\text{g}_N \text{g}_C^{-1}$
Q_1	nitrogen uptake limit of carbon-specific nitrogen quota	$\text{g}_N \text{g}_C^{-1}$
Q_{max}	maximal carbon-specific nitrogen quota	$\text{g}_N \text{g}_C^{-1}$
ψ	nitrogen-specific chlorophyll quota	$\text{g}_{\text{chl}} \text{g}_N^{-1}$
$\bar{\psi}$	maximal nitrogen-specific chlorophyll quota	$\text{g}_{\text{chl}} \text{g}_N^{-1}$
θ	carbon-specific chlorophyll quota	$\text{g}_{\text{chl}} \text{g}_C^{-1}$
D	dilution rate	s^{-1}
μ	biomass growth rate	s^{-1}
$\bar{\mu}$	biomass growth rate under nutrient-replete conditions	s^{-1}
$\mu_{\text{chl}}, \mu_{\text{chl}}^{\text{PI}}$	chlorophyll-specific photosynthesis rate	$\text{g}_C \text{g}_{\text{chl}}^{-1} \text{s}^{-1}$
$\mu_{\text{chl}}^{\text{PI}*}$	optimal chlorophyll-specific photosynthesis rate	$\text{g}_C \text{g}_{\text{chl}}^{-1} \text{s}^{-1}$
R	biomass respiration rate	s^{-1}
ρ	inorganic nitrogen uptake rate	$\text{g}_N \text{g}_C^{-1} \text{s}^{-1}$
$\bar{\rho}$	inorganic nitrogen maximal uptake rate	$\text{g}_N \text{g}_C^{-1} \text{s}^{-1}$
k_s	half-saturation constant for inorganic nitrogen uptake rate	$\text{g}_N \text{m}^{-3}$
ϕ	light-dependent growth term	—
k_I	saturation parameter of the nitrogen-specific chlorophyll-a quota	$\mu\text{E m}^{-2} \text{s}^{-1}$
I_g	growth irradiance	$\mu\text{E m}^{-2} \text{s}^{-1}$
I	instantaneous light intensity	$\mu\text{E m}^{-2} \text{s}^{-1}$
I^*	optimal acclimation irradiance	$\mu\text{E m}^{-2} \text{s}^{-1}$
δ	photoacclimation time constant	—
A	fraction of photosynthetic units in open state	—
A^∞	steady-state fraction of photosynthetic units in open state	—
B	fraction of photosynthetic units in closed state	—
C	fraction of photosynthetic units in inhibited state	—
σ	effective cross-section of a photosynthetic unit	$\text{m}^2 \mu\text{E}^{-1}$
τ	turnover time of a photosynthetic unit	s
k_d	damage constant of a photosynthetic unit	—
k_r	repair constant of a photosynthetic unit	s^{-1}
K	ratio of damage to repair constants	s
$\alpha, \bar{\alpha}$	initial slope of the photosynthesis-irradiance response curve	$\text{g}_C \text{g}_{\text{chl}}^{-1} \mu\text{E}^{-1} \text{m}^2$
Γ	size of a photosynthetic unit	$\text{g}_{\text{chl}} \text{PSU}^{-1}$
N	number of photosynthetic units	PSU g_C^{-1}
γ	exponent of photosynthetic unit size equation	—
σ_0	pre-exponential factor of photosynthetic unit size equation	$\mu\text{E}^{-1} \text{m}^2 \text{g}_{\text{chl}}^{-\gamma} \text{PSU}^\gamma$
κ	exponent of effective cross-section equation	—
β	pre-exponential factor of effective cross-section equation	$\mu\text{E}^{-1} \text{m}^2 \text{g}_{\text{chl}}^{1/\kappa} \text{g}_C^{-1/\kappa}$
PSI	photosystem I	
PSU	photosynthetic unit	
PI	photosynthesis-irradiance	