# Is it relevant to explicitly parameterize chlorophyll synthesis in marine ecological models?

M. Mateus [a,*], P.C. Leitão [b], H. de Pablo [a], R. Neves [a]

[a] MARETEC, Instituto Superior Técnico, Universidade Técnica de Lisboa, Av. Rovisco Pais, 1049-001, Lisboa, Portugal
[b] Rua Rui Teles Palhinha, nº4 - 1º, Leião, 2740-278 Porto Salvo, Portugal

## ARTICLE INFO

## ABSTRACT

Oceanographers and modelers often relate chlorophyll concentrations with phytoplankton carbon invoking a suitable C:Chla ratio. However C:Chl ratios are not constant in natural systems, thus making chlorophyll a deceptive measure of true biomass.

In this paper we report on the adaptation of an algorithm for chlorophyll synthesis to a complex ecological model for the marine environment. Based on this model we have developed several simulation experiments to assess the performance of the chlorophyll synthesis and the phytoplankton photoadaptation strategy. The model was applied to three distinct settings, comprising distinctive model geometries and ambient conditions: a schematic setting corresponding to a virtual mesocosm without any transport scheme (0D), a 1D vertical open-ocean application to a 150 m deep water-column, and an application to an estuary using a 2D configuration. Conditions vary from spatially stable in the first case to a strong spatial and temporal heterogeneity in the case of the estuary. Our results fall within the range and reproduce some of the trends found in published data, supporting the idea that when conditions have strong changes of nutrient availability and light conditions, a photoacclimation mechanism becomes an essential requirement for reliable chlorophyll biomass estimates. This is particularly relevant if model simulations are to be used to study natural systems complemented by data retrieved from direct measurements.

## 1. Introduction

Ecological models are expected to be as simple as possible and yet convey the complexity of living systems. A challenge in marine ecological modeling has been to identify which processes must be included in model simulations to address this complexity in a realistic way. The explicit inclusion of chlorophyll dynamics in models is a common example of this challenge. Chlorophyll a (named Chl, hereafter) has been used for long time as a measure of algal biomass, especially for its measurement simplicity and because it is a common pigment to all phytoplankton species. Oceanographers and modelers often relate Chl concentrations to phytoplankton biomass by means of empirical factors, using it as a proxy to carbon biomass. The canonical C:Chl of 60 is commonly used in estimations of C biomass from Chl readings (Cloern et al., 1995). But because this ratio can change in time (see Domingues et al., 2008 and references therein), chlorophyll is a deceptive measure of true biomass, and so this procedure has been recognized to be doubtful given the lack of precision of these empirical factors.

This limitation hinders the use of spatial chlorophyll maps obtained by remote sensing techniques to estimate biomass. Similar

drawbacks are expected from ecological models that do not address chlorophyll synthesis and calculate this index from fixed C:Chl ratios. In these cases, light is used to calculate a limitative factor to production and chlorophyll does not play any role in the model performance. This has been the paradigm of marine ecological models for long time (Fasham et al., 1990).

Photosynthesis is broadly described as the carbon fixation mediated by Chl, a pigment that is common to all planktonic autotrophs. The fundamental relationship governing the photosynthetic process is usually expressed by the following equation:

$$n\text{CO}_2 + 2n\text{H}_2\text{O} \xrightarrow{\text{light}} n(\text{CH}_2\text{O}) + n\text{O}_2 + n\text{H}_2\text{O}$$
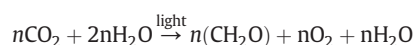
However, the whole photosynthetic process is not a single reaction, but rather the result of distinct steps. These can be broadly summarized as: (i) capturing and transferring light energy into chemical forms, (ii) further changes in the chemical forms into a suitable chemical form for biochemical reactions, and (iii) fixing carbon using the energy produced by the former steps (Parsons et al., 1984).

Mechanistic models account for much of the details of the photosynthesis process, modeling the Photosynthetically Available Radiation (PAR), i.e., the wavelength spectra used by chlorophyll and pigments during photosynthesis, and the different chemical compounds

* Corresponding author. Tel.: +351 21 8419436; fax: +351 21 8419423.
*E-mail address:* mmateus.maretec@ist.utl.pt (M. Mateus).

produced in the process. Yet, this level of details is not suitable for ecological models because they add complexity in the parameterization and require more computer power. Several approaches have been used to simulate the role of photosynthesis and account for primary production in phytoplankton (Behrenfeld and Falkowski, 1997). In most models, primary production is generally summarized as a relationship between carbon assimilation and incident light intensity by assuming that the rate of photosynthesis $P(t)$ is directly proportional to the available light energy $I(t)$. These relationships are mainly derived empirically, although some may have a physiological background (Eilers and Peeters, 1988; Megard et al., 1984). Basically this means that primary production is modeled by converting the absorbed radiation into net photosynthesis, either by using light as a forcing function that drives the C-fixation or in a stoichiometric conversion of the flux of light into chemical compounds (Kooijman, 2000).

The trend has been to increase the degree of sophistication in models, merging biological, physical and chemical processes, to open their scope of simulation purposes. Chl has become a standard feature in more recent marine ecological models incorporation. However, degree of sophistication in models dealing with chlorophyll dynamics vary significantly, from more detailed mechanistic approaches (Baird and Emsley, 1999) to chlorophyll assessment using diagnostic methods (Ebenhoh et al., 1997). With the increase complexity of ecological models during the last decades, much as a reflex of the natural increase in experimental knowledge, particular attention has been devoted to the explicit parameterization of intracellular Chl production and variable Carbon to Chl quotas (expressed as C:Chl ratios, or simply, C:Chl).

The knowledge that the C:Chl ratio is not constant but varies in response to light levels and cell physiological state, has paved the way to the incorporation of acclimation mechanisms into the modeled processes of phytoplankton dynamics (Behrenfeld et al., 2005; Faugeras et al., 2004). This acclimation of the photosynthetic apparatus, expressed not only in the variability of C:Chl but also of Nitrogen:Chl (N:Chl), is a physiological response to external conditions, namely the variations in irradiance and nutrient availability (Domingues et al., 2008). In addition, phytoplankton specific composition is also a relevant driver of C:Chl ratios (Chan, 1980). In response to the growing awareness of photo adaptation importance, over the past decade a number of models have been developed to account for variable chlorophyll content in algae (Sathyendranath et al., 2009; Wang et al., 2009). Light history is reflected in C:Chl fluctuations in these models, which in turn affects the instantaneous photosynthesis-light response (C-fixation).

In this paper we report on the adaptation of an algorithm for chlorophyll synthesis to a complex ecological model for the marine environment. Based on this model we have developed several simulation experiments to assess the performance of the chlorophyll synthesis and the phytoplankton photoadaptation strategy. This work was developed in the context of EU project Data Integration System for Eutrophication Assessment in Coastal Waters (INSEA), a collaborative project to develop a coastal management system based on the efficient integration of observations and biophysical models. Since many ecosystem models are not based on Chl, but on carbon, a suitable C:Chl ratio has is usually invoked to estimate Chl for comparison with remote sensing data. In the context of the project this work is a contribution to understand the factors that influence C:Chl ratios, thus providing relevant insights on the choice of adequate ratios.

## 2. Material and methods

### 2.1. Chlorophyll synthesis formulation

The chlorophyll synthesis algorithm (Geider et al., 1996, 1997, 1998) was adapted to fit an ecological model made from scratch (Mateus, 2012-this issue) inside the MOHID modeling system

(Leitão et al., 2008), a community model shared by a large user group around the world. The ecological model reflect the current trends and paradigms of marine ecological models (Baretta-Bekker et al., 1997), with explicit modeling of carbon and nutrient cycles, variable stoichiometry in organism and organic matter components, and different phytoplankton groups. With this formulation, chlorophyll is explicitly modeled allowing the adaptation to different ambient light, temperature and nutrient conditions. This adaptation is expressed in variable C:Chl ratios. Unless stated otherwise, parameter values have been taken from Mateus et al. (2012-this issue).

Phytoplankton growth rates (C-fixation) are determined by available light and nutrients using a modified form of a growth model taken from the literature (Geider et al., 1996, 1997, 1998). The model parameterization includes the following regulatory features: (a) Chl synthesis requires N assimilation, (b) the carbon-specific, light-saturated photosynthetic rate depends on the internal nitrogen status of the cell, (c) the carbon-specific, light-limited photosynthetic rate depends on the C:Chl ratio, and (d) Chl synthesis is downregulated when the rate of light absorption exceeds the rate of utilization of photons for carbon fixation, with the extent of downregulation being governed by the imbalance between rates of light absorption and photosynthesis.

The actual specific assimilation/photosynthesis rate is described by:

$$P_c^{\text{phot}} = P_c^{\text{max}} \left[ 1 - \exp\left( \frac{-\alpha^{\text{chl}} \cdot X_{\text{chl}}^* \cdot I_0}{P_c^{\text{max}}} \right) \right] \quad (1)$$

where $\alpha^{\text{chl}}$ is the chlorophyll light absorption coefficient, $X_{\text{chl}}^*$ the chlorophyll cell quota or Chl:C, and $I_0$ the available irradiance in the cell. $P_c^{\text{max}}$, the maximum rate of C-specific photosynthesis is a function of temperature $\Omega_T$, a dimensionless function that can have different forms (Arrhenius, Q10, optimal interval, etc.), ranging between 0 (total limitation) and 1 (no limitation), and the maximum daily assimilation rate $r$ at a reference temperature:

$$P_c^{\text{max}} = r \cdot \Omega_T \quad (2)$$

Allowing for phytoplankton acclimation to light and nutrients, the light history is reflected on growth by the variation of the Chl:C. To keep the nomenclature of the original model the Chl:C ratio ($X_{\text{chl}}^*$) is used in the equations, but the inverse C:Chl ratio ($X_{\text{chl}}$) is used elsewhere since it is the most common ratio found in the literature (Domingues et al., 2008; Sathyendranath et al., 2009; Wang et al., 2009). A short description of all parameters and their units is provided in Table 1.

The model of phytoplankton growth and physiological acclimation treats nutrient uptake and photosynthesis rates as functions of both environmental factors and cellular chemical compositions (Chl:C and N:C). Chl synthesis, $P_{ac}$, is regulated by the balance between photosynthetic carbon fixation and light absorption (the ratio of energy assimilated to energy absorbed). This regulation term, $\rho_{\text{chl}}$, is formulated as:

$$\rho_{\text{chl}} = X_{\text{chl:n}}^{\text{max}} \frac{P_c^{\text{phot}}}{\alpha^{\text{chl}} \cdot X_{\text{chl}}^* \cdot I_o} \quad (3)$$

where $X_{\text{chl:n}}^{\text{max}}$ is the maximum value of Chl:N ratio. The remaining variables have already been defined for Eq. (1). The Chl synthesis parameterization is then:

$$P_{ac} = \frac{\rho_{\text{chl}} \cdot \nu_n}{X_{\text{chl}}^*} - \phi_{\text{chl}} \quad (4)$$

Chl synthesis is assumed to be proportional to nitrogen uptake, $\nu_n$, reflecting the need for the synthesis of proteins used in light