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Dynamic Effect of Light and Turbulence on Algal Photosynthetic Rate: A Water-Quality Model

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Dynamic Effect of Light and Turbulence on Algal Photosynthetic Rate: a Water-Quality Model

BY

Andres Rivas

A research project report submitted in partial fulfillment of the requirement for the degree of

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IN
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Project Advisor:
Dr. Scott Wells

Portland State University
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ABSTRACT

Several studies provide evidence that algal photosynthetic rates depend on various changing factors such as light attenuation, temperature, and nutrient limitation (Chapra, 1997). However, recent papers show that turbulence and photosynthetic rate dynamics is also important (Ross, 2006). In this study, the photosynthetic rate model used is the one proposed by Chapra (1997), where it depends directly on temperature, nutrient and light limitation factors. At the same time, the effect of turbulence or random-walk of algae particles in the water column was also introduced in this model. To account for this factor, the model added was that proposed by Ross (2006), in which the random movement of an algae particle depends on an initial position, a sinking or swimming velocity, an advective term and a random term related to probability. An example test is proposed to evaluate the model and all the parameters and variables are pre-established to show a natural example commonly found in nature. The values of photosynthetic rate were obtained on average and point by point, the photosynthetic rate evolution with time was evaluated. Simulations results are consistent with literature, specifically the photosynthetic rate dynamic behavior, and wereas compared with the results obtained by Harris (1977), Marra (1978), and Ross (2006). Some aspects of the dynamic effect of light attenuation and turbulence on photosynthetic rate are investigated through the model.
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1.0 Introduction

Modeling algae is one of the most important analyses that can be done on waterbodies to study the equilibrium of ecosystems. As Wehr et al (1975) states, algae are the starting point for many trophic chains and provide good knowledge about the state of the system. In this way, it is common in water quality modeling to focus on algae known as phytoplankton, they consist of a variety of species, such as dinoflagellates, diatoms, and cyanobacteria. In a balanced marine ecosystem, phytoplankton provide food for a wide range of aquatic life including whales, shrimp, snails, and jellyfish (NOAA 2014). Similarly, algae provide water quality information on non-marine systems such as lakes, ponds and rivers. Some of the data that can be found by analyzing algae on lakes vary from nutrients such as phosphorus or nitrogen to information on optimal temperature in the system.

The phytoplankton production, photosynthetic rate, and biomass in most lentic systems are controlled by P (phosphorus) supply (Van den Hoek, 1995). However, other factors such as grazing, light availability (irradiance), and temperature also affect phytoplankton.

Therefore, it is well known that phytoplankton distribution modeling depends on nutrients, light, and temperature as main factors. But recent studies indicate that the effect of turbulence is also crucial to simulate correctly such distributions in a water column. As Goshal et al. (2000) explains, phytoplankton productivity is strongly constrained by the need for light which is only available in the upper layers, and the need for mineral nutrients. Vertical upwelling and turbulent transport to dredge up nutrients from the deeper waters is also an important process for algae growth.

Several models have been developed to simulate the behavior of algae, photosynthetic rates and algae production. These models take as a main factor the relationship between photosynthetic rate and irradiance (Steele, 1962; Platt and Jassby, 1976; Kiefer and Mitchell, 1983; Olson et al., 1996). However, some issues arise when applying these models to simulate algae behavior. First, most of the models take the irradiance in a static way (Han et al., 2000). The water systems are often affected by non-constant physical factors (e.g. mixing process, turbulence) and weather factors (e.g. cloudiness or precipitation) that lead phytoplankton to
experience important changes on irradiance. In consequence, a taking in the variance on irradiance is necessary for such simulations (Steeman-Nielsen et al., 1962; Harris, 1978).

Other factors involved in simulating algae growth are temperature and nutrients availability (Chapra, 1997). Temperature affects algae at the cellular scale (Van den Hoek, 1995). At the same time, inclusion of temperature in water-quality models is necessary to determine their effect on competition among groups (e.g. what type of algae is developing). In the same way, nutrient limitation is also important since it contributes to algae growth (Wehr, 1975).

Turbulence or randomness also affect algae simulations. Most of the models used take algae particles movement as a predictable function along depth (Goshal et al., 2000). However, some studies provides good evidence that random-walk of algae particles in the water column may affect such simulation at the same level as light, nutrients and temperature (Visser, 1997; Ross, 2006). Several approaches for random-walk have been developed (Goodwin, 2001; Guha, 2007), most of them use particle tracking theory to develop the models tracking algae particle position along the water column at each time iteration.

In the present study, a model to simulate photosynthetic growth is developed to investigate the dynamic effect of irradiance and turbulence. In the same way, the effects of temperature and nutrients limitation are also included. First, the limits to phytoplankton growth are outlined, providing the equations and models to simulate algae, growth rate, temperature, and nutrients. Secondly, the models to predict the effect of light on phytoplankton growth is computed for both, an approximation to a point and to the averaged water column depth. Then, the main relations for primary production and photosynthetic rate are used to compute the growth rate. Also, a random-walk model is used to simulate the vertical movement of algae particles. Finally, the results are compared with the data obtained by Ross (2006).
2.0 Limits to phytoplankton growth

The development of models for phytoplankton growth is often used to predict the behavior of algae (Chapra, 1997; Ross, 2006). The framework of these models includes nutrient limitation, effects of light, and temperature. Chapra (1997) states that the first step to characterize algae is similar as the one in the approaches of characterizing organic matter and microorganisms. For a batch system, with a first order decay reaction, the mass balance can be written as

\[
\frac{da}{dt} = k_g a
\]

where \(a\) is the concentration of algae (mgChla m\(^{-3}\)), and \(k_g\) is the first order growth rate (d\(^{-1}\)). Applying initial conditions of \(a_0 = 0\) at \(t = 0\), then Equation 1 has the analytical solution

\[
a = a_0 e^{k_g t}
\]

By inspection of Equation 2, it is evident that at long times the concentration of algae will be extremely high. Thus, along with the growth there must be a process that limits growth of algae (Chapra, 1997). In consequence, to incorporate this effect 2 new processes are added to Equation 1. First, the growth rate is expanded by showing that is a function of temperature, nutrients, and light limitation. Later it will be shown that light limitation is also affected by turbulence. Secondly, a loss rate term is added to Equation 1, which in the present study is considered as a constant. This rate represents the losses by respiration, excretion, and predatory losses (Chapra, 1997). Now the governing equation for algae growth takes the form

\[
\frac{da}{dt} = k_g(T, N, I) a - k_d a
\]

Where \(k_g(T, N, I)\) is the growth rate as a function of temperature \(T\), nutrients \(N\), and light \(I\), and \(k_d\) is the loss rate. Now expanding the term of growth (Chapra, 1997), the expression now takes the following form

\[
k_g(T, N, I) = k_{g,T} \phi_N \phi_L
\]
Where \( k_{g,T} \) is the maximum growth rate at a particular temperature \((d^{-1})\), \( \varphi_N \) is the attenuation factor for nutrients limitation, and \( \varphi_L \) is the attenuation factor for light limitation. The attenuation factors are dimensionless, and they can take values from 0 (total limitation) to 1 (no limitation). In the next section of the study, each of these terms are explained.

### 2.1 Temperature effect

Including the effect of temperature in a water-quality model is necessary to determine the influence of this characteristic on the different groups of algae (Van den Hoek, 1995). The temperature defines if a certain group of algae is favored among others in the water system. Different types of algae have different optimal temperatures at which the growth rate is higher.

Several models have been proposed to represent the effect of temperature on phytoplankton growth (Epply, 1972; Vogel, 1974; Chapra, 1997). The simplest is explained by Chapra (1997), which is a linear model with minimum temperatures below which growth does not occur

\[
k_{g,t} = k_{g,\text{ref}} \frac{T - T_{\text{min}}}{T_{\text{ref}} - T_{\text{min}}}
\]

(5)

Where \( k_{g,t} \) is the growth rate \((d^{-1})\) at a temperature \( T \) (Celsius), \( k_{g,\text{ref}} \) is the growth rate \((d^{-1})\) at a reference temperature \( T_{\text{ref}} \) (Celsius), and \( T_{\text{min}} \) is the temperature below which growth ceases.

However, the most common model used is also stated by Chapra (1997), commonly known as the theta model. This is also the approach used in the present study. This model is expressed by

\[
k_{g,T} = k_{g,20} \Theta^{T-20}
\]

(6)

where \( k_{g,T} \) is the growth rate \((d^{-1})\) at \( T \) (°C), \( k_{g,20} \) is the growth rate \((d^{-1})\) at 20 °C, and based on literature (Epply, 1972) a value of \( \Theta = 1.066 \) is often used. This value is based on a large number of studies involving many species of phytoplankton.
2.2 Nutrients limitation effect

Nutrients also impact the growth rate of algae. The main nutrients used by phytoplankton on their process are phosphorus, nitrogen, and silica (Van den Hoek, 1995). Nutrient limitation affects algae on providing or limiting resources that develop the algae growth rate. The most common approach for handing nutrient limitation is the Michaelis-Menten equation (Chapra 1997), described by

\[ \phi_N = \frac{N}{k_{SN} + N} \]

Where \( N \) is the concentration of the limiting nutrient, and \( k_{SN} \) is the half-saturation constant. Chapra 1997, states that some typical values for \( k_{SN} \) are for phosphorus 1-5 \( \mu \)P L\(^{-1}\), for nitrogen 5-20 \( \mu \)N L\(^{-1}\), and for silica 20-80 5-20 \( \mu \)Si L\(^{-1}\). The values for the half saturation constant may vary depending on the form of the nutrient that is limiting. In the same way, this equation is linearly proportional to concentration at low nutrient levels and approaches a constant value of one at high levels.

In any water system there will usually be more than one type of nutrient that is at some level limiting the growth rate (Walker, 1983). In this case, there are multiple approaches that may be used, such as multiplicative approach, the minimum approach, and the harmonic mean approach (Chapra, 1997). However, in this study the most commonly accepted method will be used, the minimum limitation nutrient approach. This method states that when there is more than one nutrient that is affecting growth rate, the nutrient in shortest supply controls growth

\[ \phi_N = \min\{\phi_p, \phi_n\} \]  

where the minimum between P and N is taken as the nutrient that controls growth, in this example we will be using just phosphorus or nitrogen even though other nutrients could also limit growth.
2.3 Light limitation effect

The effect of light on phytoplankton growth is always difficult to estimate by the fact that several factors have to be taken in consideration to come up with the total effect (Chapra, 1997). The main factors impacting light limitation effect are surface-light variation, light attenuation with depth, dependence of the growth rate on light, and at some level that will be stated below, turbulence present in the water column.

According to Chapra (1997), one of the most used methods to estimate the light limitation on algae modeling is the Steele (1965) approach. This model states that growth is inhibited at high light levels, and is given by

\[ F(I) = \frac{I}{I_s} e^{-\frac{I}{I_s} + 1} \]  \hspace{1cm} (9)

where \( I \) is the light level and \( I_s \) is the optimal light level (ly d\(^{-1}\)). Now, the spatial variation of light down through the water column can be modeled by the well-known Beer-Lambert law, which says

\[ I(z) = I_0 e^{-k_e z} \]  \hspace{1cm} (10)

where \( I_0 \) is the solar radiation at the surface (ly d\(^{-1}\)) and \( k_e \) is the extinction coefficient (m\(^{-1}\)). The extinction coefficient can be related to more fundamental quantities (Riley, 1956) by

\[ k_e = k_e' + 0.0088a + 0.54a^{2/3} \]  \hspace{1cm} (11)

Where \( k_e' \) is the light extinction due to factors other than phytoplankton. These values are often found on literature (Di Toro, 1978; Chapra, 1997). At this point, Equations 9 and 10 can be coupled to express the general equation for the light limitation factor at any depth “z” along the water column, this will be the model used to estimate the light limitation factor in the present study. The equation on discussion is given by

\[ F(I) = \frac{I_a e^{-k_e z}}{I_s} e^{-\frac{I_a e^{-k_e z}}{I_s} + 1} \]  \hspace{1cm} (12)
The above Equation 12 is evaluated at a point, i.e. it is estimating the light attenuation factor for a given depth in the water column. However, in the present study the averaged light attenuation factor for the entire water body will also be calculated. According to Chapra (1997), Equation 12 can now be integrated over depth and time to develop the mean value for the light attenuation factor. The integration is expressed as

$$\phi_L = \frac{1}{H} \int_{H_1}^{H_2} \int_{T_p}^{T} \left[ \frac{I_a e^{-k_e z}}{I_s} e^{-\frac{I_a e^{-k_e z}}{I_s}} - 1 \right] dt \, dz$$

(Equation 12)

Evaluating this double integral and taking as $H_1$ the water surface and $H_2$ the depth of the water column, it is obtained the mean value for the light attenuation factor. After evaluating and applying the integration limits, the resulting equation is

$$\phi_L = \frac{2.718 f}{k_e H} (e^{-\alpha_1} - e^{-\alpha_0})$$

(Equation 13)

Where $f$ is the photoperiod (fraction of day), and

$$\alpha_0 = \frac{I_a}{I_s} e^{-k_e H_1}$$

(Equation 14)

$$\alpha_1 = \frac{I_a}{I_s} e^{-k_e H_2}$$

(Equation 15)

where $I_a$ is the average light over the daylight hours (ly d$^{-1}$), $I_s$ is the optimal light level (ly d$^{-1}$), and $H_1$ and $H_2$ depend on the reference system used (H is the total height). The above Equations 13 is used in the model to estimate the averaged light attenuation factor. Also, it is important to address that the light values used in all preceding equations are visible, photosynthetically available light (Chapra, 1997). This value is typically about 40% to 50% of the energy in the complete standard spectrum used in this type of calculations.
3.0 Growth rate model

Now with every term stated, the complete model of phytoplankton growth rate can be developed. Equation 16 is the model applied to a point “z” in the water column, and Equation 17 is applied to the averaged water column depth. The two mentioned equations are respectively given by

\[ k_g = k_{g,20}1.066^{T-20} \left[ \frac{l_a e^{-k_e z}}{l_s} e^{-\frac{l_a e^{-k_e z}}{l_s} + 1} \right] \min(\phi_N, \phi_p) \]  \hspace{1cm} (16)

\[ k_g = k_{g,20}1.066^{T-20} \left( \frac{2.718 f}{k_g H} (e^{-\alpha_1} - e^{-\alpha_2}) \right) \min(\phi_N, \phi_p) \]  \hspace{1cm} (17)

Where \( k_g \) is the growth rate as a function of temperature, light limitation, and nutrient limitation. At this point, it can be also calculated the primary production and the oxygen produced by photosynthesis (Chapra, 1997), these equations are respectively

\[ Pr = a_{ca} k_g H a \]  \hspace{1cm} (18)

\[ P = r_{oc} a_{ca} k_g a \]  \hspace{1cm} (19)

Where \( Pr \) is the primary production (gC m\(^{-2}\) d\(^{-1}\)), \( a_{ca} \) is the rate of milligrams of carbon by \( \mu g \) of Chla (1/20 mgC \( \mu g \text{Chla}^{-1} \)), \( P \) is the oxygen produced (gO m\(^{-2}\) d\(^{-1}\)), and \( r_{oc} \) is the rate of grams of oxygen by grams of carbon (2.69 gO gC\(^{-1}\)). However, for showing the results on graphs and plots, the photosynthetic rate from Equation 19 is reduced to

\[ P = r_{oc} a_{ca} k_g \]  \hspace{1cm} (20)

With Equation 20 the model is now able to estimate the photosynthetic rate with units of molO\(_2\) mgChl\(_a\)\(^{-1}\) h\(^{-1}\), which is the most used unit to express photosynthetic rate when plotting against time and light (Ross, 2006).
4.0 Turbulence effect on the growth rate model

Turbulence takes a meaningful role on the simulation of phytoplankton behavior. Particles of algae in the water column will tend to a random movement through the system. This random movement impact then the light attenuation factor at each point “z” along the water column, and therefore, the photosynthetic rate. (Visser, 1997). To address this effect, several models have been proposed to simulate the vertical random-walk of particles in water systems (Dimou, 1993; Visser, 1997; Goodwin, 2001; Ross, 2006; Guha, 2008). However, in the present study the model proposed by Visser (1997) and then modified by Ross (2006) was used.

Random walks techniques or the computer simulation of the movement of individual particles in a turbulent environment is becoming a much used tool in investigating environmental processes (Visser, 1997). In this way, the distribution of planktonic cells is just one of the processes that can be simulated by using random walk models.

Most authors researching in this area state that the most crucial question to be addressed in such simulations is how individual particles move in response to turbulent diffusion. The random walk model is often used to address this question. Visser (1997) explains that the main premise of a random walk simulation is that, given a diffusivity $K \text{ (m}^2 \text{ s}^{-1})$, the ensemble average of the square of the particle displacement $Z$ is given by

$$\frac{d}{dt} \langle Z^2 \rangle = 2K \tag{21}$$

Equation 1 is given for a 1-dimensional process. In consequence, for an individual particle, this can be translated to a change in position with time, from $Z_n$ to $Z_{n+1}$, over a finite time step $\delta t$, given by

$$Z_{n+1} = Z_n + R(2r^{-1}K\delta t)^{1/2} \tag{22}$$

Where $R$ is a random process with mean $\langle R^2 \rangle = 0$, and standard deviation $r$, if $R$ is a uniform distribution between +1 and -1, then $r = 1/3$. Equation 22 is also known as the naïve random walk formulation.
In this way, Ross (2006) seeks to simulate with a random walk model that two cases can be reproduced with the same approximation. These cases are when the diffusivity term is taken to be a constant and when is not. The random walk scheme used was very similar to the model used by Visser (1997), but now a new particle sinking term is introduced, the equation is given by

\[ Z_{n+1} = Z_n - w_p \delta t + K'(Z_n) \delta t + R \{ 2 r^{-1} K \left[ Z_n + \frac{1}{2} K'(Z_n) \delta t \right] \delta t \}^{1/2} \]  

(23)

Where the new term \( w_p \delta t \) is the sinking term, and \( w_p \) is the vertical sinking/swimming velocity. The rest of the variables and coefficients are treated as in the model of Visser (1997). In the same hand, Ross (2006) also compared the results of this equation with the same model, but now taking the diffusivity term \( K' \) as a constant, the model then takes the form

\[ Z_{n+1} = Z_n - w_p \delta t + R \{ 2 r^{-1} K[Z_n] \delta t \}^{1/2} \]  

(24)

which is the naive random walk formulation with the extra sinking term. This model will be one of the most used in the present study to represent turbulence in the model of light attenuation factor. Furthermore, the diffusivity profile used by Ross (2006), and also used in this model has the form

\[ K(Z) = K_{bg} + \frac{K_m}{2} \left[ 1 - \cos \left( \frac{2 \pi Z}{H} \right) \right] \]  

(25)

Where \( K_{bg} \) is a background diffusivity which quantifies the amount of turbulent mixing in the thermocline and near the surface, and \( K_m \) is the maximum diffusivity at the center of the mixed layer.
5.0 Simulation and results

Parameterization

Several studies can be used to determine the parameters in the model expressed by the equations stated above. Values for an example test of the model will be stated to verify validity. The main model are equations 16 and 17, which are the point and averaged growth rate respectively, and also equation 20 which represents the photosynthetic rate. Most of the parameters are estimated indirectly in the literature (Chapra, 1997; Visser, 1997; Ross, 2006). In consequence, their exact meaning and dimensions are easily confused. The parameters used in this study and their possible ranges are listed on Table I.

As suggested by Chapra (1997), the value used for the optimal light ($I_s$) was picked from the range proposed, this value is 300 Ly d$^{-1}$. The values for light at the surface ($I_a$) were stated at 3 cases, 100, 500, and 800 Ly d$^{-1}$ respectively, since they are common values found on optimal weather conditions (Chapra, 1997), as well as they provide different cases to contrast. Also, the values for $K_{g,20}$, $\Theta$, $T$, $N$, $K_{SN}$, $k_e$, $a$, and $f$ were all used by taking the most common values found in literature as stated by Chapra (1997) and Ross (2006), as well as to describe a common situation of a water system.

Table 1. Parameters values and ranges used in the model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Range/Value</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_a$</td>
<td>Ly d$^{-1}$</td>
<td>500</td>
<td>Irradiance</td>
</tr>
<tr>
<td>$I_s$</td>
<td>Ly d$^{-1}$</td>
<td>100-500(300)</td>
<td>Optimal Irradiance</td>
</tr>
<tr>
<td>$K_{g,20}$</td>
<td>d$^{-1}$</td>
<td>2</td>
<td>Growth rate at 20 °C</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>Dimensionless</td>
<td>1.066</td>
<td>Theta coefficient</td>
</tr>
<tr>
<td>$T$</td>
<td>°C</td>
<td>25</td>
<td>Water temperature</td>
</tr>
<tr>
<td>$N$</td>
<td>mg m$^{-3}$</td>
<td>3</td>
<td>Concentration of limiting nutrient</td>
</tr>
<tr>
<td>$K_{SN}$</td>
<td>mg m$^{-3}$</td>
<td>2</td>
<td>Half saturation constant for limiting nutrient</td>
</tr>
<tr>
<td>$k_e$</td>
<td>m$^{-1}$</td>
<td>0.3</td>
<td>Extinction coefficient</td>
</tr>
<tr>
<td>$a$</td>
<td>mgChla m$^{-3}$</td>
<td>4</td>
<td>Chlorophyll a concentration</td>
</tr>
<tr>
<td>$f$</td>
<td>Dimensionless</td>
<td>0.5</td>
<td>Photoperiod</td>
</tr>
<tr>
<td>$H$</td>
<td>m</td>
<td>30</td>
<td>Water Column depth</td>
</tr>
<tr>
<td>$\alpha_{ca}$</td>
<td>mgC μgChla$^{-1}$</td>
<td>1/20</td>
<td>Carbon-to-chlorophyll ratio</td>
</tr>
<tr>
<td>$r_{oc}$</td>
<td>mgO mgC$^{-1}$</td>
<td>2.69</td>
<td>Oxygen-to-carbon ratio</td>
</tr>
<tr>
<td>$w_p$</td>
<td>m s$^{-1}$</td>
<td>$10^3$</td>
<td>Sinking velocity</td>
</tr>
<tr>
<td>$\delta t$</td>
<td>s</td>
<td>0.1</td>
<td>Time step</td>
</tr>
<tr>
<td>$K_{bg}$</td>
<td>m s$^{-1}$</td>
<td>$10^6$</td>
<td>Experimental constant for diffusivity</td>
</tr>
<tr>
<td>$K_m$</td>
<td>m s$^{-1}$</td>
<td>$0.9 \times 10^6$</td>
<td>Experimental constant for diffusivity</td>
</tr>
</tbody>
</table>
Furthermore, a standard water column depth of 30 m was selected to fix in the model. This value was in concordance with the previous parameters stated above. As it is to express a common example of a water column with typical values at normal weather, physical, and chemical conditions. In the same way, the values for the constants $a_{ca}$, $r_{oc}$, were selected in agreement with the values stated by Chapra (1997). Finally, the values for the random walk model were selected by following the common values found on literature (Visser, 1997; Ross, 2006), the values on discussion are $w_p$, $\delta t$, $K_{bg}$, and $K_m$.

The model was developed by writing a code in Haskell, an emergent programing language widely used in research (see www.haskell.org to find more information about the language), and Fortran90, a well-used language in the engineering field. The script of it along with the functions constructed can be seen in the Appendix.

**Description of the example experiment used to test the model**

The model consists on equations 16 and 17 which predict the punctual and averaged growth rate respectively. Equation 20 that estimates the photosynthetic rate. And equation 24 that is the random walk model to predict the particle movement along the water column.

![Figure 1](image-url)  
**Figure 1.** Movement prediction for the algae particle along the vertical axis. Note that the display was reduced to a quadrant of 0.1 meters x 0.3 hours to illustrate the turbulence effect.
The example experiment to test the model is the release of one algae particle at the top of a 30 meters deep pool. The vertical movement was predicted with equation 24, and the behavior of the particle can be seen on Figure 1. The whole model was run with a time step of 0.1 seconds for 12 hours.

As stated earlier, Visser (1997) and Ross (2006) explain that turbulence plays an important role on particle movement along a water column. Visser (1997) describes that particles under the influence of turbulence can either accelerate or retard their sedimentation rate as a consequence of the randomness of turbulence. The turbulent eddies provides friction forces on particles that affect directly their settling. Ross (2006) developed a model to prove that both cases, acceleration and retardation of particles can be predicted by using the same random walk model, the results obtained by this author satisfied the theory that turbulence has a direct impact on particle movement along the water column.

*Photosynthetic rate evolution with constant irradiance*

The time course of photosynthesis under constant irradiance can show decay of the photosynthetic rate when photoinhibition occurs (Ross, 2006). Thus, to show this the model was run at 3 constant irradiance levels: 100, 500, and 800 ly d⁻¹. The first value corresponds to the low boundary of $I_s$ and the second to the high boundary of the same range (See Table 1). The third value is chosen to test the model prediction outside this range, at normal weather conditions and with the same parameters values stated at Table 1. The photosynthetic rate evolution at all three irradiances levels are shown in Figure 2.
Figure 2. Photosynthetic rate evolution under constant light intensity, turbulent field, and at three light levels, (1) 100, (2) 500, and (3) 800 ly d\(^{-1}\) respectively. Note: on segment 1 the effect of photoinhibition is showed.

**Diurnal change on photosynthetic rate**

The daily change of light has also an effect on photosynthetic rate. To represent this, the daily light course was set to be expressed by the function

\[
I_p \sin^3(\pi t/12) \text{ ly d}^{-1}
\]

(26)

Being the peak light intensity \(I_p\) of 100, 500, and 800 ly d\(^{-1}\), to represent three example cases and contrast the results for a period “t” of 12 hours. The model was run to simulate diurnal change in photosynthetic rate, all the parameters used were the pre-established for the example test (See Table 1), with the exception of light intensity, which was simulated by the sinusoidal function stated above.
The change in photosynthetic rate from morning to afternoon is symmetrical, being the peak at noon. In natural aquatic environments, light intensity experienced by phytoplankton is usually coupled with physical processes, according to Ross (2006) some processes such as mixing and weather conditions may also affect the water column. The diurnal change on photosynthetic rate can be seen on Figure 3.

**Figure 3.** Photosynthetic rate evolution when the light function is defined as $I_p \sin^3(\pi t/12)$ ly d$^{-1}$. Being $I_p$ (1) 100, (2) 500, and (3) 800 ly d$^{-1}$.

Photosynthetic rates measured with a succession of increasing irradiance levels are often higher than the rates measured with a series of decreasing irradiance (Ross, 2006). This is commonly known as the hysteresis effect. How hysteresis is developed depends on various factors such as algae cell type, turbulence in the system, and fluctuating weather conditions.

Now the model was run to contrast the point and the averaged approach. The equations and parameters values stated above, including the equations for random-walk movement were used as described earlier, the irradiance used to contrast the approaches was 500 ly d$^{-1}$. The photosynthetic rate evolution was obtained and then plotted in these 2 cases. The first case was to show the photosynthetic rate evolution with time (the point approach or equation 16). The second case was the averaged approach to estimate the photosynthetic rate (equation 17). With
this, it is possible to contrast both approaches and see the correlation that arises. In the following Figure 4, both approaches are showed.

Figure 2. Photosynthetic rate evolution with time obtained by running the whole model. The curve (1) is obtained by the “point” approach, and the straight line (2) corresponds to the averaged approach (\(4.5 \times 10^{-4} \text{ moleO}_2 \text{ mgChla}^{-1} \text{ h}^{-1}\)), with irradiance of 500 ly d\(^{-1}\).
6.0 Discussion and conclusions

The validity of the model

It has to be stated that dynamics of photosynthetic rate or more specifically algae dynamics are more complicated than described by the present model. In reality, there are several more factors to take into consideration, such as photoadaptation. Thus, in order to contrast the model developed in the present study, the structure and the results of it were compared to the models developed by Harris (1977), Marra (1978), and Ross (2006). The results from Ross (2006) were the main focus since from this study several equations were used.

In this way, Harris (1977) developed a series of experiments to detail the time course of net photosynthetic rate over a period of 4 hours. The irradiances used in this study varied from 90 to 5000 μE m⁻² s⁻¹, and the model had a similar structure to the one in this study. The model of Harris (1977) shows that the photosynthetic rate rises to a maximum at 5 minutes. Afterwards, the net photosynthetic rate declines until a steady-state value is reached. Also, similar results were obtained by Marra (1978), in this study the time course of photosynthetic rate was measured at six irradiances from 5 to 100% the value of the incident irradiance on the water surface. The photosynthetic rates were decaying over time for all irradiances, and the sharpest decay occurred at the highest irradiance. Finally, the model by Ross (2006) shows similar results to the models briefly described above. In this model, the same structures were used as the ones in the present study, with the only exception of the random-walk function. Ross (2006) ran the model for 12 hours and obtained similar behaviors, the photosynthetic rate rose at the beginning and then declined again after 6 hours. In this study were also used different combinations of irradiances and growth rates to compare results.

In the present study, the structure followed in the model was very similar to the one used by Ross (2006), also it had some common items with Harris (1977) on light attenuation function used and with Marra (1978) on the averaged values. It is important to note that actual numbers or values of the results are difficult to compare since each study used different constants on each equation and the experiments developed had different characteristics. However, since the structure of each model is very similar to the one used in the present study, it is possible to
compare and contrast the behavior obtained in photosynthetic rate. That is the main goal of this study.

The time course of photosynthetic rate can be seen on Figure 2 for constant irradiances and on Figure 3 with the sinusoidal function. In the case with constant irradiances, on Figure 2, the behavior was in concordance to the ones obtained by Harris (1977), Marra (1978), and Ross (2006). The photosynthetic rate evolution presented a decay as the time increases (for $I_a$ values of 500 and 800 ly d$^{-1}$), this behavior is exactly as the tendency obtained by Ross (2006). However, when the irradiance was set to be 100 ly d$^{-1}$ the model shows the inhibition, since it starts at a low photosynthetic rate and then a peak at 0.2 h takes place, decreasing the rate afterwards, this can be due to the fact that at low irradiances the equations lose validity, also it is important to note that an irradiance of 100 ly d$^{-1}$ is the smaller value in the range showed on Table 1.

Another difference with the values obtained by Ross (2006) was on the maximum values of photosynthetic rate (for the case when the irradiances are constant), the maximum photosynthetic rates obtained in the present study were $5.7 \times 10^{-4}$, $4.8 \times 10^{-4}$, and $2.8 \times 10^{-4}$ moleO$_2$ mgChla$^{-1}$ h$^{-1}$, for the values of $I_a$ of 100, 500 and 800 ly d$^{-1}$ respectively. The maximum values obtained by Ross (2006) varied around $7 \times 10^{-4}$ moleO$_2$ mgChla$^{-1}$ h$^{-1}$. The values obtained in the present study were on the same order of magnitude, and the behavior obtained was similar.

For the second case when the irradiance varies as a sinusoidal function (see Figure 3), the photosynthetic rate behavior is also very similar to the one obtained by Ross (2006). The photosynthetic rate starts low and then has a peak, then decreasing until it approaches zero. The peaks obtained for when $I_p$ has values of 100, 500 and 800 ly d$^{-1}$, were $5.7 \times 10^{-4}$, $5.6 \times 10^{-4}$, and $1.5 \times 10^{-4}$ moleO$_2$ mgChla$^{-1}$ h$^{-1}$ respectively. These results were in concordance with the ones obtained by Ross (2006). However, when the $I_p$ is set to be 800 ly d$^{-1}$ the model seems to underestimate the photosynthetic rate, because comparing this behavior with the other two for when the peak irradiance is 100 and 500 ly d$^{-1}$ the maximum values were higher in comparison with 800 ly d$^{-1}$. This can be the effect of setting a high irradiance, since 800 ly d$^{-1}$ is beyond the range recommended in the literature, at the end this help to address the ranges in which the model is valid, irradiance ranges for this case.
The results obtained with the averaged approach when the values of $I_a$ are 100, 500 and 800 ly d\(^{-1}\), were $3.2 \times 10^{-4}$, $4.5 \times 10^{-4}$, and $0.8 \times 10^{-4}$ moleO\(_2\) mgChla\(^{-1}\) h\(^{-1}\) respectively. This result represent an under prediction by using the average approach instead of the point approach. Such values can be due to the fact that in the average approach the random-walk of particles is not considered. Finally, based in the above comparisons between the results in the present study and the results obtained by Harris (1977), Marra (1978), and Ross (2006), the behaviors obtained with the present model are in good direction, therefore, the present study proves to be acceptable to express the dynamics of photosynthetic rate when the parameters and conditions are set similar to the ones used in the literature and on this project.

*The effect of temperature, nutrient limitation, light attenuation, and random-walk of particles on photosynthetic rate*

In equation 4, it is stated that the growth rate depends directly on temperature, nutrient limitation, and light attenuation factors. Thus, if any of these variables increase the growth rate will be higher and then the photosynthetic rate will show increased values. This is also explained by Ross (2006), who showed examples, by increasing light, nutrient, or temperature factors. However, the effect of random-walk of algae particles in the water column is more difficult to address, the turbulence or chaotic behavior of particles may produce different path movements each time, which can affect other factors such as light. According to Ross (2006), more models have to be developed to be able to compare and contrast the effect of turbulence on photosynthetic rate evolution. The lack of models on phytoplankton growth dealing directly with random-walk of particles is the main issue.

*Limitation of the model*

There are some items that can be addressed as main goals to improve the model. First, the temperature and nutrient limitations factors. The water column was assumed to be well-mixed, but in reality this could not be the case. Fluctuations on temperature along the water column and variable concentration can be found on many natural water systems. In consequence, the model can be improved by introducing terms to express temperature and nutrient variations. Second, using different random-walk models is also viable, since the comparison of different results
using different approaches to count for the factor of turbulence can be essential to find the extension of its impact on photosynthetic rate.

Finally, the results obtained with the model for the example test developed in the present study must be compared to a real laboratory test, or with a real controlled water column with its own characteristics and parameters. This is essential since the model used in the present study was tested only working with pre-established parameters and variables functions. The contrast between the efficiency of the model with the example test and with a real water column can provide another item validation of the model, and at the same time, it can bring facts about which parts of the model needs to be improved.
7.0 Appendix

Code in Haskell

module Program.Types where

type Z = Double

data SimData = SimData
  { irradiance :: Double -> Double
  , optIrradiance :: Double
  , growRate :: Double
  , theta :: Double
  , waterTemp :: Double
  , nutrientConcentration :: Double
  , saturation :: Double
  , extinctionCoefficient :: Double
  , chlorophyll :: Double
  , photoperiod :: Double
  , waterDepth :: Double
  , carbonToChloroRatio :: Double
  , oxygenToCarbonRatio :: Double
  , sinkingVelocity :: Double
  , timeStep :: Double
  , diffusivity0 :: Double
  , diffusivity1 :: Double
  }

module Main where

import Data.Maybe
import System.IO
import Program.Types
import Program.Equations

-- Base test data for all test cases
testDataBase :: SimData
testDataBase = SimData
  { irradiance = const 100
  , optIrradiance = 300
  , growRate = 2
  , theta = 1.066
  , waterTemp = 25
  , nutrientConcentration = 3
  , saturation = 2
  }
, extinctionCoefficient = 0.3
, chlorophyll = 4
, photoperiod = 0.5
, waterDepth = 30
, carbonToChloroRatio = 1 / 20
, oxygenToCarbonRatio = 2.69
, sinkingVelocity = 10 ** (-3)
, timeStep = 1
, diffusivity0 = 10 ** (-6)
, diffusivity1 = 0.9 * 10 ** (-6) }

-- Test cases 0 - 5 (total 6)
testData0, testData1, testData2, testData3, testData4, testData5 :: SimData

testData0 = testDataBase { irradiance = const 100 }
testData1 = testDataBase { irradiance = const 500 }
testData2 = testDataBase { irradiance = const 800 }
testData3 = testDataBase { irradiance = \t -> 100 * (sin (\pi * t) / 12) ** 3 }
testData4 = testDataBase { irradiance = \t -> 500 * (sin (\pi * t) / 12) ** 3 }
testData5 = testDataBase { irradiance = \t -> 800 * (sin (\pi * t) / 12) ** 3 }

-- IGNORE FROM HERE
--

data StepData = StepData { stepZ :: Double, stepP :: Double }

simStep :: Int -> SimData -> Z -> IO [(Double, Double)]
simStep 0 _ _ = return []
simStep hours simData z = do
  newZ <- zStep simData z
  xs <- simStep (hours - 1) simData newZ
  return $(p simData z, z) : xs

simulation :: String -> SimData -> Int -> Maybe Handle -> IO ()
simulation name simData time mhandle = do
  let handle = fromMaybe stdin mhandle
  hPutStrLn handle >> "SIMULATION"
  hPutStrLn handle $ "Name: " ++ name
  hPutStrLn handle $ "Ia (irradiance):
  hPutStrLn handle $ "Time (seconds): " ++ show time ++ " seconds"
  hPutStrLn handle $ "Time (hours): " ++ show (time `quot` 3600) ++ " hours"
  hPutStrLn handle "Average Kg: " ++ show (kgAvg simData)
  hPutStrLn handle ""
hPutStrLn handle ">> Starting simulation...

hPutStrLn handle "P    Z"

res <- simStep time simData 0

hPutStrLn handle . unlines . map (\(p, z\) -> show p ++ "    " ++ show z) $ res

return ()

main :: IO ()
main = do
  let time = 12 * 3600
  withFile "out/data0.txt" WriteMode (\h -> simulation "Sim 0" testData0 time (Just h))
  withFile "out/data1.txt" WriteMode (\h -> simulation "Sim 1" testData1 time (Just h))
  withFile "out/data2.txt" WriteMode (\h -> simulation "Sim 2" testData2 time (Just h))
  withFile "out/data3.txt" WriteMode (\h -> simulation "Sim 3" testData3 time (Just h))
  withFile "out/data4.txt" WriteMode (\h -> simulation "Sim 4" testData4 time (Just h))
  withFile "out/data5.txt" WriteMode (\h -> simulation "Sim 5" testData5 time (Just h))

module Program.Equations where

import Control.Arrow
import Program.Types
import System.Random

e :: Double
e = exp 1

pr :: SimData -> Z -> Double
pr simData z =
  let
    aca = carbonToChloroRatio simData
    kg' = kg simData z
    h = waterDepth simData
    a = chlorophyll simData
  in
    aca * kg' * h * a

p :: SimData -> Z -> Double
p simData z =
  let
    roc = oxygenToCarbonRatio simData
    aca = carbonToChloroRatio simData
    kg' = kg simData z
  in
roc * aca * kg'

zStep :: SimData -> Z -> IO Z
zStep simData z = do
  rand <-
  (x -> fromIntegral x / fromIntegral (maxBound :: Int))
  <$> randomRIO (minBound :: Int, maxBound :: Int) :: IO Double
  let
    wp = sinkingVelocity simData
    deltaTime = timeStep simData
    r = 1 / 3
  return $ z - wp * deltaTime + rand * (2 * r ** (-1) * k simData z * deltaTime) ** (1 / 2)

k :: SimData -> Double -> Double
k simData z =
  let
    kbg = diffusivity0 simData
    km = diffusivity1 simData
    h = waterDepth simData
  in
    kbg + (km / 2) * (1 - cos ((2 * pi * z) / h))

kg :: SimData -> Z -> Double
kg simData z =
  let
    kg20 = growRate simData
    temp = waterTemp simData
    ia = irradiance simData $ (timeStep simData)
    is = optIrradiance simData
    ke' = ke simData
    -- Formula simplications
    iek = (ia * e ** (-ke simData * z)) / is
  in
    kg20 * 1.066 ** (temp - 20) * (iek * e ** (-iek + 1)) * omegaN simData

kgAvg :: SimData -> Double
kgAvg simData =
  let
    kg20 = growRate simData
    temp = waterTemp simData
    f = photoperiod simData
    h = waterDepth simData
    ke' = ke simData
    a0 = alpha0 simData
    a1 = alpha1 simData
    -- Formula simplications

\[
\text{frac} = (2.718 \times f) / (\text{ke}' \times \text{h}) \\
\text{subs} = e^{a_0} - e^{a_1} \\
\text{in} \\
k_{20} * 1.066 \times (\text{temp} - 20) \times (\text{frac} \times \text{subs}) \times \omega_N \text{simData}
\]

```haskell
ke :: SimData -> Double
ke simData =
  let
    ke' = extinctionCoefficient simData
    a = chlorophyll simData
  in
    ke' + 0.0088 * a + 0.54 * a ** (2 / 3)
```

```haskell
alpha0 :: SimData -> Double
alpha0 simData =
  let
    ia = irradiance simData $ (timeStep simData)
    is = optIrradiance simData
    ke' = ke simData
    h = waterDepth simData
  in
    (ia / is) * e ** (-ke')
```

```haskell
alpha1 :: SimData -> Double
alpha1 simData =
  let
    ia = irradiance simData $ (timeStep simData)
    is = optIrradiance simData
    ke' = ke simData
    h = waterDepth simData
  in
    (ia / is) * e ** (-ke' * 30))
```

```haskell
omegaN :: SimData -> Double
omegaN simData =
  let
    n = nutrientConcentration simData
    ksn = saturation simData
  in
    n / (ksn + n)
```
Code in Fortran90

**module** Init

```fortran
integer, parameter :: dp = kind(0.d0) ! double precision
real(dp) :: pi = 3.14159265359

! Simulation data structure
**type** :: SimData
    real(dp) :: irradiance
    real(dp) :: optIrradiance
    real(dp) :: growRate
    real(dp) :: theta
    real(dp) :: waterTemp
    real(dp) :: nutrientConcentration
    real(dp) :: saturation
    real(dp) :: extinctionCoefficient
    real(dp) :: chlorophyll
    real(dp) :: photoperiod
    real(dp) :: waterDepth
    real(dp) :: carbonToChloroRatio
    real(dp) :: oxygenToCarbonRatio
    real(dp) :: sinkingVelocity
    real(dp) :: timeStep
    real(dp) :: diffusivity0
    real(dp) :: diffusivity1
**end type** SimData

contains

!! Utility functions
!!

! Initialize random numbers
**subroutine** init_random_seed()
    integer :: i, n, clock
    integer, dimension(:,), allocatable :: seed

    call random_seed(size = n)
    allocate(seed(n))

    call system_clock(count=clock)

    seed = clock + 37 * (/ (i - 1, i = 1, n) /)
    call random_seed(put = seed)
```

26
deallocate(seed)
end

! Gets random real numbers in the given range
real(dp) function nextReal(lower, upper)
  real(dp), intent(in) :: lower, upper
  real(dp) :: r

  call random_number(r)

  nextReal = lower + (upper - lower) * r
end function nextReal

!!
!! Equations
!!

real(dp) function pr(env, z)
  type(SimData), pointer, intent(in) :: env
  real(dp), intent(in) :: z
  real(dp) :: aca, kgprime, h, a

  aca = env%carbonToChloroRatio
  kgprime = kg(env, z)
  h = env%waterDepth
  a = env%chlorophyll

  pr = aca * kgprime * h * a
end function pr

real(dp) function p(env, z)
  type(SimData), pointer, intent(in) :: env
  real(dp), intent(in) :: z
  real(dp) :: roc, aca, kgprime

  roc = env%oxygenToCarbonRatio
  aca = env%carbonToChloroRatio
  kgprime = kg(env, z)

  p = roc * aca * kgprime
end function p

real(dp) function zStep(env, z)
  type(SimData), pointer, intent(in) :: env
  real(dp), intent(in) :: z
real(dp) :: wp, deltaTime, r, kprime

wp = env%sinkingVelocity
deltaTime = env%timeStep
r = 1 / 3.0_dp
kprime = k(env, z)

zStep = z - wp * deltaTime + rand * (2 * r ** (-1) * kprime * deltaTime) ** (1 / 2.0_dp)
end function zStep

real(dp) function k(env, z)
  type(SimData), pointer, intent(in) :: env
  real(dp), intent(in) :: z
  real(dp) :: kbg, km, h

  kbg = env%diffusivity0
  km = env%diffusivity1
  h = env%waterDepth

  k = kbg + (km / 2.0_dp) * (1 - cos((2 * pi * z) / h))
end function k

real(dp) function kg(env, z)
  type(SimData), pointer, intent(in) :: env
  real(dp), intent(in) :: z
  real(dp) :: kg20, temp, ia, is, keprime, iek

  kg20 = env%growRate
  temp = env%waterTemp
  ia = env%irradiance
  is = env%optIrradiance
  keprime = ke(env)

  ! Formula simplification
  iek = (ia * exp(1.0) ** (-keprime * z)) / is

  kg = kg20 * 1.066_dp ** (temp - 20) * (iek * e ** (-iek + 1)) * omegaN(env)
end function kg

real(dp) function kgAvg(env)
  type(SimData), pointer, intent(in) :: env
  real(dp) :: k20, temp, f, h, keprime, a0, a1, frac, subs

  k20 = env%growRate
  temp = env%waterTemp
  f = env%photoperiod
  h = env%waterDepth
keprime = ke(env)
a0 = alpha0(env)
a1 = alpha1(env)

! Formula simplifications
frac = (2.718_dp * f) / (keprime * h)
subs = e ** (-a0) - e ** (-a1)

kgAvg = kg20 * 1.066_dp ** (temp - 20) * (frac * subs) * omegaN(env)
end function kgAvg

real(dp) function ke(env)
  type(SimData), pointer, intent(in) :: env
  real(dp) :: keprime, a

  keprime = env%extinctionCoefficient
  a = env%chlorophyll

  ke = keprime + 0.0088_dp * a + 0.54_dp * a ** (2 / 3_dp)
end function ke

real(dp) function alpha0(env)
  type(SimData), pointer, intent(in) :: env
  real(dp) :: ia, is, keprime, h

  ia = env%irradiance
  is = env%optIrradiance
  keprime = ke(env)
  h = env%waterDepth

  alpha0 = (ia / is) * e ** (-keprime)
end function alpha0

real(dp) function alpha1(env)
  type(SimData), pointer, intent(in) :: env
  real(dp) :: ia, is, keprime, h

  ia = env%irradiance
  is = env%optIrradiance
  keprime = ke(env)
  h = env%waterDepth

  alpha1 = (ia / is) * e ** (-keprime * 30))
end function alpha1

real(dp) function omegaN(env)
  type(SimData), pointer, intent(in) :: env
real(dp) :: n, ksn

n = env%sodiumConcentration
ksn = env%saturation

omegaN = n / (ksn + n)
end function omegaN

!!
!! Program logic
!!
subroutine simulate(env, timeSeconds)
  type(SimData), pointer, intent(in) :: env
  integer, intent(in) :: timeSeconds
  real(dp) :: z, pVal
  integer :: timeMs, elapsedTimeMs, timeStepMs, currentTimeMs

  z = 0
  pVal = 0

  timeMs = timeSeconds * 1000
  elapsedTimeMs = 0
  timeStepMs = env%simTimeStep * 1000

  open(unit = 1, file = "out/data0.txt")

  do currentTimeMs = 0, timeMs, timeStepMs
    z = zStep(env, z)
    pVal = p(env, z)
    write(1, *) pVal
  end do

  close(1)
end

end module Init

program Simulation

  use Init
  implicit none
  ! Simulation test-case
  type(SimData), pointer :: testData0
  allocate(testData0)

end
testData0%irradiance = 500
testData0%optIrradiance = 300
testData0%growRate = 2
testData0%theta = 1.066
testData0%waterTemp = 25
testData0%nirradiance = 3
testData0%saturation = 2
testData0%extinctionCoefficient = 0.3
testData0%chlorophyll = 4
testData0%photoperiod = 0.5
 testData0%waterDepth = 30
testData0%carbonToChloroRatio = 1 / 20.0
 testData0%oxygenToCarbonRatio = 2.69
 testData0%sinkingVelocity = 1E-3
 testData0%timeStep = 1
 testData0%diffusivity0 = 1E-6
 testData0%diffusivity1 = 0.9E-6

! Initialize
call init_random_seed()

! Program Logic
call simulate(testData0, 12 * 3600)

! Deallocate resources
deallocate(testData0)
end program Simulation
8.0 References


