MODELLING PRIMARY PRODUCTION

by Žarko Kovač

Part I

THEORY

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I Theory

FOREWORD

The published text is a first, out of three planned parts, which together will comprise a textbook on marine primary production. This textbook is intended to be used as educational material for students and early careers researchers in the oceanographic community. The aimed audience are students of physics that wish to learn a bit of ocean biology, as well as students of biology that wish to learn a bit of mathematical modelling, based on the approaches used in physics. It is implied that the interested reader possess basic knowledge of calculus and ocean optics, as well as rudimentary understanding of photosynthesis. The textbook is an integral part of dissemination and outreach activities within the project Fragility of Marine Photosynthesis Under Climate Change, funded by the Croatian Science Foundation. In this project we try to collect as much data as we can on marine primary production and develop new mathematical models to explain what we see in the data. If you notice any errors in the text please write to the author. Also, if you find this textbook useful, write as well!

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PHOTOSYNTHESIS IRRADIANCE FUNCTIONS

1.1 BASIC QUANTITIES

Consider a plane parallel ocean with light impinging directly overhead. Take into account the fate of photons in this ocean: some get scattered, some absorbed. Portion of the photons that get absorbed by phytoplankton pigments are used to drive photosynthesis. It is the fate of these photons we are interested in. To be more precise, our goal is to formulate a mathematical relation between the photons that find themselves below the sea surface at any time, the so called available light, and the rate of photosynthesis in the water column. Complementary to the available light, the rate of photosynthesis will undoubtedly be set by the sheer number of phytoplankton present in the water column.

Before we can even begin to quantify the rate of photosynthesis we need a measure of available light. For this we take **irradiance** I ($\mathrm{W\,m^{-2}}$), defined as light energy that in unit time passes through a unit surface [21], for now omitting the wavelength dependence. In our case this corresponds to the total energy per unit surface carried by the photons that pass a horizontal plane in our simple plane parallel ocean. Since the ocean water scatters and absorbs photons, light gets attenuated with depth and becomes a function of depth. Therefore, at any given depth z (m) we can state the following:

$$I = I(z). \tag{1.1}$$

In order to actually calculate $I(z)$ we need a light penetration model. For now, we assume $I(z)$ as given.

Knowing the underwater light filed, albeit in a rather simple form, makes our second step possible: relating light and the rate of photosynthesis. Prior to that we need to be more precise as to what is meant by the rate of photosynthesis. We define **primary production** P ($\mathrm{mg\,C\,m^{-3}\,h^{-1}}$) as the rate of inorganic carbon assimilation by phytoplankton in photosynthesis [30].

Having defined irradiance and primary production we are now in a position to formulate a relation between the two. We state this in the following form:

$$P = P(I). \tag{1.2}$$

Considering that irradiance is a function of depth (1.1), production is also a function of depth:

$$P(z) = P(I(z)). \tag{1.3}$$

This relation implicitly holds information about the physiology and the number of phytoplankton in the water column at any time. In order to model primary production we would like to have the physiological status and the concentration of phytoplankton decoupled and stated explicitly. In other words, the relation we have just stated is diagnostic, whereas we would like to have a prognostic relation.

With this goal we take Chlorophyll *a* concentration as a measure of phytoplankton **biomass** B ($\mathrm{mg\,Chl\,m^{-3}}$). This further enables us to eliminate the effect of biomass variability from (1.2) by defining **normalized production** P^B ($\mathrm{mg\,C\,(mg\,Chl)^{-1}\,h^{-1}}$) as:

$$P^B = \frac{P}{B}. \tag{1.4}$$

We now acknowledge that normalized production is a function of irradiance, dictated by the physiological status of the phytoplankton and write:

$$P^B = p^B(I). \tag{1.5}$$

The simplest of such photosynthesis light relations would be a linear one:

$$p^B(I) = \alpha^B I, \tag{1.6}$$

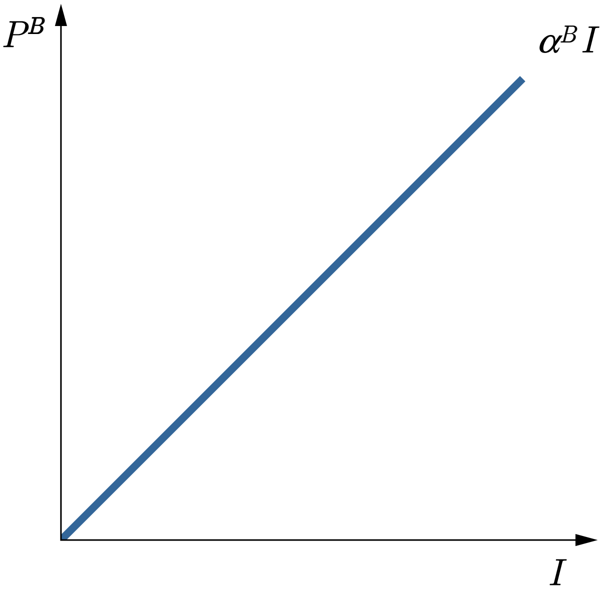

Figure 1: A linear photosynthesis irradiance function relating normalized production P^B to irradiance I. The coefficient of proportionality is the initial slope α^B.

as shown in Figure 1 [4]. The coefficient of proportionality in this relation is called the **initial slope** ($\mathrm{mg\,C\,(mg\,Chl)^{-1}\,(W\,m^{-2})^{-1}\,h^{-1}}$) and is the first physiological parameter in our model. Also, the function just presented (1.6) is our first example of a **photosynthesis irradiance function** (typically written with a lower case p^B to differentiate it from P^B).

Knowing a photosynthesis irradiance function and taking into account (1.4) we can now state our simple production model as:

$$P(z) = \alpha^B I(z) B(z), \tag{1.7}$$

where we have assumed that biomass and irradiance are depth dependent, whereas the initial slope is constant. We have therefore implicitly assumed a physiologically uniform population with vertically variable concentration. On the left hand side we have instantaneous production, whereas on the right hand side we have biomass as a state variable, initial slope as a parameter and irradiance as an argument of the photosynthesis irradiance function.

1.2 BEYOND LINEARITY

In the ocean a linear production light relation seldom holds for naturally occurring phytoplankton populations, as they are typically exposed to irradiance levels well beyond the range in which photosynthesis responds linearly to an increase in irradiance. At low irradiance a change in irradiance causes a linear response in production, which can be stated as:

$$\frac{\mathrm{d}P^B}{\mathrm{d}I} = \alpha^B, \tag{1.8}$$

and is in fact a differential form of expression (1.6). Following [6], a more realistic assumption would be to treat the rate of change in P^B with respect to I as a power series in P^B, stated mathematically as:

$$\frac{\mathrm{d}P^B}{\mathrm{d}I} = a_0 + a_1 P^B + a_2 (P^B)^2 + \ldots, \tag{1.9}$$

where a_i $(i = 1, 2, \ldots)$ are the coefficients to be determined. In this manner the linear photosynthesis irradiance function (1.6) is the solution to the previous equation with only the first parameter a_0 detained, such that (1.9) reduces to (1.8), making $a_0 = \alpha^B$.

A logical step forward would be to take into account the next factor in the power series, so that we have:

$$\frac{\mathrm{d}P^B}{\mathrm{d}I} = \alpha^B + a_1 P^B, \tag{1.10}$$

now with a_1 to be determined. This would allow the $p^B(I)$ function to have curvature (Figure 2), since the second derivative would not equal zero for $a_1 \neq 0$.

To derive the exact solution to equation (1.10) we make use of an observational fact that production saturates at high irradiance, which mathematically translates to:

$$\lim_{I \to \infty} p^B(I) = P^B_m, \tag{1.11}$$

and here we encounter a second physiological parameter called the **assimilation number** P^B_m $(\mathrm{mg\,C}\,(\mathrm{mg\,Chl})^{-1}\,\mathrm{h}^{-1})$ [30, 3]. In our current

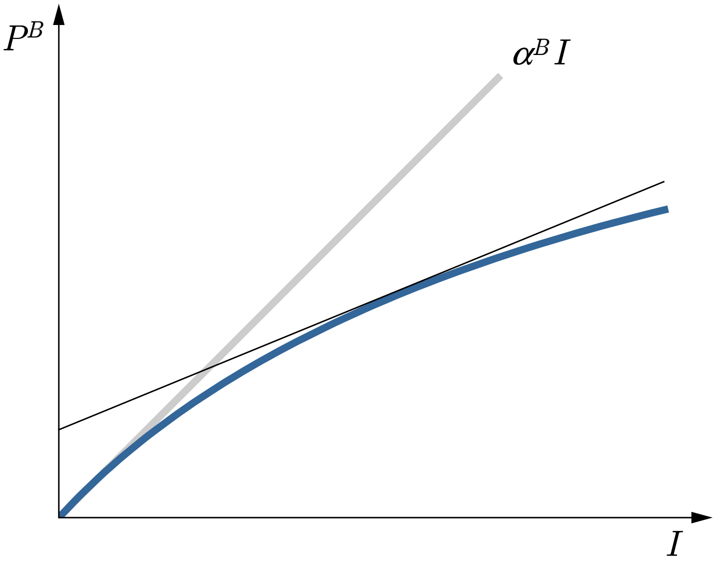

Figure 2: Curvature in the photosynthesis irradiance function exhibited with increasing irradiance.

context this condition translates to a boundary condition for equation (1.10) of the following form:

$$\lim_{I \to \infty} \frac{\mathrm{d}P^B}{\mathrm{d}I} = 0. \tag{1.12}$$

Using the previous two facts in equation (1.10) gives:

$$a_1 = -\frac{\alpha^B}{P_m^B}, \tag{1.13}$$

turning (1.10) into:

$$\frac{\mathrm{d}P^B}{\mathrm{d}I} = \alpha^B \left(1 - \frac{P^B}{P_m^B}\right). \tag{1.14}$$

Therefore, at low P^B, which occurs at low I, the response of production to a change in irradiance is highest and equals α^B. With an increase in P^B, which occurs at higher irradiance, the response declines, manifested mathematically by the decrease in $\mathrm{d}P^B/\mathrm{d}I$ (Figure 2).

Having derived equation (1.14) we now wish to solve it to obtain another photosynthesis irradiance function as its solution. By separation of variables and integration we obtain:

$$-\ln\left(P_m^B - P^B\right) = \frac{\alpha^B}{P_m^B} I + C, \tag{1.15}$$

where C is a constant of integration. Acknowledging that production ceases with no light, such that $P^B = 0$ at $I = 0$, we get:

$$C = -\ln\left(P_m^B\right), \tag{1.16}$$

transforming (1.15) into:

$$\ln\left(\frac{P_m^B - P^B}{P_m^B}\right) = -\frac{\alpha^B}{P_m^B} I. \tag{1.17}$$

After a little algebra and reintroducing the notation $P^B = p^B(I)$, yields:

$$p^B(I) = P_m^B \left(1 - \exp\left(-\alpha^B I \middle/ P_m^B\right)\right). \tag{1.18}$$

and we recognize this as the **exponential photosynthesis irradiance function** [44, 31].

The presented procedure can be extended still further [6]. For example, retaining the third term in the power series (1.9) the hyperbolic tangent photosynthesis irradiance function can be obtained:

$$p^B(I) = P_m^B \tanh\left(\alpha^B I \middle/ P_m^B\right). \tag{1.19}$$

These are but a few examples of a number of photosynthesis irradiance functions in the literature. Commonly used functions can be traced back to the following papers [4, 1, 41, 19, 31]. Extensive reviews on photosynthesis irradiance functions can for example be found in [19, 30, 13, 20]. In the literature the photosynthesis irradiance functions are also referred to as the light saturation functions, or simply as $P - I$ curves. All functions share some common properties which we now state explicitly.

1.3 PROPERTIES

The shape of the photosynthesis irradiance function expresses biophysical, biochemical and metabolic processes which regulate photosynthesis [9, 10]. Fortunately, just two parameters uniquely determine the photosynthesis irradiance function: the initial slope α^B and the assimilation number P_m^B [30, 3]. The initial slope is also referred to as photosynthetic efficiency and the assimilation number as the photosynthetic capacity [26]. Both parameters are referred to as the **photosynthesis parameters**.

Without explicitly stating the parameter values, the photosynthesis irradiance function can be written as a function of irradiance, in the following form [32]:

$$p^B(I) = p^B\left(I \mid \alpha^B, P_m^B\right), \tag{1.20}$$

highlighting the role photosynthesis parameters have. Having defining the photosynthesis irradiance function with two parameters, α^B and P_m^B, a whole family of photosynthesis irradiance functions is set. It is worth noting that the parameters are strictly positive.

The photosynthesis irradiance function itself is also positive and defined only for positive values of irradiance $I \geq 0$ [30]:

$$p^B(I) > 0. \tag{1.21}$$

For low irradiance normalized production is a linear function of irradiance with a coefficient of proportionality given by α^B, and we write:

$$\lim_{I \to 0} p^B(I) = \alpha^B I. \tag{1.22}$$

With increasing irradiance the slope of the curve drops. Finally, at high enough irradiance the slope flattens, and we have:

$$\lim_{I \to \infty} p^B(I) = P_m^B. \tag{1.23}$$

In that case light saturation takes place and normalized production stops being dependent on irradiance (Figure 3).

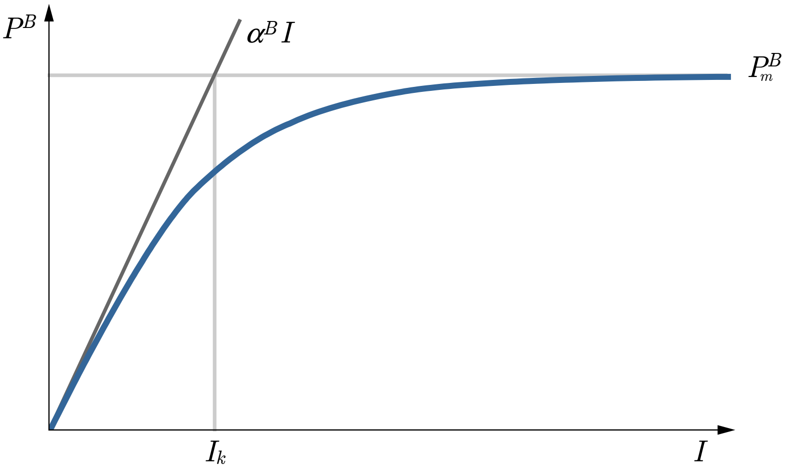

Figure 3: A typical photosynthesis irradiance function: at low light production is proportional to irradiance, as irradiance increases the response becomes nonlinear and finally for high irradiance production saturates.

Mathematically, for $I > 0$, the photosynthesis irradiance function is a strictly increasing function:

$$\frac{\mathrm{d}p^B(I)}{\mathrm{d}I} > 0, \tag{1.24}$$

with a negative second derivative:

$$\frac{\mathrm{d}^2p^B(I)}{\mathrm{d}I^2} < 0. \tag{1.25}$$

The ratio of photosynthesis parameters is called the **photoadaptation parameter**:

$$I_k = \frac{P^B_m}{\alpha^B}, \tag{1.26}$$

which is expressed in the same unit as irradiance, namely $\mathrm{W\,m^{-2}}$. In the vicinity of I_k normalized production depends on both parameters: α^B and P^B_m. With values of irradiance lower than I_k, α^B dominates, while at values higher than I_k, P^B_m dominates.

1.4 PROBLEMS

1. Derive the hyperbolic tangent photosynthesis irradiance function (1.19) by retaining the third term in the power series (1.9) and following the same procedure as used to derive the exponential photosynthesis irradiance function (1.18).

2. Below are listed some of the typical photosnthesis irradiance functions, of which some were already given in the text:

$$p^B(I) = \frac{I + P_m^B \Big/ \alpha^B - \left| I - P_m^B/\alpha^B \right|}{2 \Big/ \alpha^B}, \tag{1.27}$$

$$p^B(I) = P_m^B \frac{I}{P_m^B \Big/ \alpha^B + I}, \tag{1.28}$$

$$p^B(I) = P_m^B \frac{I}{\sqrt{I^2 + (P_m^B \Big/ \alpha^B)^2}}, \tag{1.29}$$

$$p^B(I) = P_m^B \tanh\left(\alpha^B I \Big/ P_m^B\right), \tag{1.30}$$

$$p^B(I) = P_m^B \left(1 - \exp\left(-\alpha^B I \Big/ P_m^B\right)\right). \tag{1.31}$$

By order of appearance the authors are: [4], [1], [41], [19], and finally [31]. Express all the functions using the following notation for dimensionless irradiance:

$$I^* = \frac{\alpha^B I}{P_m^B} = \frac{I}{I_k}. \tag{1.32}$$

Plot all the functions on the same graph as a function of I^*.

3. A more general form of the exponential photosynthesis irradiance function takes into account photoinhibition, a process whereby photosynthesis gets reduced at high irradiance. The mathematical expression for this function is:

$$p^B(I) = P_m^B \left(1 - \exp\left(-\alpha^B I \middle/ P_m^B\right)\right) \exp\left(-\beta^B I / P_m^B\right), \tag{1.33}$$

where β^B is the photoinhibiton parameter. Plot this function for various values of β^B starting from zero (no photoinhibiton) and gradually increasing, whilst observing the change in the shape of the function.

4. Assume that irradiance is a function of time $I = I(t)$, given by:

$$I(t) = \langle I \rangle + \delta I, \tag{1.34}$$

where $\langle I \rangle$ is the average irradiance and δI is the perturbation. Make a numerical model in which the perturbation is taken as a normally disubstituted random variable with zero mean. Set the standard deviation of the perturbation arbitrarily. Calculate production by applying (1.18) with $I(t)$ as the argument. Study the effect of light variability under low light and under high light, relative to I_k. Compare this result to the one obtained by using only average irradiance $\langle I \rangle$.

2

PRIMARY PRODUCTION PROFILE

In the sea, phytoplankton biomass and production typically have a pronounced vertical structure [24]. The structure in biomass is caused by the combined action of biological and physical processes on time scales longer than that of a day [14] while the structure of normalized production is primarily caused by available light at a given time and the physiological status of the phytoplankton population [43, 32]. The available light is determined by the optical properties of the water column and surface light, which is primarily determined by day of the year, latitude and cloud cover [21].

Having established the production-light relation in the previous chapter, we now turn our attention to the problem of modelling the vertical structure of primary production. We have already touched upon this in the previous section, namely equation (1.7), where all the basic ingredients for solving such a problem were laid out. To model the vertical profile of production, information on the following is required: biomass profile, irradiance profile and the photosynthesis irradiance function, along with the values of photosynthesis parameters. At any given time production at depth can be easily calculated by simply plugging the irradiance value at that depth into the photosynthesis irradiance function and multiplying it by biomass at the given depth. By subsequently integrating over time one can calculate daily production, taking into account that irradiance is a function of time, as well as depth. We now proceed to do just that, but first state the problem in a slightly more formal manner.

2.1 PROBLEM FORMULATION

Let the z axis, oriented downward with the origin at the surface, mark depth and let t mark time, with $t = 0$ corresponding to the timing of sunrise. Acknowledging that irradiance has both a depth and a time dependence:

$$I = I\left(z, t\right), \tag{2.1}$$

the same holds for **instantaneous normalized production at depth**:

$$P^{B}\left(z, t\right) = p^{B}\big(I\left(z, t\right)\big), \tag{2.2}$$

measured in $(\mathrm{mg\,C}\,(\mathrm{mg\,Chl})^{-1}\,\mathrm{h}^{-1})$. For generality, the explicit form of the photosynthesis irradiance function and the dependence of irradiance on depth and time will for now remain undefined. To calculate production at depth z and time t we multiply (2.2) by biomass $B\left(z, t\right)$ and obtain $P(z, t)$:

$$P\left(z, t\right) = B\left(z, t\right) p^{B}\big(I\left(z, t\right)\big), \tag{2.3}$$

referred to as the **instantaneous production at depth** $(\mathrm{mg\,C\,m^{-3}h^{-1}})$. To calculate **daily production at depth** $P_T\left(z\right)$ $(\mathrm{mg\,C\,m^{-3}})$, previous expression is integrated over time:

$$P_T\left(z\right) = \int_0^D B\left(z, t\right) p^{B}\big(I\left(z, t\right)\big)\,\mathrm{d}t, \tag{2.4}$$

with D being the time from sunrise till sunset, referred to as **daylength**. $P_T(z)$ viewed as a function of depth is the **daily production profile**.

To analytically solve the previous integral we assume that biomass does not change significantly during the course of one day, allowing it to come out the integral:

$$P_T\left(z\right) = B\left(z\right) \int_0^D p^{B}\big(I\left(z, t\right)\big)\,\mathrm{d}t, \tag{2.5}$$

which significantly simplifies the problem. In the remainder of this chapter we will continue considering biomass as time independent:

$$B(z, t) = B(z). \tag{2.6}$$

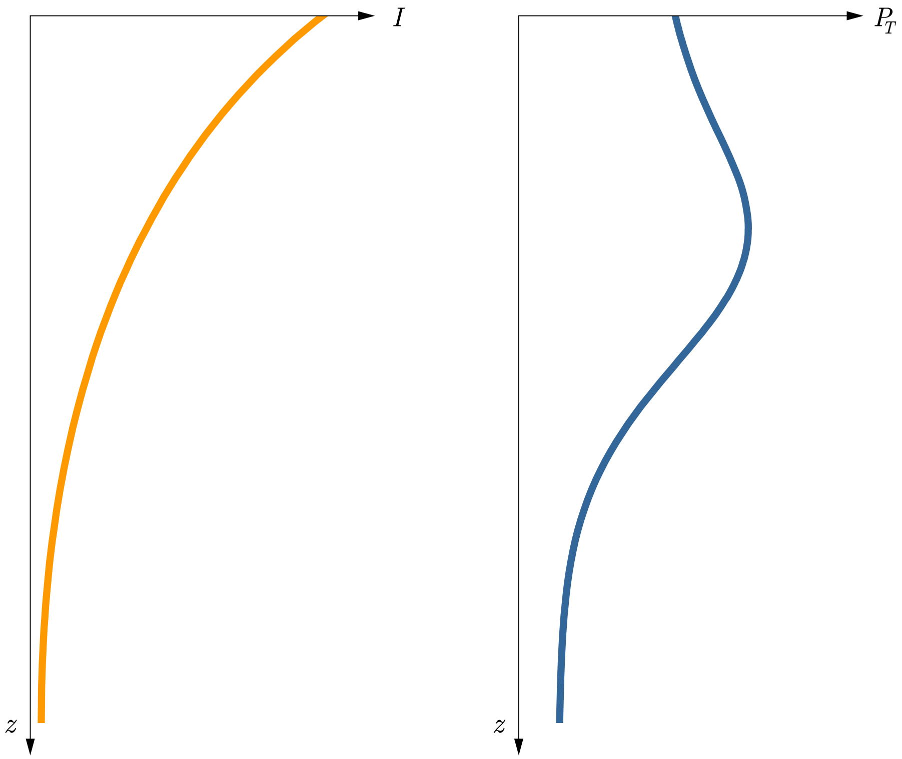

Figure 4: Sketch of the irradiance profile $I(z)$ (orange) and the daily production profile $P_T(z)$ (blue). The shape of the production profile is determined by the product of the biomass profile $B(z)$ (not shown) and the $p^B(I)$ function.

Subsequently, with biomass out of the integral, the **normalized production profile** $\left(\mathrm{mg\,C}(\mathrm{mg\,Chl})^{-1}\right)$ is obtained from (2.5) by dividing with biomass:

$$P_T^B\left(z\right) = \int_0^D p^B\left(I\left(z,t\right)\right) \mathrm{d}t, \tag{2.7}$$

which could have also been obtained by direct integration of (2.2). To solve the stated integral we need to specify irradiance as a function of depth and time, pick a photosynthesis irradiance function, and integrate over daylength. We now proceed to do just that.

2.2 UNDERWATER LIGHT FIELD

We begin by first considering a simple model for the irradiance profile. In the sea, irradiance has a pronounced vertical dependence, which is determined by the optical properties of seawater and surface radiation. The surface irradiance is simply given as a boundary condition:

$$I(0,t) = I_0(t). \tag{2.8}$$

A sine function is assumed for time dependence of surface irradiance:

$$I\left(0,t\right) = I_0^m \sin\left(\pi t/D\right), \tag{2.9}$$

where I_0^m is noon irradiance [18, 25, 21] (Figure 5). Optical properties of seawater are described by means of the **attenuation coefficient** of downward irradiance which is denoted by K (m^{-1}). It is defined as the rate of reduction of irradiance in an infinitesimally thin layer of seawater per unit depth, per unit irradiance: [21]:

$$K = -\frac{1}{I}\frac{\mathrm{d}I}{\mathrm{d}z}, \tag{2.10}$$

where the negative sign comes from the orientation of the z axis (Figure 6). As an optical medium, sea water both scatters and absorbs light, and the attenuation coefficient is the result of any combination of these two optical processes. The attenuation coefficient depends, among other things, on biomass concentration. The simplest and often used dependence of the attenuation coefficient on biomass reads:

$$K = K_w + k_B B, \tag{2.11}$$

where K_w is the seawater attenuation coefficient, which represents light attenuation processes due to scattering and absorption by pure seawater, particles and dissolved organic matter. The specific attenuation coefficient of phytoplankton k_b represents the processes of light attenuation due to absorption and scattering caused by phytoplankton [38]. The mentioned model is simple because it describes only the vertical structure of irradiance and reduces all the optical properties of sea water to the

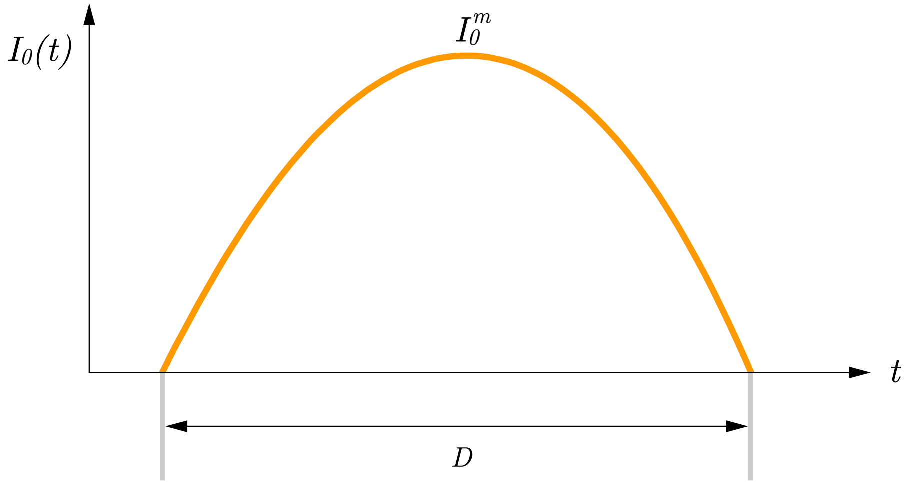

Figure 5: Idealized surface irradiance given as a sine function (2.9). Sunrise equals $t = 0$ and sunset $t = D$. Noon irradiance is given as I_0^m.

attenuation coefficient. More complex models that take into account the spatial, temporal, angular and spectral dependence of light were established [39, 8], but for pedagogical reasons for now we restrict to this model.

In case of an optically inhomogeneous water column $K = K(z)$, vertical integration of (2.10), along with the boundary condition (2.8), yields:

$$I(z,t) = I_0(t)\exp\left(-\int_0^z K(z')\,\mathrm{d}z'\right), \tag{2.12}$$

where z' is a dummy variable for integration. According to the solution (2.12) irradiance at the depth z is determined by the optical properties of the water column from the surface to that depth and the surface irradiance $I_0(t)$.

In case of an optically homogeneous water column $K \neq K(z)$, vertical integration of (2.10), along with the boundary condition (2.8), yields:

$$I(z,t) = I_0(t)\exp(-Kz). \tag{2.13}$$

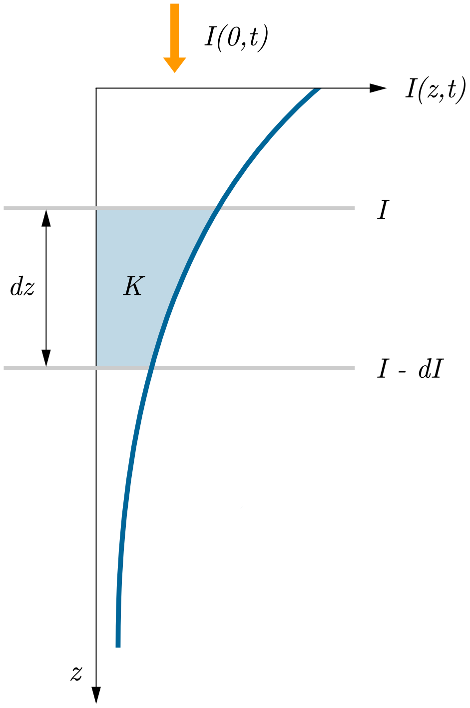

Figure 6: Water column forced by surface irradiance $I(0, t)$ and the resulting irradiance profile $I(z, t)$ (blue curve). A layer of thickness dz attenuates irradiance I by the amount dI. The attenuation coefficient K is a measure of the reduction in irradiance per unit depth per unit irradiance.

Although simple, the specified irradiance model is a commonly used model of the underwater light field when modelling primary production. The central element of the model is the attenuation coefficient, which determines the penetration depth of irradiance in the model. Taking into account the temporal dependence of surface irradiance (2.9), yields the underwater light field in our model:

$$I(z, t) = I_0^m \sin\left(\pi t / D\right) \exp\left(-Kz\right). \tag{2.14}$$

Next step in modelling the daily production profile is to use this expression in a photosynthesis irradiance function.

2.3 ANALYTICAL SOLUTION FOR THE DAILY PRODUCTION PROFILE

By taking the previous expression for irradiance (2.14) as the argument of the exponential photosynthesis irradiance function (1.18) the defining integral for daily normalized production (2.7) becomes:

$$P_T^B(z) = \int_0^D P_m^B \left[1 - \exp\left(-\alpha^B I_0^m \sin(\pi t/D) e^{-Kz} / P_m^B \right) \right] \mathrm{d}t. \tag{2.15}$$

The solution of this integral gives the amount of carbon assimilated at depth during one day per unit biomass. To solve it we begin by defining the **dimensionless noon irradiance** as:

$$I_*^m = \frac{\alpha^B I_0^m}{P_m^B} = \frac{I_0^m}{I_k}, \tag{2.16}$$

which represents the ratio of the photoadaptation parameter to noon irradiance. It simply tells us how higher noon irradiance is relative to the photoadaptation parameter. Using (2.16) translates the previous integral into:

$$P_T^B(z) = \int_0^D P_m^B \left[1 - \exp\left(- I_*^m e^{-Kz} \sin(\pi t/D) \right) \right] \mathrm{d}t. \tag{2.17}$$

To solve it, the expansion of the exponential function as an infinite sum is used:

$$\exp x = \sum_{n=0}^{\infty} \frac{x^n}{n!}. \tag{2.18}$$

After inserting this identity into the previous integral we obtain:

$$P_T^B(z) = \int_0^D P_m^B \left(1 - \sum_{n=0}^{\infty} \frac{\left(-I_*^m e^{-Kz} \sin\left(\pi t/D\right)\right)^n}{n!} \right) \mathrm{d}t, \tag{2.19}$$

which after some algebra becomes:

$$P_T^B(z) = -P_m^B \sum_{n=1}^{\infty} \frac{\left(-I_*^m e^{-Kz} \right)^n}{n!} \int_0^D \sin^n\left(\pi t/D\right) \mathrm{d}t. \tag{2.20}$$

Next step is to employ the following substitution:

$$x = \frac{\pi t}{D}, \tag{2.21}$$

by which the integral in the previous expression becomes:

$$\int_0^D \sin^n(\pi t/D)\,\mathrm{d}t = \frac{D}{\pi}\int_0^\pi \sin^n x\,\mathrm{d}x. \tag{2.22}$$

Normalized daily production is now:

$$P_T^B(z) = -P_m^B D \sum_{n=1}^{\infty} \frac{\left(-I_*^m e^{-Kz}\right)^n}{\pi \cdot n!} \int_0^\pi \sin^n x\,\mathrm{d}x. \tag{2.23}$$

The obtained integral is solved by recursive application of the following identity:

$$\int_0^\pi \sin^n x\,\mathrm{d}x = \frac{n-1}{n}\int_0^\pi \sin^{n-2} x\,\mathrm{d}x. \tag{2.24}$$

To apply it we first break the previous sum into sums over odd and even integers, to get:

$$\begin{aligned} P_T^B(z) = -P_m^B D \Bigg(&\sum_{n=1}^{\infty} \frac{\left(-I_*^m e^{-Kz}\right)^{2n-1}}{\pi(2n-1)!} \int_0^\pi \sin^{2n-1} x\,\mathrm{d}x \\ &+ \sum_{n=1}^{\infty} \frac{\left(-I_*^m e^{-Kz}\right)^{2n}}{\pi(2n)!} \int_0^\pi \sin^{2n} x\,\mathrm{d}x \Bigg). \end{aligned} \tag{2.25}$$

Going step by step, for $n = 1$ we have:

$$\int_0^\pi \sin x\,\mathrm{d}x = 2. \tag{2.26}$$

For $n = 2$ we have:

$$\int_0^\pi \sin^2 x\,\mathrm{d}x = \frac{\pi}{2}. \tag{2.27}$$

Subsequently, for several more values of n we have:

$$\text{n=3} \quad \int_0^\pi \sin^3 x \, \mathrm{d}x = \frac{2}{3} \times 2;$$

$$\text{n=4} \quad \int_0^\pi \sin^4 x \, \mathrm{d}x = \frac{3}{4} \times \frac{\pi}{2};$$

$$\text{n=5} \quad \int_0^\pi \sin^5 x \, \mathrm{d}x = \frac{4}{5} \times \frac{2}{3} \times 2;$$

$$\text{n=6} \quad \int_0^\pi \sin^6 x \, \mathrm{d}x = \frac{5}{6} \times \frac{3}{4} \times \frac{\pi}{2};$$

The interested reader can expand this still further, but for the sake of brevity we stop the explicit statement of these integrals here. For odd integers $(2n-1)$ the solution of (2.24) can be expressed as:

$$\int_0^\pi \sin^{2n-1} x \, \mathrm{d}x = 2\frac{(2n-2)!!}{(2n-1)!!}, \tag{2.28}$$

and for even integers $(2n)$ as:

$$\int_0^\pi \sin^{2n} x \, \mathrm{d}x = \pi\frac{(2n-1)!!}{(2n)!!}. \tag{2.29}$$

Combining these expressions with (2.25) we get:

$$\begin{aligned} P_T^B(z) = -P_m^B D \Bigg(& \sum_{n=1}^{\infty} \frac{2\left(-I_*^m e^{-Kz}\right)^{2n-1}}{\pi(2n-1)!} \frac{(2n-2)!!}{(2n-1)!!} \\ & + \sum_{n=1}^{\infty} \frac{\left(-I_*^m e^{-Kz}\right)^{2n}}{(2n)!} \frac{(2n-1)!!}{(2n)!!} \Bigg). \end{aligned} \tag{2.30}$$

Although cumbersome this expression is the exact solution for daily normalized production. We now proceed to write it in a more compact and comprehensive manner.

Putting the minus sing inside the brackets gives:

$$\begin{aligned}P_T^B(z) = P_m^B D \Bigg(&\sum_{n=1}^{\infty} \frac{2\left(-I_*^m e^{-Kz}\right)^{2n-1}}{\pi(2n-1)!} \frac{(2n-2)!!}{(2n-1)!!} \\ &- \sum_{n=1}^{\infty} \frac{\left(-I_*^m e^{-Kz}\right)^{2n}}{(2n)!} \frac{(2n-1)!!}{(2n)!!} \Bigg).\end{aligned} \tag{2.31}$$

We observe that the solution consists of a product of the assimilation number P_m^B, daylength D and a relatively complicated expression inside the brackets. To simplify this expression we define the $f_z\left(I_*^m e^{-Kz}\right)$ function as:

$$f_z\left(I_*^m e^{-Kz}\right) = \sum_{n=1}^{\infty} \frac{2\left(I_*^m e^{-Kz}\right)^{2n-1}}{\pi\,(2n-1)!} \frac{(2n-2)!!}{(2n-1)!!} - \sum_{n=1}^{\infty} \frac{\left(I_*^m e^{-Kz}\right)^{2n}}{(2n)!} \frac{(2n-1)!!}{(2n)!!}, \tag{2.32}$$

displayed in Figure 7 [23, 22]. This function is dimensionless and its argument is the dimensionless noon irradiance I_*^m multiplied by the e^{-Kz} term: $I_*^m e^{-Kz}$. With the given definition daily normalized production $P_T^B(z)$ now becomes:

$$P_T^B(z) = P_m^B D\, f_z\left(I_*^m e^{-Kz}\right), \tag{2.33}$$

At a given depth z, by knowing I_0^m, K, α^B and P_m^B the value of $I_*^m e^{-Kz}$ is calculated. Then the product $P_m^B D f_z(I_*^m e^{-Kz})$ gives the value of daily normalized production at depth z. To calculate production, we simply multiply (2.33) by biomass at depth $B(z)$:

$$P_T(z) = B(z) P_m^B D\, f_z\left(I_*^m e^{-Kz}\right). \tag{2.34}$$

In summary, we have derived an analytical solution for daily production at depth and now proceed to explore some of the properties of the presented solution.

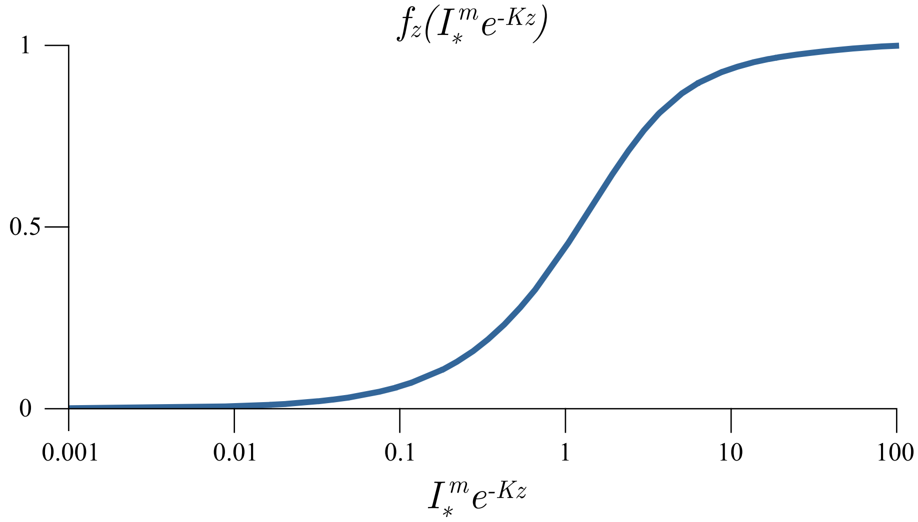

Figure 7: Dimensionless function $f_z(I_*^m e^{-Kz})$ from the analytical solution for daily production (2.33). By multiplying this function with biomass $B(z)$, the assimilation number P_m^B and daylength D daily production at depth is calculated.

2.4 PROPERTIES OF THE PRODUCTION PROFILE

In our model irradiance declines with depth, according to:

$$\frac{\mathrm{d}I}{\mathrm{d}z} = -KI. \tag{2.35}$$

Taking this into account, let us consider the change with depth of instantaneous production:

$$\frac{\mathrm{d}p^B(I(z))}{\mathrm{d}z} = \frac{\mathrm{d}p^B}{\mathrm{d}I}\frac{\mathrm{d}I}{\mathrm{d}z}. \tag{2.36}$$

The first term is positive, because the photosynthesis irradiance function is an increasing function of irradiance (1.24), whereas the second term is negative. Therefore, instantaneous production declines with depth:

$$\frac{\mathrm{d}P^B}{\mathrm{d}z} < 0. \tag{2.37}$$

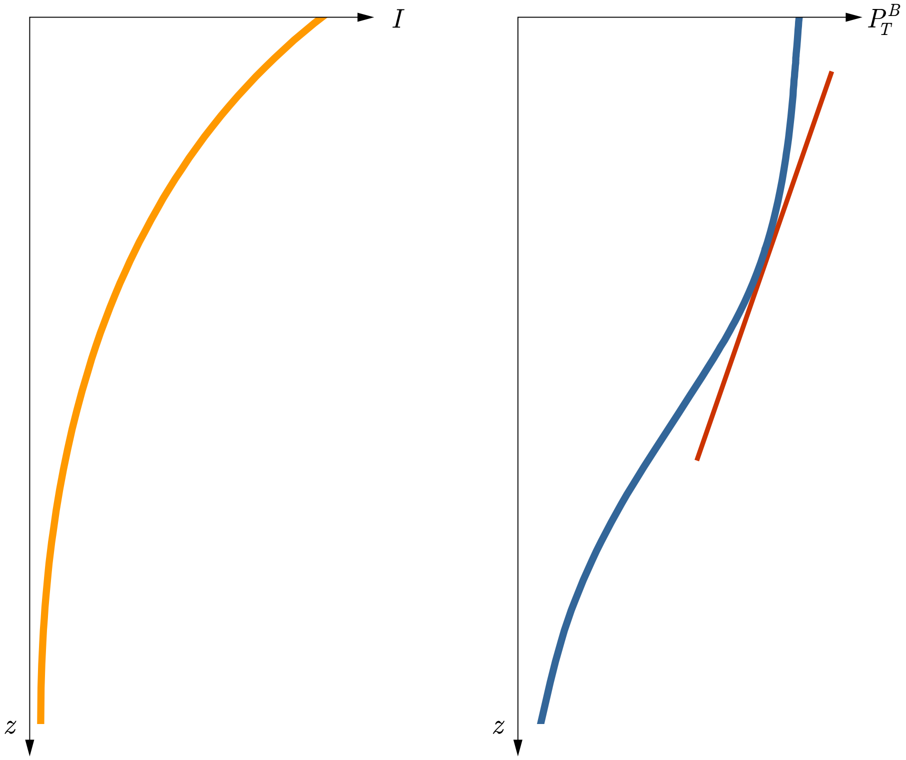

Figure 8: Decline of normalized daily production with depth (blue). Irradiance $I(z,t)$ (orange) declines exponentially with depth causing normalized production to also decline with depth, making the tangent to $P_T^B(z)$ (red line) have a negative slope with respect to depth.

Normalized daily production, being the integral over time of instantaneous production, also declines with depth (Figure 8):

$$\frac{\mathrm{d}P_T^B}{\mathrm{d}z} < 0, \tag{2.38}$$

which is easy to show by simply taking the derivative of f_z:

$$\frac{\mathrm{d}}{\mathrm{d}z} f_z(I_*^m e^{-Kz}) < 0. \tag{2.39}$$

Looking now at daily production we have:

$$P_T(z) = B(z)P_T^B(z), \tag{2.40}$$

the derivative of which with respect to depth reads:

$$\frac{\mathrm{d}P_T}{\mathrm{d}z} = \frac{\mathrm{d}B}{\mathrm{d}z}P_T^B + B\frac{\mathrm{d}P_T^B}{\mathrm{d}z}, \tag{2.41}$$

which due to (2.38) can be both positive and negative and subsequently production can acquire a subsurface maximum, in contrast to normalized production which can not.

The rate of change in daily production with respect to depth is positive if the rate of increase in biomass with depth, multiplied by normalized production, outpaces the rate of decline in normalized production multiplied by biomass:

$$\frac{\mathrm{d}B}{\mathrm{d}z}P_T^B + B\frac{\mathrm{d}P_T^B}{\mathrm{d}z} > 0. \tag{2.42}$$

By using (2.33) we derive the following condition:

$$\frac{1}{B}\frac{\mathrm{d}B}{\mathrm{d}z} > -\frac{\mathrm{d}}{\mathrm{d}z}f_z\left(I_*^m e^{-Kz}\right)\Big/ f_z\left(I_*^m e^{-Kz}\right). \tag{2.43}$$

Therefore, the relative increase in biomass with depth has to be higher than the relative decrease in production with depth. Since (2.39) is always negative the right hand side is positive.

However, it is worth noting that the given conclusions are valid for vertically uniform photosynthesis parameters, which implies a vertically uniform phytoplankton population. However, the solution (2.34) also holds in case of non-uniform photosynthesis parameters $\alpha^B = \alpha^B(z)$ and $P_m^B = P_m^B(z)$, changing the solution (2.34) to:

$$P_T(z) = B(z)P_m^B(z)D\, f_z\left(I_*^m(z)e^{-Kz}\right), \tag{2.44}$$

where now the normalized noon irradiance is also a function of depth $I_*^m(z) = \alpha^B(z)I_0^m/P_m^B(z)$. Knowing how to model the daily production profile, we now turn our attention to the biomass profile and explore how its vertical dependence is typically specified in models.

2.5 SHIFTED GAUSSIAN BIOMASS PROFILE

A prototypical function most often used to describe the biomass profile in the ocean is the Shifted Gaussian:

$$B(z) = B_0 + \frac{h}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(z - z_m)^2}{2\sigma^2}\right), \qquad (2.45)$$

where the biomass beneath the Gaussian curve is given by h, the depth of the maximum is at z_m and the width of the biomass peak is determined by σ. B_0 is the background biomass (Figure 9). The height of the peak biomass at z_m is $H = h/\sigma\sqrt{2\pi}$.

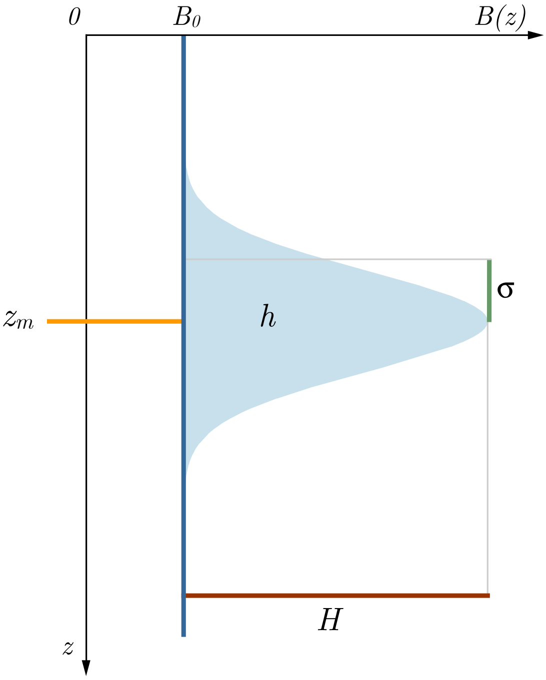

Figure 9: Sketch of the shifted Gaussian biomass profile. Integral biomass beneath the Gaussian curve is given by h (blue shaded region), depth of the maximum by z_m (orange mark) and the width of the biomass peak by σ (green line). B_0 is the background biomass (dark blue line), here equal to the surface biomass. The height above the background biomass is given by $H = h/\sigma\sqrt{2\pi}$ (red line).

The Gaussian function is suitable for describing the vertical structure of biomass and has been accepted as a standard profile for a long time [32]. It is a simple function that allows the description of the vertical structure of phytoplankton biomass for different geographical areas and seasons [29]. It has been used in many models as an initial condition for biomass, and the forms it describes are often obtained as results of numerical models [16] and measurements [34]. It is suitable for describing the structure of the deep chlorophyll maximum, which is an ubiquitous phenomenon throughout the world's oceans [7, 2].

With the shifted Gaussian biomass, daily production profile equals:

$$P_T(z) = \left[B_0 + \frac{h}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} \right) \right] P_m^B D\, f_z\left(I_*^m e^{-Kz}\right), \qquad (2.46)$$

which was obtained by direct application of (2.33) and (2.45) in (2.40). It is evident that the production profile now consists of the profile associated with the vertically uniform term in the Gaussian, namely B_0 and the vertically non-uniform term, namely the exponential component, which is dictated by three parameters: σ, z_m and h. Depending on the values of these parameters the shape of the production profile will change.

The first term will create a declining production profile, due to $B_0 \neq B(z)$, whereas the second term may create an increasing production profile. This implies that production may acquire a subsurface maximum with a shifted Gaussian biomass profile. The depth of the maximum in biomass need not coincide with the depth of maximum production. Below the maximum, both terms need to give diminishing production with increasing depth. At great depth ($z \to \infty$) normalized production and the shifted Gaussian both go to zero, but the background biomass B_0 does not. However, when multiplied to calculate daily production at great depth, their product is zero:

$$\lim_{z\to\infty} P_T(z) = B_0 P_m^B D\, f_z\left(I_*^m e^{-K\infty}\right) = 0. \qquad (2.47)$$

Having background biomass constant is an unrealistic assumption for great depth and is in contradiction with observations. A remedy to this issue was proposed by [5] in the form of a Sigmoid function, which we now explore.

2.6 SHIFTED SIGMOID BIOMASS PROFILE

The Shifted Sigmoid function proposed by [5] is of the following form:

$$B(z) = B_0\left[1 - \frac{1}{1 + \exp\big(-\sigma(z - z_m)\big)}\right], \tag{2.48}$$

where now B_0 is not the background biomass, but the surface biomass. The parameter σ dictates the slope of the biomass profile and z_m gives the mid point depth of the slope (Figure 10).

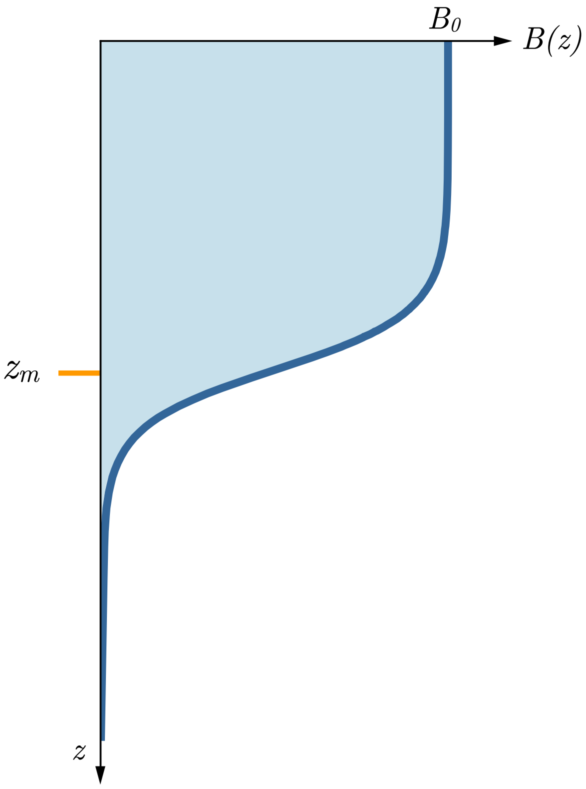

Figure 10: Sketch of the shifted Sigmoid biomass profile. Surface biomass is given by B_0, depth of the mid point by z_m (orange mark) and the slope of the biomass profile is dictated by σ. Total biomass is given by the blue shaded area.

The total biomass is now given as:

$$\int_0^\infty B(z)\,\mathrm{d}z = \frac{1}{\sigma}\ln\left(1+\exp(\sigma z_m)\right), \tag{2.49}$$

which in the limit of high σ becomes simply:

$$\lim_{\sigma\to\infty}\int_0^\infty B(z)\,\mathrm{d}z = B_0 z_m. \tag{2.50}$$

With the shifted Sigmoid daily production profile now reads:

$$P_T(z) = B_0 P_m^B D\, f_z\left(I_*^m e^{-Kz}\right)\left[1-\frac{1}{1+\exp\left(-\sigma(z-z_m)\right)}\right]. \tag{2.51}$$

Once again, in the limit of high σ we have

$$\lim_{\sigma\to\infty} P_T(z) = B_0 P_m^B D\, f_z\left(I_*^m e^{-Kz}\right), \tag{2.52}$$

which is valid from the surface up to the mid point depth z_m.

2.7 RELATION TO GROWTH MODELS

Phytoplankton growth models are dynamic models that describe the spatial-temporal distribution of biomass [45]. A typical model of this type consists of a differential equation that describes the biomass dynamics [15]. Such equations form an integral part of ecological models in which hydrodynamic equations and equations describing the rest of the ecosystem are combined [11]. In the phytoplankton growth equation, the basic term is the light saturation function, which describes the biomass growth caused by photosynthesis. The solution of the equation gives the time development of biomass which is related to primary production [17].

In order to demonstrate the connection between growth models and primary production, a simple growth model of the following form will be considered:

$$\frac{\partial}{\partial t}B(z,t)=\frac{1}{\chi}P^B(z,t)B(z,t), \tag{2.53}$$

where the normalized production is equal to $P^B(z,t)=p^B\left(I\left(z,t\right)\right)$, and χ is the carbon to chlorophyll ratio [40]. For the purposes of this demonstration, χ is constant. The equation simply states that carbon assimilated in photosynthesis increases biomass. The solution of this equation at time D (daylength) reads:

$$B(z,D)=B(z,0)\exp\left(\frac{1}{\chi}P_T^B(z)\right). \tag{2.54}$$

By writing the exponential function as a sum (2.18), previous expression becomes:

$$B(z,D)=B(z,0)+B(z,0)\left[\frac{1}{\chi}P_T^B(z)+\sum_{n=2}^{\infty}\frac{1}{n!}\left(\frac{1}{\chi}P_T^B(z)\right)^n\right]. \tag{2.55}$$

The terms in this sum have a fairly simple interpretation. Each term of the sum represents the total synthesized biomass in case the initial biomass were equal to the previous term:

$$B(z,0)\left(\frac{1}{\chi}P_T^B(z)\right)^n=\left[B(z,0)\left(\frac{1}{\chi}P_T^B(z)\right)^{n-1}\right]P_T^B(z). \tag{2.56}$$

Since primary production is the only process by which biomass accumulates in this simple growth model, all terms inside the parentheses in expression (2.55) correspond to primary production at depth z. Primary production is a process with a finite energy source that takes place in the finite dimensions of the water column, and therefore the terms in the series expansion (2.55) should converge. The exponential function is convergent over the entire set of real numbers, implying this series expansion is indeed convergent, which means that terms of higher order can be ignored in first approximation.

Keeping only the first term inside the parentheses yields a first-order approximation of the biomass at time D:

$$B(z, D) \approx B(z, 0) + \frac{1}{\chi} B(z, 0) P_T^B(z). \tag{2.57}$$

This implicitly assumes that the accumulation of biomass is dominantly caused by initial biomass, and the contribution from the newly synthesized biomass itself is negligible. The second term on the right is the daily production defined by (2.5), divided by χ. Therefore, the production profile provides a first approximation of the change in the biomass profile caused by primary production if biomass growth is allowed in the model.

Apart from the effect on biomass, there is also an effect growth has on the production profile. According to (2.54), for time-dependent biomass, the daily production profile is equal to:

$$P_T(z) = \chi B(z, 0) \left[\exp\left(\frac{1}{\chi} P_T^B(z) \right) - 1 \right], \tag{2.58}$$

which is basically the difference between the final and initial biomass, multiplied by χ. We notice that there is an additional parameter χ in this expression. How big an influence χ has on the production profile in the growth model can be easily analysed by expressing the exponential function in the previous expression as a sum and rearranging:

$$P_T(z) = \left[1 + \sum_{n=2}^{\infty} \frac{1}{n! \chi^{n-1}} \left(P_T^B(z) \right)^{n-1} \right] B(z, 0) P_T^B(z). \tag{2.59}$$

The influence of χ on the production profile is manifested only as a second-order factor. The conclusion is that the two models give an equivalent production profile in first approximation.

2.8 PROBLEMS

1. Assume the attenuation of irradiance with depth is described by the following equation:

$$\frac{\mathrm{d}I}{\mathrm{d}z} = -KI, \tag{2.60}$$

where K is the diffuse attenuation coefficient for downwelling irradiance and the z axes is positive downwards. Taking the surface irradiance just below the sea surface ($z = 0$) as known I_0 derive the solution for the irradiance profile (2.13). Subsequently use the irradiance profile to calculate $P^B(z)$ first by means of (1.6) and second by means of (1.18). Plot the two results and their difference.

2. Assume the attenuation of irradiance with depth is again described by (2.60). Restate this expression as

$$\mathrm{d}I = -KI\,\mathrm{d}z, \tag{2.61}$$

and use it in (1.14) to derive $P^B(z)$. The result should match the one obtained in the first problem, where the irradiance profile is directly used in the exponential photosynthesis irradiance function.

3. Use the photosynthesis irradiance functions given in Problem 2 of Chapter 2 in a numerical model and solve for the daily production profile for each. The irradiance profile is given by (2.14) in each case. Compare the results by plotting the numerical solutions as a function of I_*^m in the same manner that the analytical solution (2.33) is presented in Figure 7.

4. Build a numerical model in which the effect of biomass on the attenuation of irradiance with depth is taken into account with (2.11) such that the irradiance profile is given by (2.12). Calculate the daily production profile in this case and compare it to the analytical solution in which $K = K_w$. Use multiple values for k_B to explore its effect on the shape of the daily production profile.

5. Employ the shifted Gaussian in calculation of the daily production profile by using (2.46). Based on (2.41) state the condition for the maximum production at depth and derive the condition that is satisfied at that depth. Express the first derivative with respect to depth of the daily production profile in case of the shifted Gaussian and following (2.41) consider under which scenario does the production profile decrease/increase with depth. Explore the effect depth z_m and width of the maximum σ have on the shape of the production profile and the depth of the maximum in daily production.

6. Build a model of the daily production profile using the shifted Sigmoid (2.48) as the model for the biomass profile. For the normalized daily production profile use expression (2.33). Explore the effect σ and z_m have on the shape of the biomass profile as well as the production profile.

7. Build a numerical model that solves equation (2.53). Explore how the biomass profiles evolves under variable surface irradiance given by (2.14) and contrast it with the evolution over time under constant surface irradiance equal to the average daily irradiance $I_0^m \pi/2$.

3

WATERCOLUMN PRODUCTION

Having described the vertical structure in biomass and production we are now in a position to calculate the total amount of carbon assimilated in photosynthesis in the entire water column. This quantity is called watercolumn production and is of paramount importance in oceanography. In standard oceanographic practice watecolumn production is quantified by the amount of carbon assimilated during the day in the photic zone. Measurements of watercolumn production have been carried out at sea after the introduction of the radioactive carbon method in 1952 by Steeman Nielsen [42]. Since then, the development of mathematical models of watercolumn production has been of high interest to oceanographers.

In modern times remotely sensed data are merged with state of the art models to calculate global estimates of marine primary production. The backbone of all such models is the functional relation between the rate of carbon assimilation and irradiance: the photosynthesis irradiance function. While the various models differ in precise detail they all share the same structure and in this chapter we explore this structure.

We build upon the previous chapter where we have shown how to calculate daily production at depth. We proceed to extend the model and demonstrate how to calculate watercolumn production. The canonical solution for unifrom biomass [36] is presented along with the solution for mixed layer production. The assumption of uniform biomass is relaxed and exact solutions for watercolumn production with a shifted Gaussian biomass and a general solution for arbitrary biomass are derived.

3.1 PROBLEM FORMULATION

We start by defining **watercolumn production** $P_{Z,T}$ ($\mathrm{mg\,C\,m^{-2}}$) as the amount of carbon assimilated in photosynthesis in the water column during one day per square meter [36, 21]. In the notation of the model developed thus far we have:

$$P_{Z,T} = \int\limits_{0}^{\infty} \int\limits_{0}^{D} P(z,t)\,\mathrm{d}t\,\mathrm{d}z. \tag{3.1}$$

The notation $P_{Z,T}$ is also used when the upper limit over depth is not infinity. By expressing instantaneous production using (2.3) we have:

$$P_{Z,T} = \int\limits_{0}^{\infty} \int\limits_{0}^{D} B\left(z,t\right) p^{B}\left(\, I\left(z,t\right)\,\right) \mathrm{d}t\,\mathrm{d}z. \tag{3.2}$$

Further assuming time independent biomass and grouping the terms based on the definition of the normalized production profile (2.5) we have:

$$P_{Z,T} = \int\limits_{0}^{\infty} B\left(z\right) \left(\int\limits_{0}^{D} p^{B}\left(\, I\left(z,t\right)\,\right) \mathrm{d}t \right) \mathrm{d}z. \tag{3.3}$$

where the term inside the brackets is recognized as $P_T^B(z)$. Thus formulated, watercolumn production equals the vertical integral of the daily production profile $P_T(z)$ (Figure 11), that is, the vertical integral of the product between biomass $B(z)$ and normalized production $P_T^B(z)$ profiles:

$$P_{Z,T} = \int\limits_{0}^{\infty} B(z) P_T^B(z)\,\mathrm{d}z = \int\limits_{0}^{\infty} P_T(z)\,\mathrm{d}z. \tag{3.4}$$

Here we observe the importance of the production profile as it the central element in the calculation of watercolumn production.

Integration of $P(z,t)$ can also be done vertically first and then over time, a procedure that will shortly be used to find an analytical solution

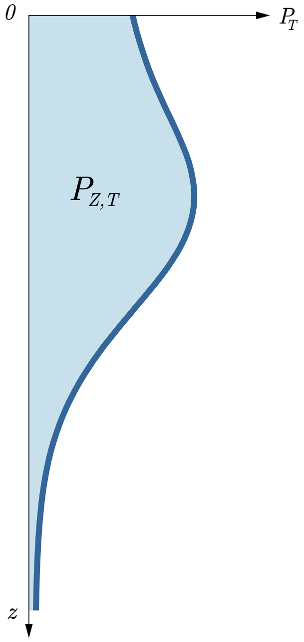

Figure 11: Sketch of watercolumn production $P_{Z,T}$ (light blue area) as the vertical integral of the daily production profile $P_T(z)$ (thick blue curve).

for watercolumn production. In this case, the vertical integral of $P(z,t)$ is the **instantaneous watercolumn production** $P_{Z,T}$ ($\mathrm{mg\,C\,m^{-2}\,h^{-1}}$):

$$P_Z(t) = \int_0^\infty B(z,t)\, p^B\big(\, I(z,t)\,\big)\, \mathrm{d}z. \tag{3.5}$$

With this definition, watercolumn production becomes an integral over daylength of instantaneous watercolumn production:

$$P_{Z,T} = \int_0^D P_Z(t)\, \mathrm{d}t. \tag{3.6}$$

The obtained expression is equal to (3.3). Having laid out the basic definitions, we now proceed to solve for $P_{Z,T}$ analytically, following [36].

3.2 ANALYTICAL SOLUTION FOR WATERCOLUMN PRODUCTION

Thus far, using the exponential photosynthesis irradiance function (1.18) and exponentially declining sinusoidal irradiance (2.13), yielded the daily normalized production profile (2.15), which we now multiply by biomass $B(z)$ to obtain:

$$P_{Z,T} = \int_0^\infty \int_0^D B(z) P_m^B \left[1 - \exp\left(-\alpha^B I_0^m \sin(\pi t/D) e^{-Kz} / P_m^B \right) \right] \mathrm{d}t \, \mathrm{d}z, \quad (3.7)$$

as the integral that needs to be solved to get watercolumn production. We begin with the simplest case, by first assuming uniform biomass:

$$B(z) = B, \quad (3.8)$$

and subsequently change the order of integration, in line with the interpretation provided in (3.6). Now we have:

$$P_{Z,T} = B P_m^B \int_0^D \int_0^\infty \left(1 - \exp\left(-\alpha^B I_0^m \sin(\pi t/D) e^{-Kz} / P_m^B \right) \right) \mathrm{d}z \, \mathrm{d}t, \quad (3.9)$$

where we have extracted B and P_m^B outside the integrals, both being independent of depth and time. With a change of variables:

$$x = I_*^m \sin(\pi t/D) e^{-Kz}, \quad (3.10)$$

the vertical integral in the expression (3.9) becomes a table integral and its solution reads:

$$\int_0^\infty \left[1 - \exp\left(-I_*^m \sin(\pi t/D) e^{-Kz} \right) \right] \mathrm{d}z = \frac{1}{K} \sum_{n=1}^\infty \frac{(-1)^{n+1}}{n \cdot n!} \left(I_*^m \sin\left(\pi t/D\right) \right)^n . \quad (3.11)$$

The obtained expression multiplied by $B P_m^B$ gives the instantaneous watercolumn production $P_Z(t)$:

$$P_Z(t) = \frac{B P_m^B}{K} \sum_{n=1}^\infty \frac{(-1)^{n+1}}{n \cdot n!} \left(I_*^m \sin\left(\pi t/D\right) \right)^n . \quad (3.12)$$

By inserting (3.11) into (3.9) we get:

$$P_{Z,T} = \int_0^D \frac{BP_m^B}{K} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n \cdot n!} \Big(I_*^m \sin\left(\pi t/D\right) \Big)^n \,\mathrm{d}t. \tag{3.13}$$

Here we recognize the same integral as in (2.23) which is again solved by the application of the recursive relation (2.24), yielding:

$$\begin{aligned} P_{Z,T} = \frac{BP_m^B D}{K} \Bigg[& \sum_{n=1}^{\infty} \frac{2\left(I_*^m\right)^{2n-1}}{\pi\left(2n-1\right)\left(2n-1\right)!} \frac{(2n-2)!!}{(2n-1)!!} \\ & - \sum_{n=1}^{\infty} \frac{\left(I_*^m\right)^{2n}}{2n\left(2n\right)!} \frac{(2n-1)!!}{(2n)!!} \Bigg]. \end{aligned} \tag{3.14}$$

The presented solution is the analytical solution for daily watercolumn production. For unit biomass it is also a solution for normalized production. The expression in parentheses in (3.14) depends only on I_*^m and can be denoted as a function $f(I_*^m)$, similar to (2.31), in order to make the solution less cumbersome. With this notation, previous expression becomes simply:

$$P_{Z,T} = \frac{BP_m^B D}{K} f(I_*^m). \tag{3.15}$$

Graph of $f(I_*^m)$ is given in Figure 12. It is clear from the given solution that daily watercolumn production has a linear dependence on biomass B and daylength D. Nonlinear dependencies arise with respect to photosynthesis parameters α^B and P_m^B, and irradiance I_0^m. It is necessary to emphasize the inverse proportionality of watercolumn production and the attenuation coefficient K.

Since it was published, solution [36] has seen many applications: in the study of the interaction of mixing depth and primary production [37], in the context of Sverdrup's critical depth theory [27], in the assessment of primary production via satellites [33], as elements of climate models [33] and for explaining the dynamics of high nutrient - low chrollophyll zones [28, 35].

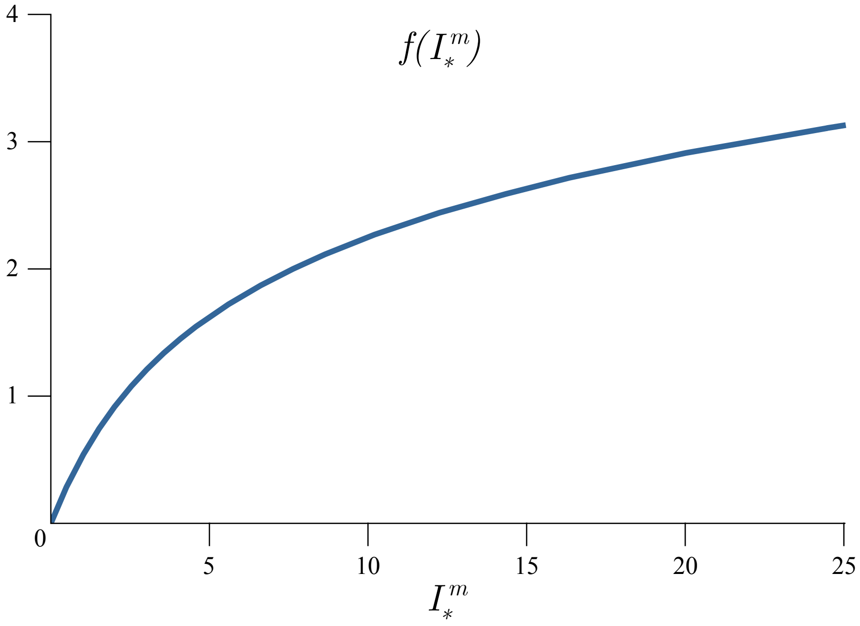

Figure 12: Dimensionless function $f(I_*^m)$ from the analytical solution for daily watercolumn production (3.15) with uniform biomass.

The assumption of an infinitely deep water column is obviously not met in the ocean. However, due to a decline in irradiance with depth, and subsequently production, the contribution of production at any given depth to watercolumn production declines with depth. Due to this, keeping infinity as the limit in the vertical integration for the open ocean is a reasonable assumption and does not lead to grave error, provided the ocean is well mixed.

Typically, the upper ocean layer is well mixed and uniform in properties, therefore the assumption of uniform biomass holds. This layer is historically referred to as the mixed layer [12]. Below the mixed layer biomass tends to be stratified, therefore the assumption of uniform biomass breaks down. We now proceed to demonstrate how to calculate mixed layer production and subsequently watercolumn production with a shifted Gaussian biomass profile.

3.3 MIXED LAYER PRODUCTION

Consider a layer in which active mixing takes place extending from the surface up to depth Z_m (Figure 13), referred to as the **mixed layer depth**. Production taking place in this layer is referred to as the **mixed layer production** ($\mathrm{mg\,C\,m^{-2}}$), stated mathematically as:

$$P_{Z_m,T} = \int_0^{Z_m} \int_0^{D} P(z,t)\,\mathrm{d}t\,\mathrm{d}z. \tag{3.16}$$

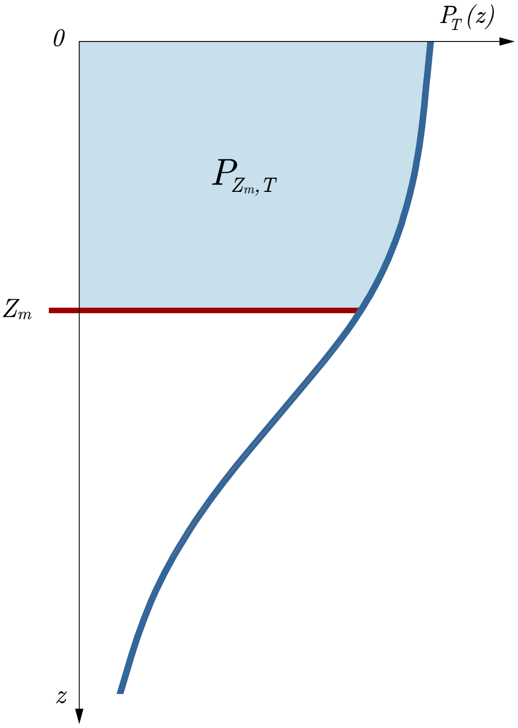

Figure 13: Sketch of mixed layer production $P_{Z_m,T}$ (light blue area) as the vertical integral of the daily production profile $P_T(z)$ (thick blue curve) from the surface $z = 0$ to the mixed layer depth Z_m (red line).

Following (3.7) the previous integral translates to:

$$P_{Z_m,T} = BP_m^B \int_0^{Z_m} \int_0^D \left[1 - \exp\left(-\alpha^B I_0^m \sin(\pi t/D) e^{-Kz} / P_m^B \right) \right] \mathrm{d}t\, \mathrm{d}z, \quad (3.17)$$

where we acknowledge biomass as being uniform in the mixed layer. To solve this integral we first observe the following:

$$P_{Z_m,T} = \int_0^{Z_m} P_T \, \mathrm{d}z = \int_0^{\infty} P_T \, \mathrm{d}z - \int_{Z_m}^{\infty} P_T \, \mathrm{d}z. \quad (3.18)$$

The first integral on the right hand side calculates watercolumn production, whereas the second one calculates production of the layer below Z_m. Given that biomass is uniform, we observe that the second integral can be interpreted as the production of an infinitely deep water column forced with surface irradiance equal to:

$$I(Z_m, t) = I_0^m e^{-KZ_m} \sin(\pi t/D), \quad (3.19)$$

as shown in Figure 14. Noon irradiance at mixed layer depth equals $I_0^m e^{-KZ_m}$. If in place of I_0^m in the expression for surface irradiance (2.9) we use $I_0^m e^{-KZ_m}$, solution (3.15) yields daily production of the layer below Z_m:

$$\int_{Z_m}^{\infty} P_T(z)\, dz = \frac{BP_m^B D}{K} f(I_*^m e^{-KZ_m}), \quad (3.20)$$

again shown in Figure 14, where in place of I_*^m we now have $I_*^m e^{-KZ_m}$. By inserting (3.15) and (3.20) into (3.18) we obtain:

$$P_{Z_m,T} = \frac{BP_m^B D}{K} \left[f\left(I_*^m\right) - f\left(I_*^m e^{-KZ_m}\right) \right], \quad (3.21)$$

as the solution for daily mixed layer production. This solution could have also been found by direct integration of (3.17) following the procedure used to solve for $P_{Z,T}$.

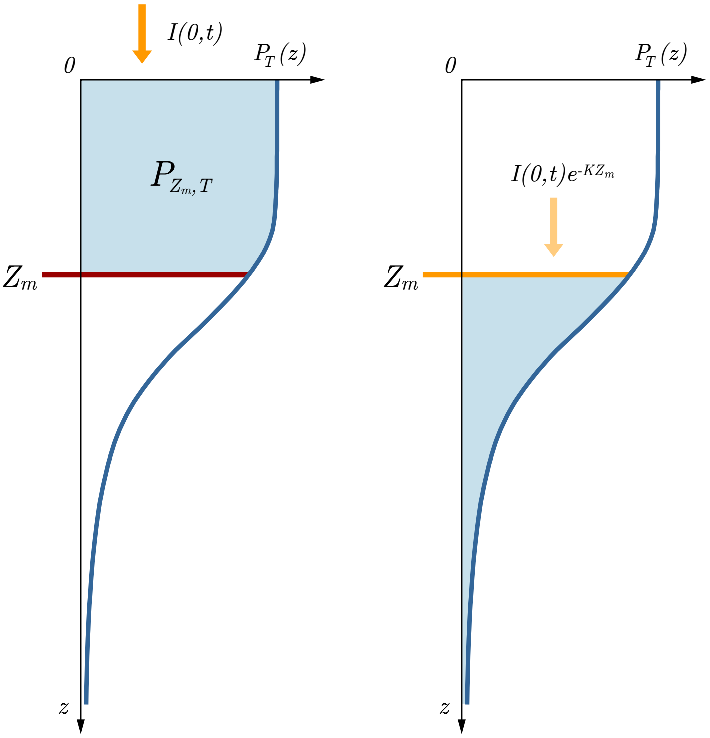

Figure 14: Mixed layer production $P_{Z_m,T}$ depicted as the difference between watercolumn production $P_{Z,T}$, forced by $I(0,t)$ and the production of the portion of the water column below the mixed layer, forced by $I(0,t)e^{-KZ_m}$.

3.4 WATERCOLUMN PRODUCTION WITH A SHIFTED GAUSSIAN BIOMASS PROFILE

The previously presented solution for the normalized production profile (2.33) can be used to solve integral (3.1) in a more general case when the biomass profile is described by the shifted Gaussian function (2.45). The contribution to watercolumn production from the constant term in the Gaussian B_0 is given by (3.15). Therefore, only the contribution from the vertically dependent term has to be found.

Following (3.4) watercolumn production equals the product of the biomass profile and the normalized production profile. Acknowledging the shifted Gasussian (2.45) in place of $B(z)$, we are interested in the solution of the following integral:

$$P_{Z,T} = \int_0^\infty \left[B_0 + \frac{h}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} \right) \right] P_m^B D\, f_z\left(I_*^m e^{-Kz}\right) \mathrm{d}z. \quad (3.22)$$

The contribution to watercolumn production from the uniform biomass term B_0 is already known, namely (3.15), therefore:

$$P_{Z,T} = \frac{B_0 P_m^B D}{K} f(I_*^m) + \int_0^\infty \frac{h}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} \right) P_m^B D f_z\left(I_*^m e^{-Kz}\right) \mathrm{d}z. \quad (3.23)$$

We label the integral on the right hand side as:

$$\Delta P_{Z,T} = \frac{P_m^B D h}{\sigma\sqrt{2\pi}} \int_0^\infty \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} \right) f_z\left(I_*^m e^{-Kz}\right) \mathrm{d}z, \quad (3.24)$$

and it gives the contribution to watercolumn production due to the non-uniformity of the Gaussian profile. For notational simplicity, the f_z function (2.32) will be written as:

$$f_z\left(I_*^m e^{-Kz}\right) = \sum_{n=1}^{\infty} M(n)\, e^{-(2n-1)Kz} - \sum_{n=1}^{\infty} N(n)\, e^{-2nKz}, \quad (3.25)$$

where $M(n)$ and $N(n)$ contain the terms that do not depend on z. With this notation, the previous integral becomes:

$$\begin{aligned} \Delta P_{Z,T} = \frac{P_m^B D h}{\sigma\sqrt{2\pi}} \int_0^\infty \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} \right) \times \\ \left[\sum_{n=1}^{\infty} M(n)\, e^{-(2n-1)Kz} - \sum_{n=1}^{\infty} N(n)\, e^{-2nKz} \right] \mathrm{d}z. \end{aligned} \quad (3.26)$$

In the obtained expression the sum and the integral can change places:

$$\begin{aligned}\Delta P_{Z,T} = P_m^B D \frac{h}{\sigma\sqrt{2\pi}} \Bigg[& \sum_{n=1}^{\infty} M(n) \int_0^{\infty} \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} - (2n-1)Kz\right) \mathrm{d}z \\ & - \sum_{n=1}^{\infty} N(n) \int_0^{\infty} \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} - 2nKz\right) \mathrm{d}z \Bigg].\end{aligned} \tag{3.27}$$

The same form of the integral appears in both terms, with a minor difference only in the $2n$ term in the place of $2n-1$ term in the second integral. We will first demonstrate how to solve this integral in case of odd integers, namely:

$$\int_0^{\infty} \exp\left(-\frac{(z-z_m)^2}{2\sigma^2} - (2n-1)Kz\right) \mathrm{d}z. \tag{3.28}$$

As a starting point we rewrite the argument of the exponential function into the following form:

$$-\frac{(z-z_m)^2}{2\sigma^2} - (2n-1)Kz = -\frac{1}{2\sigma^2}(z^2 - 2(z_m - (2n-1)\sigma^2 K)z + z_m^2). \tag{3.29}$$

We then introduce the following label:

$$z_m - (2n-1)\sigma^2 K = z_{2n-1}, \tag{3.30}$$

and after some algebra obtain:

$$\begin{aligned}-\frac{(z-z_m)^2}{2\sigma^2} - (2n-1)Kz &= -\frac{1}{2\sigma^2}(z^2 - 2z_{2n-1}z + z_m^2) \\ &= -\frac{1}{2\sigma^2}(z^2 - 2z_{2n-1}z + z_{2n-1}^2 - z_{2n-1}^2 + z_m^2) \\ &= -\frac{1}{2\sigma^2}(z^2 - 2z_{2n-1}z + z_{2n-1}^2) + \frac{1}{2\sigma^2}(z_{2n-1}^2 - z_m^2) \\ &= -\frac{1}{2\sigma^2}(z - z_{2n-1})^2 + \frac{1}{2\sigma^2}(z_{2n-1}^2 - z_m^2).\end{aligned} \tag{3.31}$$

Inserting this expression back into (3.28) yields:

$$\begin{aligned}\int_0^\infty \exp\left(-\frac{(z-z_m)^2}{2\sigma^2}-(2n-1)Kz\right)\mathrm{d}z = \\ \exp\left(\frac{z_{2n-1}^2-z_m^2}{2\sigma^2}\right)\int_0^\infty \exp\left(-\frac{(z-z_{2n-1})^2}{2\sigma^2}\right)\mathrm{d}z.\end{aligned} \tag{3.32}$$

Employing the following change of variables:

$$x=\frac{z-z_{2n-1}}{\sqrt{2}\sigma}, \tag{3.33}$$

the integral on the right hand side becomes:

$$\int_0^\infty \exp\left(-\frac{(z-z_{2n-1})^2}{2\sigma^2}\right)\mathrm{d}z=\sqrt{2}\sigma\int_{z_{2n-1}}^\infty \exp(-x^2)\,\mathrm{d}x. \tag{3.34}$$

Now again, the integral on the right hand side of this expression can be split into two integrals:

$$\int_{z_{2n-1}}^\infty \exp(-x^2)\,\mathrm{d}x=\int_{z_{2n-1}}^0 \exp(-x^2)\,\mathrm{d}x+\int_0^\infty \exp(-x^2)\,\mathrm{d}x, \tag{3.35}$$

The solutions to these integrals are given by the error function $\Phi(x)$. Finally the solution to (3.34) is:

$$\int_0^\infty \exp\left(-\frac{(z-z_{2n-1})^2}{2\sigma^2}\right)\mathrm{d}z=\sigma\sqrt{\frac{\pi}{2}}\left(1+\Phi\left(\frac{z_{2n-1}}{\sqrt{2}\sigma}\right)\right). \tag{3.36}$$

The solution for even integers is identical with the only difference that $2n$ appears in the place of $2n-1$.

At last the overall solution to (3.27) is:

$$\begin{aligned}\Delta P_{Z,T} =& P_m^B D \frac{h}{2} \times \\ & \left[\sum_{n=1}^{\infty} \exp\left(\frac{z_{2n-1}^2 - z_m^2}{2\sigma^2}\right) \frac{2\left(I_*^m\right)^{2n-1}}{\pi\,(2n-1)!} \frac{(2n-2)!!}{(2n-1)!!} \left(1 + \Phi\left(\frac{z_{2n-1}}{\sqrt{2}\sigma}\right)\right) \right. \\ & \left. - \sum_{n=1}^{\infty} \exp\left(\frac{z_{2n}^2 - z_m^2}{2\sigma^2}\right) \frac{\left(I_*^m\right)^{2n}}{(2n)!} \frac{(2n-1)!!}{(2n)!!} \left(1 + \Phi\left(\frac{z_{2n}}{\sqrt{2}\sigma}\right)\right) \right],\end{aligned} \tag{3.37}$$

where the $\Delta P_{Z,T}$ depends explicitly on the values of h, z_m, σ, α^B, P_m^B, I_0^m and D. The derived mathematical expression gives the quantity of carbon assimilated during one day per meter squared of the ocean surface, by phytoplankton distributed vertically according to the shifted Gaussian function (2.45), shown in Figure 9.

The shifted Gaussian is flexible enough to describe various features in the measured chlorophyll profiles and therefore this solution covers a wide range of situations encountered in the field. That flexibility is achieved by altering the parameters of the function, namely: B_0, z_m, σ and h. The disadvantage is that in addition to the six basic quantities: α^B, P_m^B, B_0, I_0^m, D and K, which appear in the canonical solution, the solution for the shifted Gaussian has three more: z_m, σ and h. To apply the solution, the values of these quantities need to be specified.

The solution was derived with the help of the solution for the nominalized production profile (2.33), which reduced (3.1), an integral over time and depth, to an integral over depth alone. This enabled the vertical integration of (3.22) to be carried out. However, there is a deeper connection between the analytical solution for watercolumn production with uniform biomass (3.15) and the production profile (2.33), which makes this possible. We now explore this connection and provide another way to derive the solution for the production profile, which will subsequently be used to derive a general solution for watercolumn production.

3.5 ALTERNATIVE DERIVATION OF THE PRODUCTION PROFILE

We begin by considering daily production in the layer extending from Z_1 to Z_2, such that $Z_1 < Z_2$, assuming uniform biomass (Figure 15). According to the notation used thus far, the production of an arbitrary layer that extends between depths Z_1 and Z_2 is equal to:

$$P_{Z_1,Z_2,T} = \int_{Z_1}^{Z_2} P_T(z)\,\mathrm{d}z = \int_{Z_1}^{\infty} P_T(z)\,\mathrm{d}z - \int_{Z_2}^{\infty} P_T(z)\,\mathrm{d}z. \tag{3.38}$$

Following a similar reasoning to the one presented in the derivation of the solution for mixed layer production, we first observe that light at depth Z_i equals $I(Z_i, t) = I_0^m e^{-KZ_i} \sin(\pi t/D)$. Therefore, if in place of Z_m in expression (3.20) we use Z_i, the solution still holds and we have:

$$\int_{Z_i}^{\infty} P_T(z)\,dz = \frac{BP_m^B D}{K} f(I_*^m e^{-KZ_i}), \tag{3.39}$$

where the $f(I_*^m e^{-Kz})$ reads:

$$\begin{aligned} f(I_*^m e^{-Kz}) = &\sum_{n=1}^{\infty} \frac{2\left(I_*^m e^{-Kz}\right)^{2n-1}}{\pi\,(2n-1)\,(2n-1)!}\,\frac{(2n-2)!!}{(2n-1)!!} \\ &- \sum_{n=1}^{\infty} \frac{\left(I_*^m e^{-Kz}\right)^{2n}}{2n\,(2n)!}\,\frac{(2n-1)!!}{(2n)!!}, \end{aligned} \tag{3.40}$$

and should not be confused with the f_z function from the solution for daily normalized production (2.32). By inserting (3.39) into (3.38) we get:

$$P_{Z_1,Z_2,T} = \frac{BP_m^B D}{K}\left[f\left(I_*^m e^{-KZ_1}\right) - f\left(I_*^m e^{-KZ_2}\right)\right], \tag{3.41}$$

According to expression (3.41), the solution for production of an arbitrary layer is equal to the production below depth Z_1 minus the production below depth Z_2. It is easy to check that in the case of $Z_1 = 0$ and $Z_2 = \infty$,

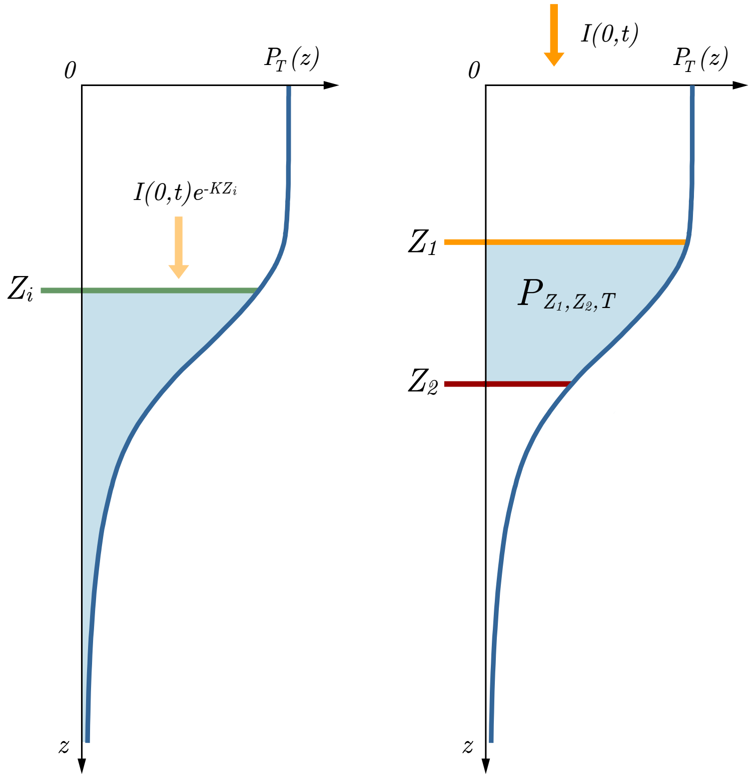

Figure 15: Production of a finite layer, from Z_1 to Z_2, depicted as the difference between watercolumn production below Z_1, forced by $I(0,t)e^{-KZ_1}$ and the production of the portion of the water column below Z_2, forced by $I(0,t)e^{-KZ_2}$

from (3.41) we get (3.15). Subsequently, by relabelling the depths Z_1 and Z_2 as:

$$\Delta Z = Z_2 - Z_1, \qquad z = Z_1, \tag{3.42}$$

we get:

$$P_{z,z+\Delta Z,T} = \frac{BP_m^B D}{K}\Big[f\big(I_*^m e^{-Kz}\big) - f\big(I_*^m e^{-K(z+\Delta Z)}\big)\Big]. \tag{3.43}$$

This expression gives the production in the layer extending from z to $z + \Delta Z$ (Figure 16).

Dividing by the layer thickness gives the average layer production per unit volume: where B is the uniform biomass in the layer. Since the biomass is uniform, the entire expression divided by B gives the average normalized production per unit volume:

$$\langle P_T^B \rangle = \frac{P_m^B D}{K} \left[\frac{f\left(I_*^m e^{-Kz}\right) - f\left(I_*^m e^{-K(z+\Delta Z)}\right)}{\Delta Z} \right]. \tag{3.44}$$

Production of each layer can be calculated separately and the biomass can vary between layers. For the accuracy of this solution, it is not necessary for the biomass to be equal in each layer. In the limit of $\Delta Z \to 0$, average normalized production $\langle P_T^B \rangle$ becomes $P_T^B(z)$ (Figure 16) and the previous expression becomes:

$$P_T^B(z) = -\frac{P_m^B D}{K} \lim_{\Delta Z \to 0} \frac{f\left(I_*^m e^{-K(z+\Delta Z)}\right) - f\left(I_*^m e^{-Kz}\right)}{\Delta Z}, \tag{3.45}$$

where the negative sign is simply extracted from the expression under the limit. The limit in the previous expression corresponds to the z derivative of the $f\left(I_*^m e^{-Kz}\right)$ function (3.40):

$$P_T^B(z) = -\frac{P_m^B D}{K} \frac{\mathrm{d}}{\mathrm{d}z} f\left(I_*^m e^{-Kz}\right). \tag{3.46}$$

Multiplying $1/K$ and $\mathrm{d}f/\mathrm{d}z$ we define $f_z\left(I_*^m e^{-Kz}\right)$ as:

$$f_z\left(I_*^m e^{-Kz}\right) = -\frac{1}{K}\frac{\mathrm{d}}{\mathrm{d}z} f\left(I_*^m e^{-Kz}\right). \tag{3.47}$$

With this definition, expression (3.46) becomes:

$$P_T^B(z) = P_m^B D\, f_z\left(I_*^m e^{-Kz}\right), \tag{3.48}$$

where $f_z\left(I_*^m e^{-Kz}\right)$ is obtained by differentiating (3.40) by z and dividing by K. By comparison with (2.33) we observe the two expressions are identical. Therefore, a mathematical relation existis between the f function (3.40) and the f_z function (2.32). Historically, this was the original derivation of the f_z function [23], hence the $_z$ in the subscript.

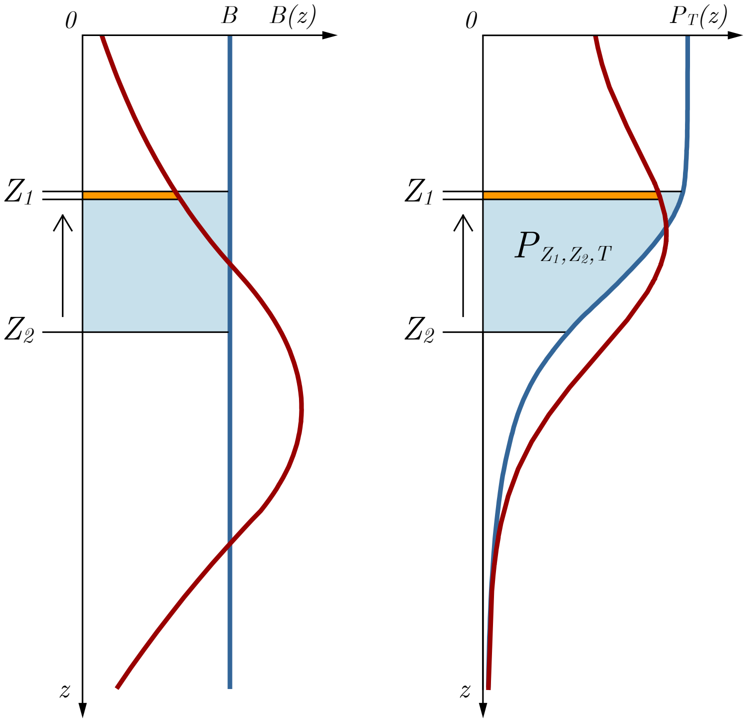

Figure 16: Illustration of the main idea in the alternative derivation of the production profile. The left image shows the biomass profiles: uniform (blue line) and non-uniform (red curve). The right figure shows the production profiles: the production profile for the uniform biomass profile (blue curve) and the production profile for the non-uniform biomass profile (red curve).

3.6 GENERAL SOLUTION

The derived relation between the f and the f_z functions enables us to find a general solution for watercolumn production in case of an arbitrary biomass profile, under the assumption that $B(z)$ is a continuous function. We start with (3.4) which we restate here for clarity:

$$P_{Z,T} = \int_0^\infty B(z) P_T^B(z)\, \mathrm{d}z. \tag{3.49}$$

By inserting (3.46) we obtain the following:

$$P_{Z,T} = -\frac{P_m^B D}{K} \int_0^\infty B(z) \frac{\mathrm{d}}{\mathrm{d}z} f\left(I_*^m e^{-Kz}\right) \mathrm{d}z. \tag{3.50}$$

Further on, proceeding with integration by parts yields:

$$P_{Z,T} = \frac{P_m^B D}{K} \left(B(0) f\left(I_*^m\right) + \int_0^\infty \frac{\mathrm{d}B(z)}{\mathrm{d}z} f\left(I_*^m e^{-Kz}\right) \mathrm{d}z \right), \tag{3.51}$$

where the following condition was used:

$$B(\infty) f(I_*^m e^{-K\infty}) = 0. \tag{3.52}$$

The derived expression (3.51) is a formal relation between the canonical solution (3.15) and any solution for watercolumn production with stratified biomass. The effect of surface biomass $B(0)$ on the magnitude of watercolumn production $P_{Z,T}$ is clearly emphasised: surface biomass is a leading factor in $P_{Z,T}$. The significance of this result is emphasized given that surface biomass is readily accessible to satellite measurement. Therefore, if the remotely-sensed surface biomass is precise, and assuming the remaining parameters of the model are characteristic of the ocean region in question, the error in the estimated watercolumn production arises solely as a consequence of the error in estimating the biomass profile, which is inaccessible to remote sensing and has to be assigned based on prior information [32].

As for the second term, it gives the contribution arising from the shape of the biomass profile. For an increase in biomass with depth, $\mathrm{d}B(z)/\mathrm{d}z > 0$, this contribution is positive. For a decline in biomass with depth, $\mathrm{d}B(z)/\mathrm{d}z < 0$, this contribution is negative. The differential change in biomass with depth $\mathrm{d}B(z)/\mathrm{d}z$ is multiplied by the $f(I_*^m e^{-Kz})$ function. The product $\mathrm{d}B(z) f(I_*^m e^{-Kz})$ gives the production that would occur below depth z in case the biomass below z were equal to $\mathrm{d}B(z)$. Total contribution from all infinitesimal changes in $B(z)$ is taken into account by the integral on the right hand side of (3.51). With increase in depth, the contribution from biomass variation decreases, simply because production declines with increasing depth (2.38).

3.7 BIOOPTICAL FEEDBACK

Thus far in calculating watercolumn production we have treated K as a constant independent of B. We now explore the effect of acknowledging K as a function of B. In this case, biomass too causes light attenuation. We only consider the case of uniform biomass and model the attenuation coefficient as a simple linear relation (2.11), restated here:

$$K = K_w + k_b B. \tag{3.53}$$

When the biomass is vertically uniform, solution (3.15) also applies to the case of the attenuation coefficient given by the previous expression and we have:

$$P_{Z,T} = \frac{B}{K_w + k_b B} P_m^B D f(I_*^m). \tag{3.54}$$

Now the dependence of $P_{Z,T}$ on biomass is not linear, which is a consequence of light attenuation caused by biomass. To analyse the dependence of $P_{Z,T}$ on biomass, we simply take the derivative of the resulting expression with respect to biomass:

$$\frac{\partial P_{Z,T}}{\partial B} = \frac{K_w}{(K_w + k_b B)^2} P_m^B D f(I_*^m). \tag{3.55}$$

If there is an upper limit on watercolumn production, with respect to biomass, the derivative of $P_{Z,T}$ should vanish for high values of biomass. That this is indeed the case can be verified easily by calculating the limit of the previous expression in the case when biomass tends to infinity:

$$\lim_{B \to \infty} \frac{\partial P_{Z,T}}{\partial B} = 0. \tag{3.56}$$

The obtained expression shows that the increase in production does not always follow linearly the increase in biomass, but production becomes limited. With the growth of biomass, light attenuation increases and the biomass itself prevents higher levels of production. At high biomass values, the attenuation coefficient can be written as [36]:

$$K \approx k_b B. \tag{3.57}$$

The upper limit of water column production in this case reads:

$$P_{Z,T} = P_m^B D f(I_*^m) \lim_{B\to\infty} \left(\frac{B}{K_w + k_b B} \right) = \frac{P_m^B D}{k_b} f(I_*^m). \tag{3.58}$$

Now the phytoplankton itself significantly limits the penetration of light through the water column and consequently limits the production of the water column. This effect is expressed only for high values of biomass, more precisely high concentrations of phytoplankton. At low phytoplankton concentrations, watercolumn production $P_{Z,T}$ is well approximated using only K_w for the attenuation coefficient. With increasing biomass, production increases, but so does the attenuation coefficient $K_w + k_b B$. Finally, the influence of light attenuation caused by a high concentration of phytoplankton dominates and the upper limit of production equals (3.58).

3.8 RELATION TO GROWTH MODELS

In the case of a mixed layer, an exact expression relating biomass accumulation and water column production can be derived. Let us consider a mixed layer of depth Z_m. To simplify notation we introduce the following label for the **total biomass in the mixed layer** ($\mathrm{mg\,Chl\,m^{-2}}$):

$$B_{Z_m}(t) = \int_0^{Z_m} B(z,t)\,\mathrm{d}z. \tag{3.59}$$

At initial time we assume biomass in the mixed layer as uniform:

$$B_{Z_m}(0) = B_0 Z_m. \tag{3.60}$$

Let us assume that mixed layer production $P_{Z_m}(t)$, given as:

$$P_{Z_m}(t) = \int_0^{Z_m} P(z,t)\,\mathrm{d}z, \tag{3.61}$$

leads to newly synthesized biomass. Let us also assume that the newly synthesized mixed layer biomass at time t is redistributed through the mixed layer during a time interval Δt, so that no stratification in biomass occurs at $t + \Delta t$. Mixed layer biomass at time $t + \Delta t$ is now:

$$B_{Z_m}(t + \Delta t) = B_{Z_m}(t) + \frac{1}{\chi} P_{Z_m}(t) \Delta t. \tag{3.62}$$

Due to vertical uniformity in biomass, instantaneous mixed layer production equals:

$$P_{Z_m}(t) = \frac{1}{Z_m} B_{Z_m}(t) P^B_{Z_m}(t), \tag{3.63}$$

so that for biomass at time $t + \Delta t$ we have:

$$B_{Z_m}(t + \Delta t) = B_{Z_m}(t) + \frac{1}{\chi Z_m} P^B_{Z_m}(t) B_{Z_m}(t) \Delta t. \tag{3.64}$$

In the limit of $\Delta t \to 0$, implying instantaneous mixing of newly synthesized biomass, the previous equation becomes:

$$\frac{\partial}{\partial t} B_{Z_m}(t) = \frac{1}{\chi Z_m} P^B_{Z_m}(t) B_{Z_m}(t). \tag{3.65}$$

The solution to this equation at time D is:

$$B_{Z_m}(D) = B_{Z_m}(0) \exp\left(\frac{1}{\chi Z_m} \int_0^D P^B_{Z_m}(t)\, \mathrm{d}t \right). \tag{3.66}$$

The integral in the exponential function is given in (3.21):

$$\int_0^D P^B_{Z_m}(t)\, \mathrm{d}t = \frac{P^B_m D}{K} \left[f(I^m_*) - f(I^m_* e^{-K Z_m}) \right]. \tag{3.67}$$

Taking into account the initial condition (3.60) along with the previous expression, the solution to (3.65) reads:

$$B_{Z_m}(D) = B_0 Z_m \exp\left[\frac{P^B_m D}{\chi Z_m K} \left[f(I^m_*) - f(I^m_* e^{-K Z_m}) \right] \right]. \tag{3.68}$$

Mixed layer production is now the difference between $B_Z(D)$ and $B_Z(0)$ multiplied by χ:

$$P_{Z_m,T} = \chi B_0 Z_m \left[\exp\left[\frac{P_m^B D}{\chi Z_m K} \left(f(I_*^m) - f(I_*^m e^{-KZ_m}) \right) \right] - 1 \right]. \quad (3.69)$$

The implicit assumption worth stating here is that all production goes to newly sensitized biomass. If this were not the case an additional loss term should be added to the equation, which will be done if later chapters.

3.9 PROBLEMS

1. Build a numerical model for calculating watercolumn production (3.1). First, split the water column into layers, each of Δz depth. Second, split daylength D into discrete time intervals, each of Δt duration. Use all the other assumptions as in the analytical model. Now watercolumn production is given as:

$$P_{Z_m,T} = \sum_{n=1}^{N}\sum_{j=1}^{J} P_n^j \Delta t \Delta z, \tag{3.70}$$

where we have labelled production at depth z_n and time t_j as P_n^t:

$$P_n^t = P(z_n, t_j) = B(n\Delta z)\left[1 - \exp\left(-\alpha^B I_0^m \sin(\pi j \Delta t/D) e^{-Kn\Delta z} \Big/ P_m^B\right)\right], \tag{3.71}$$

where $z_n = n\Delta z$, with $n = 1, 2, ..., N$ and $t_j = j\Delta t$, with $j = 1, 2, ..., J$. Test the numerical model by calculating watercolumn production for uniform biomass. Plot the numerical solution as a function of dimensionless irradiance I_*^m in the same manner as the canonical solution shown in Figure 12.

2. Use the model from the previous problem with different photosynthesis irradiance functions (1.27, 1.28, 1.29, 1.30, 1.31). Set biomass as uniform and plot the obtained numerical solutions together with the canonical solution. Calculate the difference between the canonical solution and the numerical ones.

3. Use the model from the first problem to calculate wattercolumn production with the shifted Gaussian biomass profile (2.45). Fix all the Gaussian parameters apart from the depth of the maximum z_m, which you vary. Calculate watercolumn production as a function of z_m, by varying it from $z_m = 0$ to $z_m = 200$.

4. Use the model from the first problem with the shifted Sigmoid biomass profile (2.48). Set the mid point z_m equal to the mixed layer depth Z_m and explore the behaviour of the numerical solution for watercolumn production by varying σ. Observe the model behaviour as $\sigma \to \infty$. Compare the numerical solution to the analytical solution for mixed layer production (3.21) with a fixed $z_m = Z_m$ and a sequence of values for σ.

5. Plot the solution for mixed layer production (3.21) as a function of mixed layer depth. Calculate the average mixed layer production $P_{Z_m,T}/Z_m$ and plot it, also as a function of mixed layer depth. Discuss the difference between the two plots.

6. Calculate watercolumn production by acknowledging the dependence of the attenuation coefficient on biomass in the light penetration model (2.11). Employ uniform biomass, the shifted Gaussian biomass profile and the shifted Sigmoid biomass profile. Calculate production by varying B_0 from $B_0 = 0.01\ \mathrm{mg\,Chl\,m^{-3}}$ to $B_0 = 10\ \mathrm{mg\,Chl\,m^{-3}}$.

7. Build a numerical model that solves equation (3.65). Explore how the biomass evolves over time with two models for the attenuation coefficient, first $K = K_w$ and second $K = K_w + k_B B(t)$. Plot biomass as a function of time for both cases.

4

MATRIX MODEL

The previously presented model of primary production and analytical solutions form a closed whole. With the knowledge of the values of the model parameters, daily production profile and daily watercolumn production can be calculated. The common limitation of the analytical solutions is the simple treatment of surface irradiance and the vertical uniformity of photosynthetic parameters, which somewhat limits the range of applicability of the model.

Also, the solutions are only valid for the exponential photosynthesis irradiance function [44, 31]. Other functions are also used in practice, but no analytical solutions for the daily production profile or daily watercolumn production are known for them. Therefore, the application of the model in more complex situations and with other photosynthesis irradiance functions is naturally realized by numerical methods. This chapter describes the discretization of the analytical model and the development of the matrix formalism for calculating the daily production profile and daily watercolumn production.

In a numerical model continuous time and continuous space become discrete. Consequently, integrals become sums and derivatives are expressed algebraically. In matrix notation these sums become matrix products, which are simpler to handle, both mathematically and numerically when implementing the model. The matrix equations are concise and the notation elegantly packs rather long algebraic expressions into short ones. This adds clarity to the model structure. It also simplifies model implementation.

4.1 DISCRETIZATION OF THE ANALYTICAL MODEL

Let the numerical model have N vertical levels at depths z_n, indexed by n, and J time intervals indexed by j. The depth z is positive downwards and n increases with depth so that:

$$z_n < z_{n+1}, \tag{4.1}$$

holds, as shown in Figure 17, with $n = 1, 2, ..., N$. The water column is of depth Z, such that the depth interval between two consecutive model levels is equal to:

$$\Delta z = \frac{Z}{N}. \tag{4.2}$$

The first model level is set to:

$$z_1 = \frac{\Delta z}{2}. \tag{4.3}$$

Each time interval is equal to:

$$\Delta t = \frac{D}{J}, \tag{4.4}$$

such that discrete time t_j is defined as:

$$t_j = j\Delta t, \tag{4.5}$$

with $j = 1, 2, ..., J$. The described spatial and temporal discretization enables us to rewrite the analytical expressions for the model in numerical form. We begin with the discretization of the expression for daily production (2.5) at depth z_n:

$$P_T(z_n) \approx B(z_n) \sum_{j=1}^{J} p^B\big(I(z_n, t_j)\big)\Delta t. \tag{4.6}$$

The right hand side of this expression uses biomass at depth z_n (Figure 17) and approximates daily production as a sum, rather than as an integral, like in (2.5). This sum can be denoted by $P_{n,T}$. In the limit of Δt going to zero, we have:

$$\lim_{\Delta t \to 0} P_{n,T} = P_T(z_n). \tag{4.7}$$

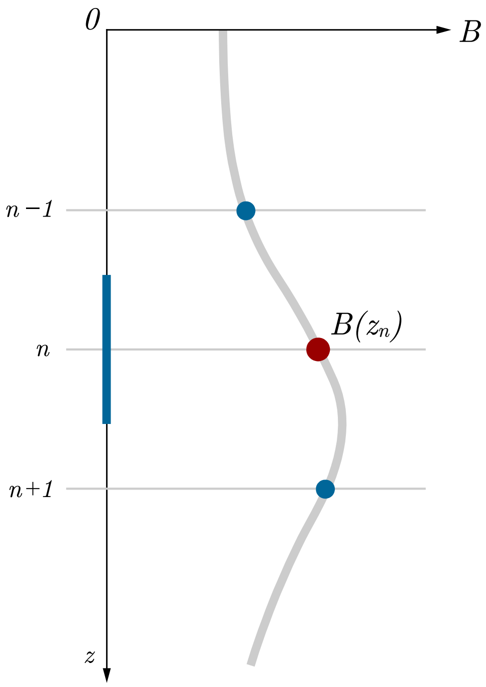

Figure 17: Vertical discretization of the biomass profile in the vicinity of depth z_n. The distance between two arbitrary vertical levels Δz need not be equal. Biomass $B(z_n)$ (red dot) represents the biomass for the entire Δz layer centred around z_n (blue line). The same holds for the vertical discretization of the production profile (not shown).

The sum on the right side of expression (4.6) approximates daily normalized production $P_T^B(z_n)$ and is denoted here by $P_{n,T}^B$:

$$P_{n,T}^B = \sum_{j=1}^{J} p^B\big(I(z_n, t_j)\big)\Delta t. \tag{4.8}$$

In this case also, in the limit when Δt tends to zero, it holds:

$$\lim_{\Delta t \to 0} P_{n,T}^B = P_T^B(z_n). \tag{4.9}$$

Therefore, both numerical expressions converge to the analytical ones in the limit of small Δt, as expected. Hence, the accuracy of the numerical calculations for a given depth z_n is dictated, and can be improved by, decreasing Δt.

Next, to numerically calculate watercolumn production $P_{Z,T}$, expression (3.1) needs to be discretized. Its discretization reads:

$$P_{Z,T} \approx \sum_{n=1}^{N} B(z_n) \left[\sum_{j=1}^{J} p^B \big(I(z_n, t_j) \big) \Delta t \right] \Delta z. \tag{4.10}$$

The double sum on the right hand side of the expression (4.10) approximates daily watercolumn production $P_{Z,T}$. In the limit when both Δt and Δz tend to zero, (4.10) goes to (3.1).

The model can also be amended such that the vertical intervals are not equal. The reason for doing this is the fact that in field work primary production measurements are often not distributed at equal depths from each other. Therefore, a given measurement is representative of a layer extending from halfway between the level, above the given level, to halfway between the given level, to the level below. Also, when the model is used to compare measurements with model predictions, setting model depths equal to the measurement depths is preferable. In this case each level z_n is assigned a depth interval Δz_n:

$$\Delta z_n = \frac{z_{n+1} - z_{n-1}}{2}, \tag{4.11}$$

for $n = 2, 3, ..., N-1$. The first vertical increment is set to:

$$\Delta z_1 = \frac{z_1 + z_2}{2}, \tag{4.12}$$

and the last one to:

$$\Delta z_N = z_N - z_{N-1}. \tag{4.13}$$

Having described the discretization of the analytical model, we now proceed to present the matrix formalism for calculating the daily production profile and watercolumn production. The formalism holds for both arbitrary and uniform vertical increments, but for pedagogical reasons will be presented with with uniform vertical increments.

4.2 MATRIX FORMALISM

With a few additional definitions, the previous sums can be concisely written using matrix formalism. We begin by first observing that irradiance at the depth z_n at the time t_j can be denoted simply as:

$$I_{nj} = I\left(z_n, t_j\right). \tag{4.14}$$

The **irradiance matrix I** (dimension $N \times J$) is defined as a matrix whose elements are I_{nj} (Figure 18). Therefore, irradiance conditions of the entire model are contained in the irradiance matrix:

$$\mathbf{I} = \begin{bmatrix} I_{11} & I_{12} & \dots & I_{1j} & \dots & I_{1J} \\ I_{21} & I_{22} & \dots & I_{2j} & \dots & I_{2J} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ I_{n1} & I_{n2} & \dots & I_{nj} & \dots & I_{nJ} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ I_{N1} & I_{N2} & \dots & I_{Nj} & \dots & I_{NJ} \end{bmatrix}. \tag{4.15}$$

Each row of the irradiance matrix is equal to the time series of irradiance at depth z_n, while each column is equal to the vertical profile of irradiance at time t_j. Elements of the irradiance matrix can be calculated with any optical model. For example, by using (2.13) we have:

$$I_{nj} = I_{0j} \exp\left(-K z_n\right), \tag{4.16}$$

where the surface irradiance now is given as:

$$I_{0j} = I_0\left(t_j\right). \tag{4.17}$$

Unlike the idealized surface irradiance model (2.9), surface irradiance here I_{0j} can now be any function, even discontinuous.

Next, we observe that when an individual element of the irradiance matrix I_{nj} is taken as an argument of the photosynthesis irradiance function we obtain normalized production at depth z_n and time t_j, which we label p^B_{nj}:

$$p^B_{nj} = p^B\left(I_{nj}\right). \tag{4.18}$$

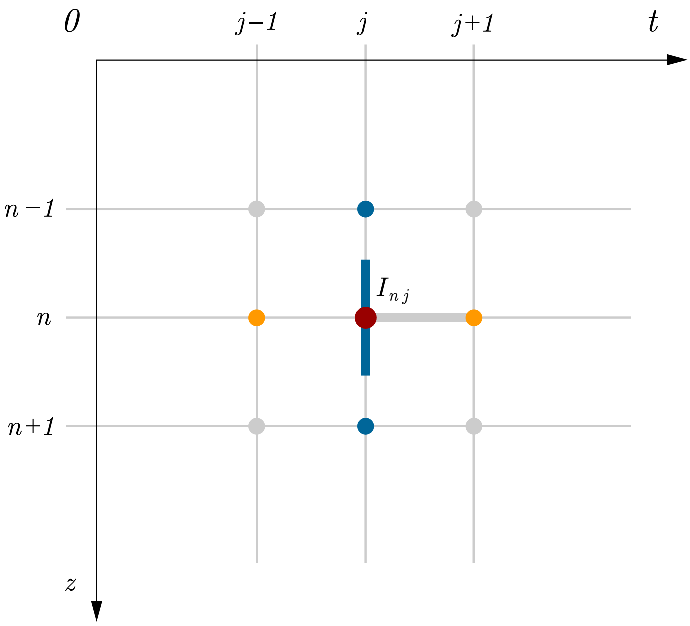

Figure 18: Sketch of the irradiance matrix $\mathbf{I}$ which collects irradiance values at depths z_n and times t_j, such that its elements are $I_{nj} = I\left(z_n, t_j\right)$ (red point). In the (z, t) plane the blue line equals Δz and the grey line equals Δt.

Subsequently, **normalized production matrix $\mathbf{P}^B$** (dimension $N \times J$) is defined as a matrix whose elements are p^B_{nj} (Figure 19):

$$\mathbf{P}^B = \begin{bmatrix} p^B_{11} & p^B_{12} & \cdots & p^B_{1j} & \cdots & p^B_{1J} \\ p^B_{21} & p^B_{22} & \cdots & p^B_{2j} & \cdots & p^B_{2J} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ p^B_{n1} & p^B_{n2} & \cdots & p^B_{nj} & \cdots & p^B_{nJ} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ p^B_{N1} & p^B_{N2} & \cdots & p^B_{Nj} & \cdots & p^B_{NJ} \end{bmatrix}. \tag{4.19}$$

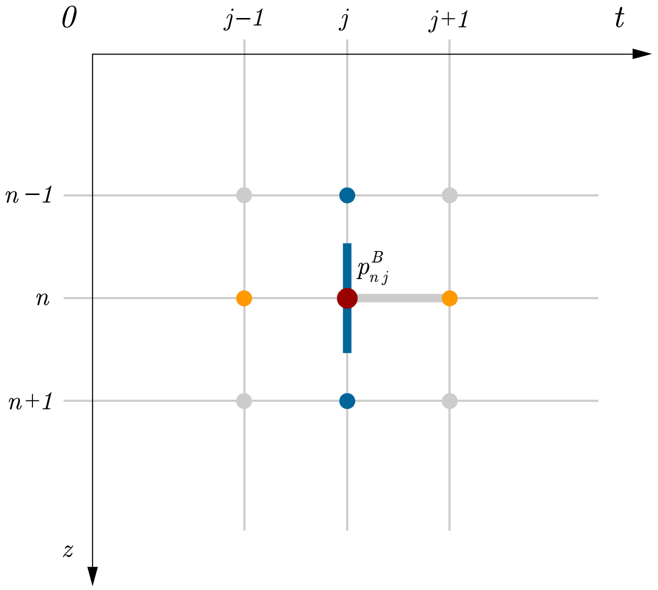

Figure 19: Sketch of the normalized production matrix $\mathbf{P}^B$ which collects normalized production values at depth z_n and time t_j, such that its elements are $p^B_{nj} = p^B(I_{nj})$. In the (z,t) plane the blue line equals Δz and the orange line equals Δt.

Each row of this matrix is equal to the time series of normalized production at depth z_n, while each column is equal to the vertical profile of normalized production at time t_j. To calculate production at depth z_n and time t_j we simply multiply each row of this matrix by the corresponding biomass at that depth:

$$P(z_n, t_j) = B\left(z_n\right) p^B\left(I_{nj}\right), \tag{4.20}$$

This expression is a discrete version of expression (2.3), now with biomass independent of time. To write the previous expression in matrix form we define the **biomass matrix B** (dimension $N \times N$) as a diagonal matrix whose elements are equal to:

$$b_{nm} = \delta_{nm} B(z_n), \tag{4.21}$$

where δ_{nm} is the Kronecker delta symbol. Written out in matrix notation the biomass matrix **B** reads:

$$\mathbf{B} = \begin{bmatrix} B(z_1) & 0 & \dots & 0 \\ 0 & B(z_2) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & B(z_N) \end{bmatrix}. \tag{4.22}$$

Now, in analogy to how production at depth is calculated by multiplying biomass with normalized production, we extend the concept to matrix form in the following manner. We recognize that the matrix product of the biomass matrix with the normalized production matrix gives the **production matrix P** (dimension $N \times J$) :

$$\mathbf{P} = \mathbf{B}\mathbf{P}^B, \tag{4.23}$$

whose elements are:

$$p_{nj} = B(z_n)p^B(I_{nj}). \tag{4.24}$$

Each row of the production matrix is equal to the time series of production at depth z_n, while each column is equal to the vertical profile of production at time t_j. Therefore, the production matrix contains all the information needed to calculate watercolumn production and the daily production profile numerically. To carry out these calculations in matrix form we proceed to define another two matrices.

By defining the **time matrix** $\boldsymbol{\tau}$ (dimension $J \times 1$), which has all its elements equal and given as:

$$\tau_j = \Delta t, \tag{4.25}$$

time integration it is simply carried out as:

$$\mathbf{p}_T = \mathbf{P}\boldsymbol{\tau}, \tag{4.26}$$

and thus a **discrete daily production profile** $\mathbf{p}_T$ is obtained (dimension $N \times 1$), whose elements are equal to (4.6). The **discrete normalized daily production profile** $\mathbf{p}_T^B$ (dimension $N \times 1$) is obtained simply as:

$$\mathbf{p}_T^B = \mathbf{P}^B\boldsymbol{\tau}, \tag{4.27}$$

whose elements are equal to (4.8). Having a model for the discrete production profile, we can now move forward and calculate watercolumn production $P_{Z,T}$ in line with the double sum (4.10). To achieve this, vertical integration of $\mathbf{p}_T$ is required. The **vertical increments matrix** $\boldsymbol{\zeta}$ (dimension $1 \times N$) is defined as a matrix whose elements are equal to the vertical increment Δz around the vertical level z_n, as defined in (4.2):

$$\zeta_n = \Delta z. \tag{4.28}$$

For $\boldsymbol{\zeta}$ the following holds:

$$\sum_{n=1}^{N} \zeta_n = Z, \tag{4.29}$$

where Z is the depth of the water column. Finally, daily watercolumn production is now given as:

$$P_{Z,T} = \boldsymbol{\zeta}\mathbf{P}\boldsymbol{\tau}. \tag{4.30}$$

The given expression is analogous to expression (3.1) and is equal to its numerical counterpart (4.10). Expressions (4.26) and (4.30) are two fundamental relations of the matrix model for daily primary production. The two can be combined into the following expression for daily watercolumn production:

$$P_{Z,T} = \boldsymbol{\zeta}\mathbf{p}_T. \tag{4.31}$$

Written in this form it is obvious that the vertical increments matrix $\boldsymbol{\zeta}$ is in fact a row vector. It enables vertical summation of the daily production profile $\mathbf{p}_T$ to be carried out simply as a matrix product of $\boldsymbol{\zeta}$ with it. In the same manner the time matrix $\boldsymbol{\tau}$ is a column vector, which enables the summation over time to be carried out simply as a matrix product in (4.26).

All of the above matrix expression are mathematically equivalent to the numerical form of the basic integrals, such as (2.5) and (3.1), in the limits of small Δt and Δz_n. To demonstrate in more detail that these matrix expressions translate to the their numerical counterparts, (4.6) and (4.10), we now present a detailed derivation of the matrix model.

4.3 DERIVATION OF THE MATRIX MODEL

The expression for $P^B_{n,T}$ (4.8) can be written as a scalar product of two vectors:

$$P^B_{n,T} = \begin{bmatrix} p^B_{n1} & p^B_{n2} & \dots & p^B_{nT} \end{bmatrix} \begin{bmatrix} \Delta t & \Delta t & \dots & \Delta t \end{bmatrix}^T, \tag{4.32}$$

where:

$$p^B_{nj} = p^B\big(I(z_n, t_j)\big). \tag{4.33}$$

The given expression is valid for each vertical level z_n. Collecting p^B_{nj} elements into a matrix yields:

$$\begin{bmatrix} P^B_{1,T} \\ P^B_{2,T} \\ \vdots \\ P^B_{n,T} \\ \vdots \\ P^B_{N,T} \end{bmatrix} = \begin{bmatrix} p^B_{11} & p^B_{12} & \cdots & p^B_{1j} & \cdots & p^B_{1T} \\ p^B_{21} & p^B_{22} & \cdots & p^B_{2j} & \cdots & p^B_{2T} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ p^B_{n1} & p^B_{n2} & \cdots & p^B_{nj} & \cdots & p^B_{nT} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ p^B_{N1} & p^B_{N2} & \cdots & p^B_{Nj} & \cdots & p^B_{NT} \end{bmatrix} \begin{bmatrix} \Delta t \\ \Delta t \\ \vdots \\ \Delta t \\ \vdots \\ \Delta t \end{bmatrix}. \tag{4.34}$$

The given expression can be abbreviated as:

$$\mathbf{p}^B_T = \mathbf{P}^B \boldsymbol{\tau}, \tag{4.35}$$

where $\mathbf{p}^B_T$ is the normalized discrete production profile, $\boldsymbol{\tau}$ is the time matrix, and $\mathbf{P}^B$ is the normalized production matrix. Further, using (4.8), the expression (4.10) can be written as:

$$P_{Z,T} \approx \sum_{n=1}^{N} B(z_n) P^B_{n,T} \Delta z, \tag{4.36}$$

which is equal to the following dot product:

$$P_{Z,T} = \begin{bmatrix} \Delta z & \Delta z & \dots & \Delta z \end{bmatrix} \begin{bmatrix} B(z_1)P^B_{n,T} & B(z_2)P^B_{n,T} & \dots & B(z_N)P^B_{N,T} \end{bmatrix}^T. \tag{4.37}$$

The elements of the rightmost vector in the given expression correspond to the daily production at the vertical level z_n:

$$P_{n,T} = B(z_n) P^B_{n,T}. \tag{4.38}$$

Using the biomass matrix $\mathbf{B}$, defined in the previous subsection as a diagonal matrix with biomass values on the diagonal, the previous expression can be written for each vertical level and summarized as:

$$\mathbf{p}_T = \mathbf{B}\mathbf{p}^B_T, \tag{4.39}$$

where $\mathbf{p}_T$ is the discrete production profile. Inserting (4.35) for $\mathbf{p}^B_T$ yields:

$$\mathbf{p}_T = \mathbf{B}\mathbf{P}^B\boldsymbol{\tau}. \tag{4.40}$$

The given expression corresponds to the right vector in expression (4.37), while the left vector in expression (4.37) corresponds to the row matrix of vertical increments $\boldsymbol{\zeta}$. Now, daily watercolumn production as expressed by (4.37) can be written in matrix form as:

$$P_{Z,T} = \boldsymbol{\zeta}\mathbf{B}\mathbf{P}^B\boldsymbol{\tau}. \tag{4.41}$$

Expanded, the matrix product $\mathbf{B}\mathbf{P}^B$ reads:

$$\mathbf{B}\mathbf{P}^B = \begin{bmatrix} B(z_1) & 0 & \dots & 0 \\ 0 & B(z_2) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & B(z_N) \end{bmatrix} \begin{bmatrix} p^B_{11} & p^B_{12} & \cdots & p^B_{1T} \\ p^B_{21} & p^B_{22} & \cdots & p^B_{2T} \\ \vdots & \vdots & \ddots & \vdots \\ p^B_{N1} & p^B_{N2} & \cdots & p^B_{NT} \end{bmatrix} \tag{4.42}$$

Next, $\mathbf{B}\mathbf{P}^B$ is denoted by $\mathbf{P}$, which is recognized as the production matrix:

$$\mathbf{B}\mathbf{P}^B = \mathbf{P}. \tag{4.43}$$

Expanded the production matrix reads:

$$\mathbf{P} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1T} \\ p_{21} & p_{22} & \cdots & p_{2T} \\ \vdots & \vdots & \ddots & \vdots \\ p_{N1} & p_{N2} & \cdots & p_{NT} \end{bmatrix}. \tag{4.44}$$

Taking all of this into account we get the expression for daily watercolumn production as:

$$P_{Z,T} = \zeta \mathbf{P} \boldsymbol{\tau}. \tag{4.45}$$

Since according to (4.33) each element of the normalized production matrix is obtained using $p^B(I)$, it is necessary to know the irradiance at the vertical level z_n at the time instant t_j, that is $I(z_n, j\Delta t)$. Denoting $I(z_n, j\Delta t)$ with I_{nj} and collecting all elements into a matrix of the same size as $\mathbf{P}^B$, the irradiance matrix $\mathbf{I}$ emerges. Subsequently, treating $p^B[\cdot]$ as an elementwise operator acting on each element of the irradiance matrix, in accordance with (4.18), we can write the following:

$$\mathbf{P}^B = p^B[\mathbf{I}], \tag{4.46}$$

such that (4.45) becomes:

$$P_{Z,T} = \zeta \mathbf{B} p^B[\mathbf{I}] \boldsymbol{\tau}. \tag{4.47}$$

Using the same notation the expression for the discrete production profile (4.40) can be written as:

$$\mathbf{p}_T = \mathbf{B} p^B[\mathbf{I}] \boldsymbol{\tau}. \tag{4.48}$$

Stated in this form the expression highlights the central role of the irradiance matrix in the model. We now look in more detail how to calculate its elements.

4.4 CALCULATING THE IRRADIANCE MATRIX

We have observed in the prior section that the irradiance matrix plays a central role in the matrix model. We now emphasise in more detail how to calculate its elements. In general, any optical model can be used to do this, but for simplicity we will limit ourselves here to the already used model (2.13), according to which the elements of the irradiance matrix are given as:

$$I_{nj} = I_{0j} \exp\left(-K z_n\right). \tag{4.49}$$

To implement it, the model requires information on surface irradiance:

$$I_{0j} = I_0\left(t_j\right). \tag{4.50}$$

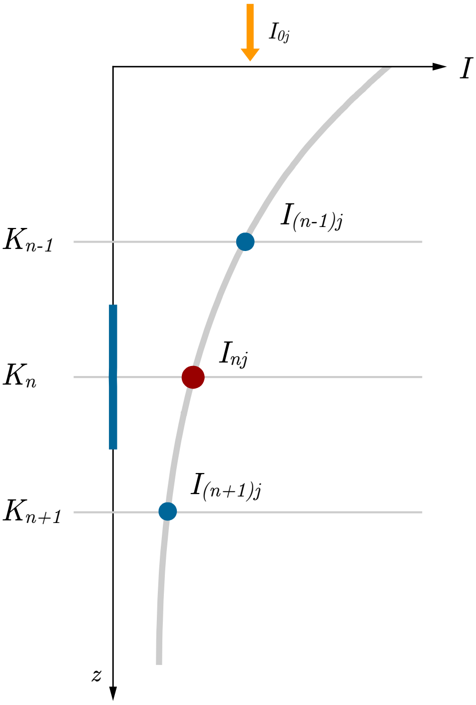

Figure 20: Calculation of irradiance at level z_n by knowing irradiance at the level above z_{n-1} for vertically dependent attenuation coefficient. Irradiance at z_n is calculated by first attenuating the irradiance at the level above $I(z_{n-1})$ over depth $\Delta z/2$ with K_{n-1} and then subsequently attenuating the obtained irradiance still further over $\Delta z/2$ with K_n.

It treats the attenuation coefficient as a constant, whereas in general the attenuation coefficient is not constant, but changes with depth. To take this into account, a simple remedy is to assign different values of the attenuation coefficient for each model layer, such that K becomes K_n:

$$K_n = K(z_n). \tag{4.51}$$

Next, we recognize that irradiance at a given model level can be calculated from knowing the irradiance at the level above and the attenuation coefficient in between. If to each level a K_n value is assigned (Figure 20) it is then valid in the depth range of that level, which is Δz_n as defined in (4.2). Therefore, to get at irradiance at the level z_n we need irradiance value at the top of that layer, which is at $z_n - \Delta z/2$ and is given as:

$$I\left(z_n - \frac{\Delta z}{2}\right) = I_{(n-1)j} \exp\left(-K_{n-1}\frac{\Delta z}{2}\right). \tag{4.52}$$

Next, having irradiance at the top of the layer, it is straightforward to calculate it at the depth z_n, by simply attenuating it with K_n for half a layer depth:

$$I_{nj} = I_{(n-1)j} \exp\left(-K_{n-1}\frac{\Delta z}{2}\right) \exp\left(-K_n\frac{\Delta z}{2}\right). \tag{4.53}$$

In this manner irradiance at each level can be calculated and the irradiance matrix values populated.

4.5 ANALOGY AMONGST THE MODELS

To gain deeper insight into the mathematical structure of both the continuous and the matrix models we now employ the notion of the scalar product of functions to highlight the mathematical symmetry amongst the models. One form in which the watercolumn production integral can be written is as the vertical integral of the production profile, which itself is given as a product of the biomass profile and the normalized production profile as $P_T(z) = B(z)P_T^B(z)$, therefore we have:

$$P_{Z,T} = \int_0^\infty B(z)P_T^B(z)\,\mathrm{d}z. \tag{4.54}$$

Mathematically, the above integral is the inner product of the two functions: $B(z)$ and $P_T^B(z)$. In discrete form the approximation to this integral reads:

$$P_{Z,T} \approx \sum_{n=1}^{N} B(z_n)P_T^B(z_n)\Delta z. \tag{4.55}$$

If we now treat $B(z_n)$ and $P_T^B(z_n)$ as vectors in an N dimensional space, we can consider the above sum as a scalar product of the two vectors, analogously to the just mentioned interpretation of (4.54). To unveil where in the matrix model this analogy lies we consider equation (4.41), which by using (4.35) we unpack here as:

$$P_{Z,T} = \boldsymbol{\zeta}\mathbf{B}\mathbf{p}_T. \tag{4.56}$$

The matrix product of $\boldsymbol{\zeta}$ and $\mathbf{B}$ reads:

$$\boldsymbol{\zeta}\mathbf{B} = \begin{bmatrix} B(z_1)\Delta z & B(z_2)\Delta z & \dots & B(z_N)\Delta z \end{bmatrix}. \tag{4.57}$$

This is a row vector of the same size as $\mathbf{p}_T$ and we label it as $\mathbf{b}$, such that elementwise we have:

$$b_n = B(z_n)\Delta z. \tag{4.58}$$

Using $\mathbf{b}$ enables expression (4.56) to be rewritten as a scalar product of $\mathbf{b}$ and $\mathbf{p}_T$:

$$P_{Z,T} = \mathbf{b}\mathbf{p}_T. \tag{4.59}$$

By way of analogy this expression has the same mathematical structure as (4.54). Namely, both expressions, (4.54) and (4.56), can be thought of as inner products, with the difference that the first is an inner product over a continuous variable z and the second one is an inner product over a discrete space in which each dimension corresponds to a model depth located at z_n. In the limit of ever smaller depth intervals Δz the two expression should be equal to each other:

$$\lim_{\Delta z \to 0} \mathbf{b}\mathbf{p}_T = \int_0^\infty B(z) P_T^B(z)\, \mathrm{d}z. \tag{4.60}$$

Therefore, both models for watercolumn production can be thought of in a similar fashion, as inner products, be it over a continuous space (4.54), or over discrete space (4.56). The advantage of the matrix model comes to the fore when using measured biomass profiles, or measured surface irradiance. It is however, slightly more difficult to implement than the analytical model in case the photosynthesis parameters are depth dependent, which we now discuss.

4.6 VERTICALLY DEPENDENT PHOTOSYNTHESIS PARAMETERS

For calculating daily production at depth with vertically dependent photosynthesis parameters we have to first state the photosynthesis parameters as functions of depth. For a depth dependent initial slope we have:

$$\alpha^B = \alpha^B(z), \tag{4.61}$$

and for a depth dependent assimilation number we have:

$$P_m^B = P_m^B(z). \tag{4.62}$$

As such it is simple to include it in the analytical model for the daily production profile (2.34), by simply stating the parameters as functions of depth:

$$P_T(z) = B(z)P_m^B(z)D\, f_z\big(I_*^m(z)e^{-Kz}\big), \tag{4.63}$$

where now the dimensionless irradiance also becomes a function of depth:

$$I_*^m(z) = \frac{\alpha^B(z)I_0^m}{P_m^B(z)}. \tag{4.64}$$

However, it is now more difficult to calculate daily watercolumn production analytically. However, in the matrix model the procedure for calculating watercolumn production is straightforward, but including vertically dependent photosynthesis parameters is a bit more tricky and can done in a number of ways.

The easiest way to proceed is to amend (4.48), the matrix model analogue to (4.63), by taking into account the vertical dependence of photosynthesis parameters. Subsequently, we have $p^B[\cdot]$ act on each row of the normalized production matrix with different values of photosynthesis parameters:

$$\mathbf{P}^B = \sum_{n=1}^{N} p^B\Big[\mathbf{EI}\big|\ \alpha^B(z_n), P_m^B(z_n)\Big], \tag{4.65}$$

where $\mathbf{E}$ is a matrix with a single unit element on the diagonal in the row corresponding to the model level n. In such a way $\mathbf{E}$ is used to select each row of the irradiance matrix. This expression corresponds to:

$$p_{nj}^B = p^B\Big(I_{nj}\big|\ \alpha^B(z_n), P_m^B(z_n)\Big), \tag{4.66}$$

where we have used the notation from (1.20) to highlight the vertical dependence of the photosynthesis parameters. In this manner each row of the production matrix can have different values of photosynthesis parameters. Whilst the construction of the normalized production matrix $\mathbf{P}^B$, as stated in (4.65), takes a bit more effort, the remainder of the model stays the same.

4.7 PROBLEMS

1. Build the irradiance matrix as defined in (4.16). Write a code which plots the irradiance profile at a desired time step, corresponding to a matrix column. Write a code which plots the irradiance time series at a desired depth, corresponding to a matrix row. Finally plot the the entire irradiance matrix. Observe how changing surface irradiance and the attenuation coefficient changes the light field and the irradiance matrix.

2. Build a normalized production matrix by using the photosynthesis irradiance function directly on the irradiance matrix (4.18). Write a code which accepts various photosynthesis irradiance functions (1.27, 1.28, 1.29, 1.30, 1.31). Plot the the normalized production matrices and the differences amongst each. Change the values of the photosynthesis parameters to observe how the production matrix changes.

3. Write a code which builds the biomass matrix (4.2) with biomass given by either the shifted Gaussian (2.45) of the shifted Sigmoid function (2.48). Use the biomass matrix to calculate the production matrix as defined in (4.23). Plot the the production matrix for different photosynthesis irradiance functions (1.27, 1.28, 1.29, 1.30, 1.31).

4. Build the irradiance matrix by acknowledging the effect of biomass on the underwater light field. Use this irradiance matrix to calculate the production matrix. Alter the parameters of the biomass profile to observe how the production matrix changes with the shape of the biomass profile.

5. Using the matrix model calculate the production profile (4.26) and watercolumn production (4.30). Also implement the code using loops, as in (4.6) and (3.1). Contrast the code with the code for the matrix model.

6. Amend the irradiance model (4.53) to take into account non uniform model level separations as stated in (4.11). Subsequently, write out the matrix model equations given in section 5.3 now using non uniform model level separations. Start with equation (4.37) and work your way through to equation (4.45).

7. Build the normalized production matrix with depth dependent photosynthesis parameters, as stated in (4.65), and use it to calculate the daily production profile and daily watercolumn production. Study the effect of using depth dependent photosynthesis parameters on both the shape of the production profile and the magnitude of daily watercolumn production.

BIBLIOGRAPHY

[1] E. C. C. Baly. The kinetics of photosynthesis. *Proceedings of the Royal Society of London*, 117B:218–239, 1935.

[2] A. Beckman and I. Hense. Beneath the surface: Characteristics of oceanic ecosystems under weak mixing conditions - A theoretical investigation. *Progress in Oceanography*, 75:771–796, 2007.

[3] M. J. Behrenfeld, O. Prasil, M. Babin, and F. Bruyant. In search of a physiological basis for covariations in light-limited and light-saturated photosynthesis. *Journal of Phycology*, 40:4–25, 2004.

[4] F. F. Blackman. Optimal and limiting factors. *Annals of Botany*, 19:281–295, 1905.

[5] Dall'Olmo G. Brewin, R. J. W., J. Gittings, X. Sun, P. K. Lange, D. E. Raitsos, H. A. Bouman, I. Hoteit, J. Aiken, and S. Sythyendranath. A conceptual approach to partitioning a vertical profile of phytoplankton biomass into contributions from two bcommunities. *Journal of Geophysical Ressearch: Oceans*, 127:e2021JC018195, 2022.

[6] B. E. Chalker. Modelling light saturation curves for photosynthesis: An exponential function. *Journal of Theoretical Biology*, 84:205–215, 1980.

[7] J. J. Cullen. The deep chlorophyll maximum: Comparing certical profiles of chlorophyll *a*. *Canadian Journal of Fisheries and Aquatic Sciences*, 39:791–803, 1982.

[8] Mobley Cutris D. *The Oceanic Optics Book.* International Ocean Colour Coordinating Group, 1.0 edition, 2022.

[9] P. G. Falkowski. Molecular ecology of phytoplankton photosynthesis. In *Primary productivity and biogoechemical cycles in the sea*, pages 47–68. Plenum Press, New York, 1992.

[10] P. G. Falkowski and J. A. Raven. *Aquatic Photosynthesis.* Princeton University Press, 2nd edition, 2007.

[11] P. J. S. Franks. NPZ models of plankton dynamics: Their construction, coupling to physics, and application. *Journal of Oceanography*, 58:379–387, 2002.

[12] P. J. S. Franks. Has sverdrup's critical depth hypothesis been tested? mixed layers vs. turbulent layers. *ICES Journal of Marine Science*, 72:1897–1907, 2015.

[13] J. Frenette, S. Demers, and L. Legendre. Lack of agreement among models for estimating the photosynthetic parameters. *Limnology and Oceanography*, 38:679–687, 1993.

[14] A. Gargett and J. Marra. Effects of upper ocean physical processes (turbulence, advection and air-sea interaction) on oceanic primary production. In *The sea*, pages 19–49. John Wiley & Sons, New York, 2002.

[15] W. Gentleman. A chronology of plankton dynamics in silico: How computer models have been used to study marine ecosystems. *Hydrobiologia*, 480:69–85, 2002.

[16] B. A. Hodges and D. L. Rudnick. Simple models of steady deep maxima in chlorophyll and biomass. *Deep Sea Research Part I: Oceanographic Research Papers*, 51:999–1015, 2004.

[17] A. Huppert, B. Blasius, and L. Stone. A model of phytoplankton blooms. *The American Naturalist*, 159:156–171, 2002.

[18] M. Iqbal. *Introduction to solar radiation*. Academic Press, 1st edition, 1984.

[19] A. D. Jassby and T. Platt. Mathematical formulation of the relationship between photosynthesis and light for phytoplankton. *Limnology and Oceanography*, 21:540–547, 1976.

[20] C. T. Jones, S. E. Craig, A. B. Barnett, H. L. MacIntyre, and J. J. Cullen. Curvature in models of the photosynthesis-irradiance response. *Journal of Phycology*, 50:341–355, 2014.

[21] J. T. O. Kirk. *Light and photosynthesis in quatic ecosystems*. Cambridge University Press, 3rd edition, 2011.

[22] Z. Kovač, T. Platt, S. Antunović, S. Sathyendranath, M. Morović, and C. Gallegos. Extended formulations and analytic solutions for watercolumn production integrals. *Frontiers in Marine Science*, 4:163, 2017.

[23] Z. Kovač, T. Platt, Shubha S., and M. Morović. Analytical solution for the vertical profile of daily production in the ocean. *Journal of Geophysical Research: Oceans*, 121, 2016.

[24] A. R. Longhurst and W. G. Harrison. The biological pump: Profiles of plankton production and consumption in the upper ocean. *Progress in Oceanography*, 22:47–123, 1989.

[25] J. L. Monteith and M. H. Unsworth. *Principles of environmental physics*. Academic Press, Elsevier, 4th edition, 2008.

[26] D. H. Peterson, M. J. Perry, K. E. Bencala, and M. C. Talbot. Phytoplankton productivity in relation to light intensity: A simple equation. *Estuarine, Coastal and Shelf Science*, 24:813–832, 1987.

[27] T. Platt, D. F. Bird, and S. Sathyendranath. Critical depth and marine primary production. *Proceeding of the Royal Society B*, 246:205–217, 1991.

[28] T. Platt, D. S. Broomhead, S. Sathyendranath, A. M. Edwards, and E. J. Murphy. Phytoplankton biomass and residual nitrate in the pelagic ecosystem. *Proceeding of the Royal Society A*, 459:1063–1073, 2003.

[29] T. Platt, C. Caverhill, and S. Sathyendranath. Basin-scale estimates of oceanic primary production by remote sensing: The North Atlantic. *Journal of Geophysical Research*, 96:15147–15159, 1991.

[30] T. Platt, K. L. Denman, and A. D. Jassby. Modelling the productivity of phytoplankton. In *The sea: ideas and observations on progress in the study of the seas*, pages 807–856. Wiley, New York, 1977.

[31] T. Platt, C. L. Gallegos, and W. G. Harrison. Photoinsmihibition of photosynthesis in natural assemblages of marine phytoplankton. *Journal of Marine Research*, 38:687–701, 1980.

[32] T. Platt and S. Sathyendranath. Oceanic primary production: Estimation by remote sensing at local and regional scales. *Science*, 241:1613–1620, 1988.

[33] T. Platt and S. Sathyendranath. Biological production models as elements of coupled, atmosphere-ocean models for climate research. *Journal of Geophysical Research*, 96:2585–2592, 1991.

[34] T. Platt, S. Sathyendranath, C. M. Caverhill, and M. R. Lewis. Ocean primary production and available light: Further algorithms for remote sensing. *Deep-Sea Research*, 35:855–879, 1988.

[35] T. Platt, S. Sathyendranath, A. M. Edwards, D. S. Broomhead, and Ulloa. Nitrate supply and demand in the mixed layer of the ocean. *Marine Ecology Progress Series*, 254:3–9, 2003.

[36] T. Platt, S. Sathyendranath, and P. Ravindran. Primary production by phytoplankton: Analytic solutions for daily rates per unit area of water surface. *Proceeding of the Royal Society B*, 241:101–111, 1990.

[37] T. Platt, J. D. Woods, Sathyendranath, and W. Barkmann. Net primary production and stratification in the ocean. *Geophysical Monograph*, 85:247–254, 1994.

[38] S. Sathyendranath, G. Cota, V. Stuart, H. Maass, and T. Platt. Remote sensing of phytoplankton pigments: A comparison of empirical and theoretical approaches. *International Journal of Remote Sensing*, 22:249–273, 2001.

[39] S. Sathyendranath and T. Platt. Computation of aquatic primary production: Extended formalism to include the effect of angular and spectral distribution of light. *Limnology and Oceanography*, 34:188–198, 1989.

[40] S. Sathyendranath, V. Stuart, A. Nair, K. Oka, T. Nakane, H. Bouman, M. Forget, H. Maass, and T. Platt. Carbon-to-chlorophyll ratio and growth rate of phytoplankton in the sea. *Marine Ecology Progress Series*, 383:73–84, 2009.

[41] E. L. Smith. Photosynthesis in relation to light and carbon dioxide. *Proceedings of the National Academy of Science of the United States*, 22:504–511, 1936.

[42] E. Steemann Nielsen. The use of radioactive carbon (^{14}C) for measuring organic production in the sea. *Journal du Conseil International pour l'Exploration de la Mer*, 18:117–140, 1952.

[43] J. F. Talling. The phytoplankton population as a compound photosynthetic system. *New Phytologist*, 56:133–149, 1957.

[44] W. L. Webb, M. Newton, and D. Starr. Carbon dioxide exchange of Alnus Rubra: A mathematical model. *Oecologia (Berl.)*, 17:281–291, 1974.

[45] B. J. Williams. *Hydrobiological Modelling*. University of Newcastle, NSW, Australia, 1st edition, 2006.

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