**Mediterranean Institute of Oceanography**

# MODELLING: METHODS & APPLICATIONS, Main concepts and contributions to oceanography

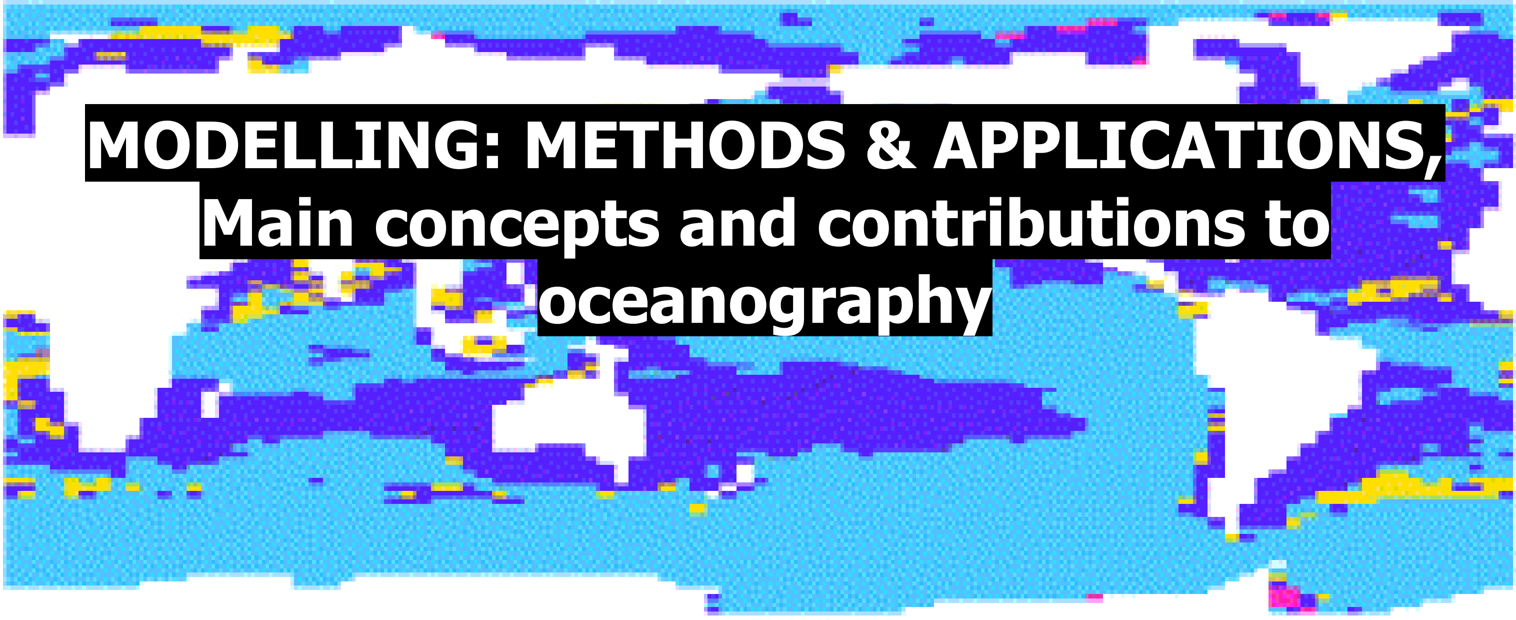
**Copernicus Academy-**

***Frédéric DIAZ***

A) Diatom Nutrient Limitation

Nitrogen 50.04%, Iron 38.75%, Silica 10.57%, Phosphorus 0.548%, Replete 0.0

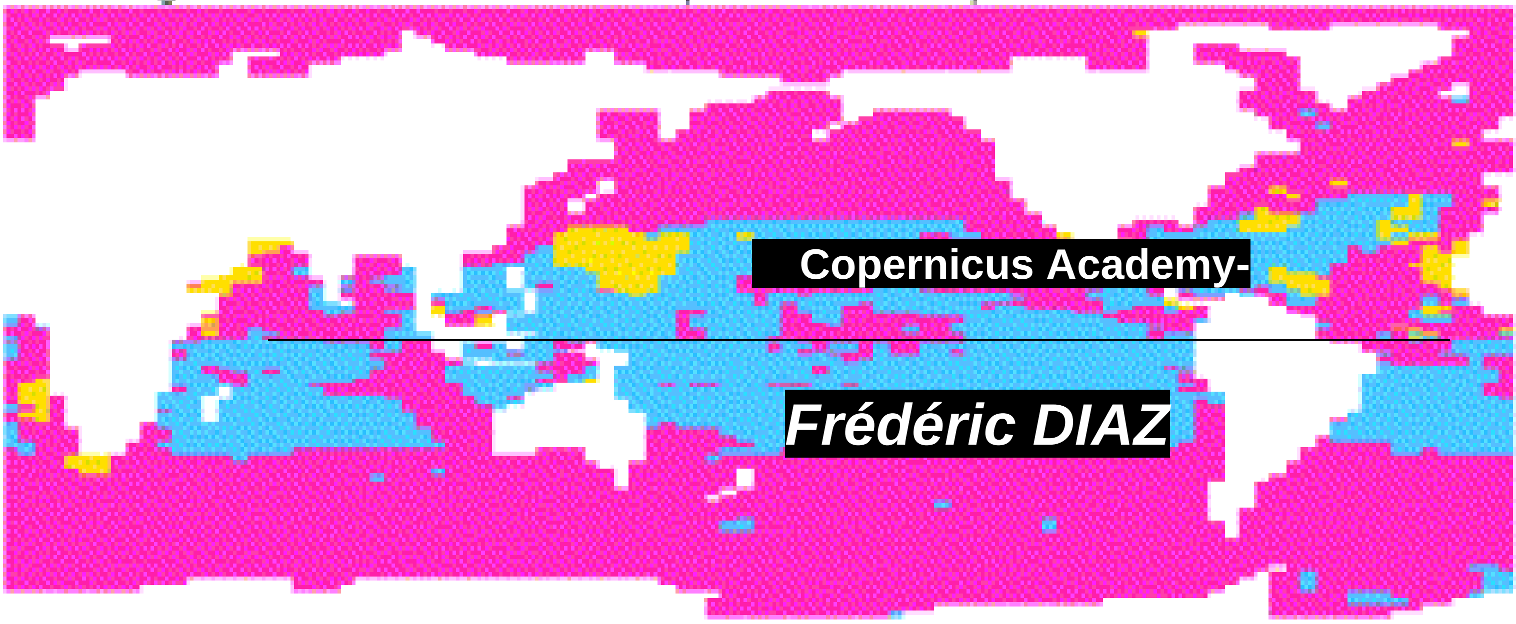
■ Nitrogen ■ Iron ■ Phosphorus ■ Silica ■ Replete



B) Small Phytoplankton Nutrient Limitation

Nitrogen 45.29%, Iron 50.20%, Phosphorus 4.405%, Replete 0.089%

■ Nitrogen ■ Iron ■ Phosphorus ■ Replete



C) Diazotroph Nutrient Limitation

Nitrogen 0.000%, Iron 35.33%, Phosphorus 3.539%, Replete 61.12%

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# MODELLING: METHODS & APPLICATIONS
# Main concepts and contributions to oceanography

## Course by F. DIAZ

## Mediterranean Institute of Oceanography

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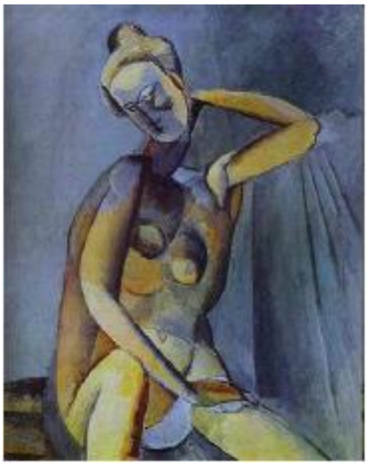
# I. INTRODUCTION

## I.1. What is modelling?

Always keep in mind what a model is: ***a model is a representation of reality***. Pablo Picasso, towards the end of his life, said: “Art is a lie which helps us to understand reality”. Modelling is exactly the same thing…

**Reality**



**Model**

The model captures the specific/essential aspects of reality. Hence, for the same “reality”, we can have several different models.

## I.2. Why we use models in oceanography

The understanding and quantitative description of marine ecosystems requires the integration of hydrodynamics, marine chemistry, and marine biology. The coupling with hydrodynamics, which determines, for instance, the availability of nutrients and the physical positioning of many marine planktonic organisms in the water column, whether on a small or large spatial or temporal scale, is particularly important as these processes cannot be described using just the biology. As it turns out, the most appropriate tool for theoretical investigations on marine ecosystems are coupled models that integrate interactions between hydrodynamics, marine chemistry, and marine biology.

Coupling biological and physical oceanography in a single model has many advantages. For example, we can perform numerical experiments on a system that we can normally only observe at discrete points in time but not manipulate. We can also use the predictive capabilities of models for environmental management applications in coastal areas, for example. On a larger scale, we can study the past and future developments of an ecosystem using experimental diagnostic or predictive simulations. The model is thus used as a tool to improve our understanding of ecosystem functioning. In addition, the use of three-dimensional models can provide an overall synthesis of sparse data by extrapolating the data in a consistent manner. Marine ecosystem models are now widely used for ecological studies, the quantifications of biogeochemical/biological fluxes, or the management of fishery resources. Nevertheless, the implementation of complex coupled models and even the analysis of model output requires some very specific knowledge and skill set, especially with respect to multidisciplinarity. To develop the skills needed to work with coupled models, we will proceed gradually, starting with rather simple models before proceeding to more complex examples. Multidisciplinarity is a requirement that stems from both the diversity of the models used and in the research issues to which modelling is applied (**Figure 1**).

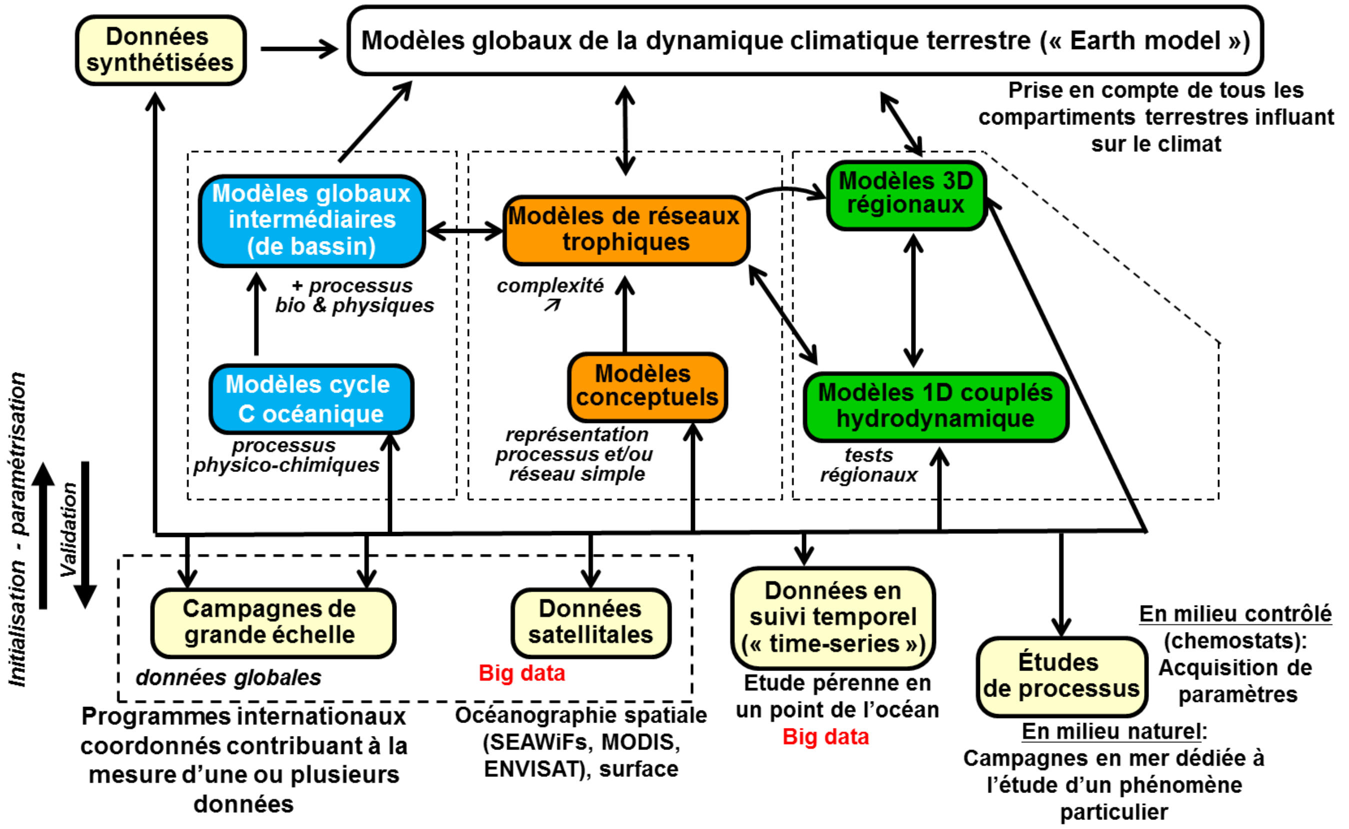


*Figure 1: Relationships between models and data (after the US-JGOFS modelling programme, DONEY et al., 2002).*

## II. GENERAL CHARACTERISTICS OF BIOLOGICAL MODELS APPLIED TO MARINE ECOSYSTEMS

First, how do we define a biological model that is applied to marine ecosystems? We use the word “model” synonymously with theoretical descriptions in terms of sets of differential equations that describe the dynamics of marine food webs. Marine food webs are relatively complex systems that can simply be represented by flows of matter: nutrients to phytoplankton, zooplankton to fish, and the recycling of detritus back to nutrients (**Figure 2**). Phytoplankton communities consist of a wide range of microscopic unicellular plants. They exists in both marine and freshwater systems where they are typically primary producers that convert carbon dioxide and various nutrients dissolved in the water into organic compounds. Phytoplankton have an enormous size range (**Figure 3**). The captured solar energy travels higher up in the aquatic food web through the grazing of phytoplankton by zooplankton. Zooplankton are then consumed by crustaceans and fish which are in turn consumed by humans. There are also return pathways from the various trophic levels back to nutrients through the processes of respiration, excretion, and the remineralization of detrital organic matter through microbial activity. This regeneration of nutrients provides renewed fuel to the photosynthesising primary producers.

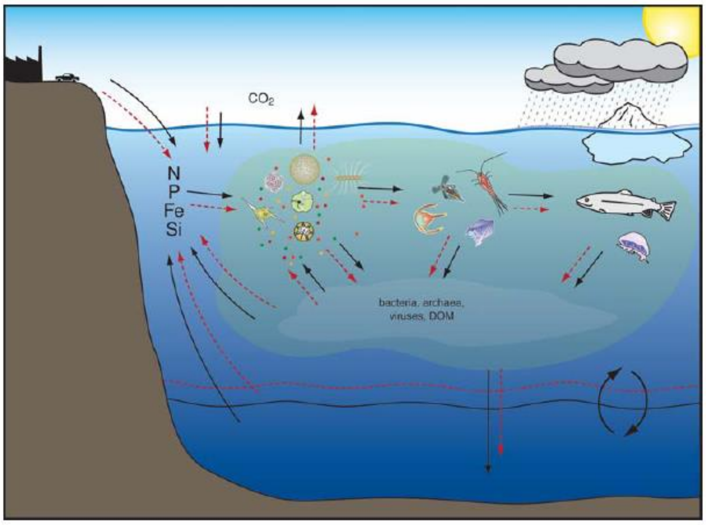


*Figure 2. Schematic of a marine ecosystem: from dissolved nutrients to carnivorous predators. Finkel et al. (2010).*

It is obvious that models cannot possibly capture the entire complexity of the marine food web, given its diversity in life cycles, behaviours, and wide range of scales (**Figure 4**). Plankton are therefore not usually represented as individuals, like fish capable of swimming. Several different kinds of models have been developed to represent particular trophic levels or parts of the ecosystem. In these models, the links between higher (HTL) and lower trophic levels (LTL) is usually directly prescribed or parameterized in a manner that delivers tangible results (we will return to this topic later on in the context of LTL–HTL linkages). To construct such a model, we need to consider the *state variables* that characterize a system. A state variable is what we would like to represent in a model (chemical elements, organisms, etc.). State variables should be well defined and represent measurable quantities such as nutrient or biomass concentrations or abundances such as the number of animals per unit volume.

The dynamics of state variables (i.e., their evolution in time and space) is driven by processes such as nutrient uptake, respiration, predation, and physical processes such as variations in light, turbulence, and advection (the movement of water masses).

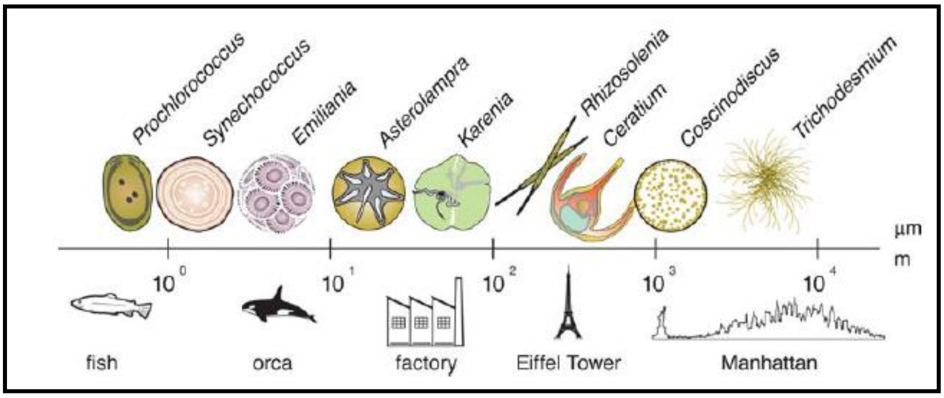


*Figure 3: Relating the wide range of phytoplankton sizes to macroscopic objects (Finkel et al., 2010).*

The different types of ecosystem models can be characterised in terms of their complexity, i.e., by the number of variables represented in the model and the level of resolution of the individual processes (in a sense the level of precision of their representation). The resolution of processes can be reduced/increased by combining several variables/increasing the number of variables. For instance, zooplankton can be implemented as a single biomass compartment or can be described using a series of variables that correspond to the developmental stage of the animal (*cf., also the example later on in the course*). Those models that include a large number of variables are not necessarily "better" than those with a smaller number of variables (*as we will see later on*). The higher the number of variables represented in a model, the more difficult it is to understand and master the internal dynamics in a model. Especially if certain processes are only poorly understood, there is no point in increasing the number of variables if the underlying ecosystem parameters are only poorly constrained (*here, field-model link*). Moreover, in order to gain a deeper understanding of an ecosystem it may not be necessary to represent all processes at a high resolution, and the use of aggregated variables may prove sufficient depending on the question one wishes to address. Before developing a model the goals and questions to be addressed need to be clearly defined so an appropriate methodological approach can be chosen.

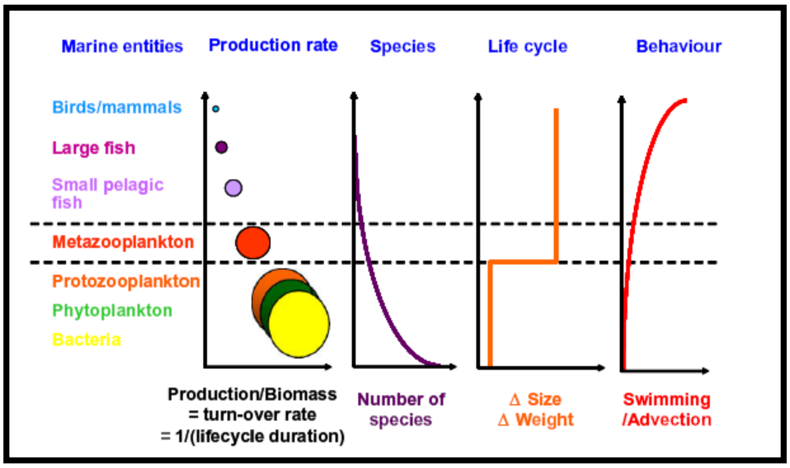


*Figure 4: Schematic showing key differences (production, number of species, life cycles, and swimming behaviour) between different trophic levels in marine ecosystems (Carlotti & Poggiale 2010).*

Models can also be characterized by their spatial coverage, ranging from zero-dimensional box-models (depending only on time) to large-scale 3D models. In box models both the physical processes are greatly simplified while the biology and chemistry may be fairly complex. Such models are easy to use and can serve as a test bed for the development of more complex models. The next level of complexity includes 1D models of the water column (vertical) that allow a more accurate and detailed representation of how physical processes such as vertical mixing or the penetration of sun light affect the biogeochemistry. Such models can be used in areas where horizontal advection is negligible. For the case of coupled 3D physical and biogeochemical model, the biological processes are often represented in a more simplified manner. For example, if we know that in a particular scenario advection plays an important in or even dominates the life cycle of a certain plankton species, then the representation of the biology can be greatly simplified or even omitted entirely (e.g., larvae transported by a current). It is a question of time scale of the biological processes vis-à-vis the physical processes (**Figure 5**). An extreme example of the simplification of the biological processes in a coupled model are simulations of mere particle trajectories where the cells or animals are treated as passive and inert drifting particles (i.e., without any biology).

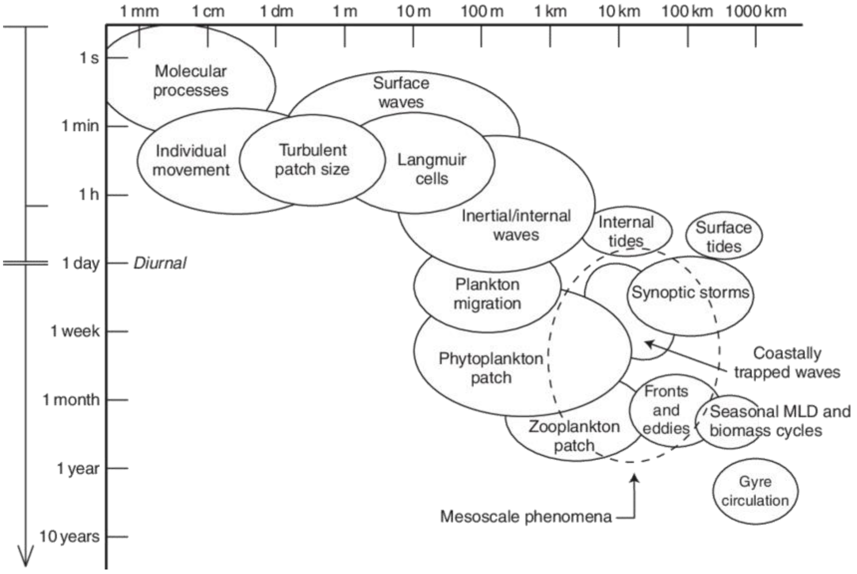


*Figure 5: Spatial and temporal scales for some physical and biological processes in the ocean (adapted from Dickey, 1991).*

Experimental marine ecologists are often uncomfortable with the many simplifying assumptions that go into most models, even with relatively complex models. However, the modelling of marine ecosystems may benefit from the participation of physicists and bio-mathematicians who may help to demonstrate how simplified formulations of causal relationships in these models may be able to reproduce the dominant characteristics of observable phenomena.

In this context, it is very interesting to reread the point made by Gordon Riley, one of the pioneers of marine plankton modelling. In his famous 1946 paper (Riley, 1946) he wrote: “In this respect physical oceanography, one of the youngest branches in actual years is more mature than the much older study of marine biology. This is perhaps partly due to the complexities of the material. More important, however, is the fact that physical oceanography has aroused the interest of a number of men of considerable mathematical ability, while on the other hand marine biologists have been largely unaware of the growing field of bio-mathematics, or at least they have felt that the synthetic approach will be unprofitable until it is more firmly backed by experimental data.”

Another important problem that complicates the use of coupled models is that biological/biogeochemical processes are typically governed by equations that are highly nonlinear and cannot be solved analytically in a straightforward manner. Thus, the first attempts to represent the dynamics of marine ecosystems were delayed or even halted due to mathematical difficulties. These problems could only be overcome in the mid-1980s with the advent of more powerful computers and the implementation of numerical methods to solve the associated equations. This frustrating situation could have been one of the reasons why marine biologists did not pay much attention to mathematical models for several decades.

With computers becoming increasingly powerful, the technical problems were gradually overcome, although interdisciplinary discussions on modelling did not develop until much later. Although models have been widely accepted and the benefits been recognised by a growing community, many marine biologists still doubt whether we can learn anything from models.

So why do we need models? There are several reasons:

1. To improve our understanding of ecosystems (using models as tools),
2. To provide a quantitative description of certain processes (production, respiration) at scales that differ from those at which they are typically observed (integrative tools),
3. To synthesize knowledge in a spatial and/or temporal manner, budgets,
4. To establish a link between theory and observations,
5. To respond to societal demands for forecasts; be that in the form of operational models for weather forecasts (short term up to a few days) or to produce medium/long term predictions (simulating different scenarios of the future evolution of ecosystems).

<u>*Note*</u>. It is also possible to create hindcasts, *i.e.,* retrospective “predictions” of the past. We can study a particularly important event or period in the past ecosystem in order to gain a better understanding of the future.

Models are mathematical tools that allow us to analyse, synthesize, and test our understanding of the dynamics of a system through predictive and retrospective simulations. The comparison of modelling results with experimental data allows models to be ***validated*** (how realistic is the model compared to observations). Due to the sub-sampling of field data, models usually cannot be fully validated. Most of the time, model validation simply quantifies the fit between the model and the data. Unfortunately, until fairly recently a common approach was to optimize the fit by adjusting the parameters (i.e., changing them in a trial-and-error fashion, the so-called tuning) of the mathematical formulas of the modelled processes, often termed model calibration (**Figure 6**). It is crucial that the number of fitted parameters is not too large because a fitted model with too many parameters that is tuned expressly for a comparison with existing observational data has no predictive capabilities. It only works well for a given situation, the one for which it was calibrated, but fails for any other type of situation. There are solutions in the form of mathematical methods to obtain the best set of parameters in a model (data assimilation using optimal control theory). The best set of parameters is the one for which the sum of errors between the data and the model is minimal.

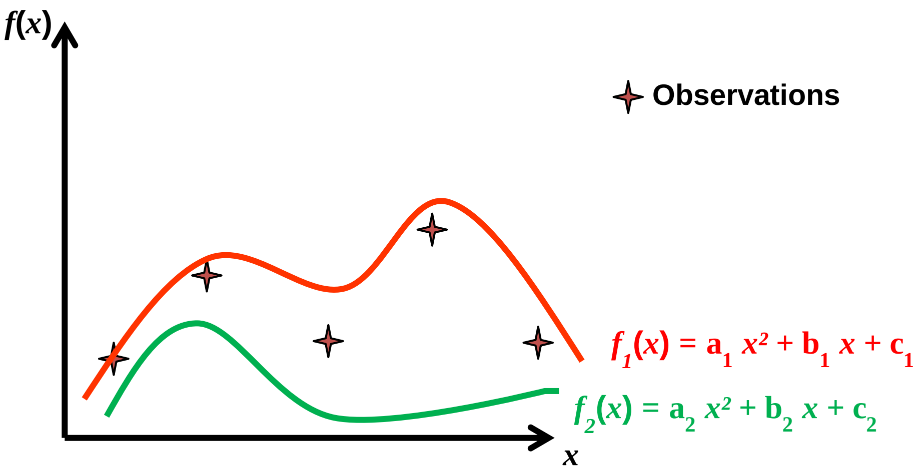


*Figure 6: Principle of model calibration and the tuning of parameters to fit a set of observations. a, b, and c are the parameters of the mathematical function (f, here a polynomial) used to describe the process (observations); two sets of parameters have been tested: ($a_1$, $b_1$, $c_1$) and ($a_2$, $b_2$, $c_2$).*

Most modellers nowadays have a good knowledge of physics and mathematics and the modelling of marine ecosystems is, in essence, multidisciplinary. This branch of contemporary oceanography requires a close collaboration between biogeochemists/biologists and modellers in order to be able to ask the right questions and develop theoretical descriptions of the most important processes in order to improve our understanding of ecosystem dynamics (e.g., nitrogen fixation, schools of fish, etc.). The development of this interdisciplinary dialogue must begin at the level of universities where students in biogeochemistry/marine biology must acquire the theoretical bases in mathematics and physics to be able to build a biological/biogeochemical model, or at least, to be able to closely cooperate with modellers. These are the ultimate goals of this course. Furthermore, you will learn how to critically assess model results and the way how models are constructed.

## III. FROM NUTRIENT MODELS TO MODELS OF HIGHER TROPHIC LEVELS

If we assume that all processes in the marine ecosystem would be perfectly known and described by a set of mathematical equations, one would expect to be able to predict the state of an ecosystem by solving the equations for an initial state and given external forces. Unfortunately, while this may be possible for a non-biological physical system (such as an inert particle), systems that include interactions between chemistry and biology pose problems that are much more complex to solve than non-living systems. Why? Because the equations governing biochemical dynamics cannot be derived explicitly from the conservation laws of Newtonian mechanics or from fluid dynamics. The biological equations are typically derived from observations and are therefore of an empirical nature. Do not confuse this with what is often termed **mechanistic** approach, which refers to models that simulate a process using laws that precisely describe the underlying mechanisms. A mechanistic approach requires a very detailed knowledge of the process and its mathematical representation should therefore be very similar if not identical is different models as the equations are meant to represent the mechanism; the parameters used in the mathematical formulation may still vary though. In biology, the mechanistic approach is rarely used because the mechanisms within cells or the interactions between organisms are not sufficiently well known to be represented in this way. Whatever approach is considered, observational knowledge must be transcribed into mathematical formulations in order to be able to simulate the process ($f(x) = ax+b$ **or** $g(x) = e^{ax}$) and to access the parameter values used in these formulations.

### III.1. Models of individuals, populations, and biomass

In the natural world, aquatic ecosystems are made up of individuals (unicellular organisms like phytoplankton, metazoans like copepods or fish) that have a certain biomass and can form so-called populations.

Thus, we can differentiate between different types of aquatic ecosystem models:

- Individual based models (IBMs),
- Population models (modelling ensembles of individuals as a shoal of fish),
- Biomass models (simulating the biomass of certain species or communities expressed as mass/number per unit volume or total mass),
- A combination of IBMs and population models,
- Models that combine dynamic aspects of populations, biomass, and individuals.

IBMs thus try to simulate the basic units of biological systems while biomass or population models represent the number or the mass of many individuals per unit volume. IBMs can account for genetic variations among individuals or individual behaviour in response to environmental cues while population or biomass models represent the ensemble average of the individuals.

Although individuals are the basic units of ecosystems, it is not always necessary to resolve individual properties. Biomass models are robust and often have an experimental significance as the use observable quantities (the amount of chlorophyll is a proxy for phytoplankton biomass, groups of individual cells) as state variables.

There is no general rule for how a system can be simplified. A common sense rule states that models should be as simple as possible and as complicated as necessary to answer a given specific question. Simple models containing just one state variable only need one mathematical equation but require a larger dataset to function.

Let us consider the concrete example of a model that is trying to describe the dynamics of a marine species using the biomass of that species as its only state variable. This species interacts with the surrounding environment: it feeds and releases organic or inorganic compounds into the environment. For a phytoplankton/fish species, the mathematical function that describes the uptake of nutrients/predation needs to know the abundance of nutrients/prey in order to function; i.e., we may need to use maps of monthly averaged *in-situ* nutrient concentrations/prey abundances. Likewise, mathematical models describing the movement of copepods (zooplankton), jellyfish, or fish larvae (including biological processes such as individual growth) require knowledge of available food or prey for the entire modelled domain. The need for such data corresponds to the notions of *boundary conditions*, *initial conditions*, and *validation* (for the latter, see above). The initial conditions correspond to the starting point of the model, i.e., the data that the model uses at start-up. Care must be taken with these initial conditions as they can significantly affect the simulation outcome if the model does not perform very well. In this context, we speak of the model sensitivity to initial conditions. In general, the more robust a model, the less sensitive it will be to the initial conditions requiring only a short spin-up time. The spin-up time is the time it takes the model to become independent of the initial conditions. We therefore never use the model output from the spin-up period. We must also consider that the model needs data at the borders of the model domain irrespective of whether it is a 1D or 3D model. During a simulation, the model needs to be “fed” with data at the model boundaries. Most 1D or 3D models only represent a small part of the ocean, but we cannot usually neglect exchanges across the model boundaries since the ocean is an open environment. The modelled quantities can leave or enter the modelled domain. Thus, there is a need for observational data to be able to prescribe these inputs/outputs at the model boundaries. When exchanges are allowed to happen, we speak of open boundaries. In a coastal scenario, land would represent a closed boundary but may still have some input locally, e.g., through a river flowing into the sea adding sediments, chemicals, etc.

The more complex the model, the more state variables we have and the greater the data requirements. Therefore, it would be wrong to assume that the more sophisticated a model, the less data you need. Today, and particularly in oceanography, we often do not collect sufficient amounts of data (because of the high cost involved) and rely quite strongly on model results which can be a mistake. In general, the more complex the model, the more information it needs to function (parameters, initial conditions, validation, boundary conditions).

Coming back to the question of model complexity and simplification, models with several state variables can describe complex dynamic interactions. For example, the interactions between food resources and predators can be modelled in such a way that any variations in fluxes can be calculated internally within the model. We will see later that coupling biomass or population models with IBMs may reduce the need for observational data (external forcing). Due to the advent of ever more powerful computers, it is increasingly easy to envisage the implementation of integrated models with these kinds of connections between sub-models.

### III.2. Modelling the low trophic levels (LTL)

A certain class of model that will be of particular interest to us in this course is the models dealing with the low trophic levels of the marine ecosystem, i.e., from nutrients to zooplankton. These types of models are typically "cut off" at the zooplankton level. Any activities and dynamics of higher trophic levels are usually implicitly prescribed using a so-called top-down approach. Implicit means that zooplankton predation by fish is included in the zooplankton mortality term, i.e., without explicitly representing any fish. Why do we cut at the zooplankton level? Simply because it is a key level that combines characteristics (**Figure 4**) that belong to both to the smallest organisms (plankton) and largest ones (multicellular with different stages of development, capabilities of migration, etc.).

Many biological models describe plankton dynamics in marine ecosystems in terms of biomass, and we can cite several seminal papers: Riley (1946), Cushing (1959), Steele (1974), Wroblewski & O'Brien (1976), Jansson (1976), Evans & Parslow (1985), or Radach & Moll (1990).

For instance, the ecological model by RILEY (**Figures 7 & 8**) is based on some fundamental work by Riley and Sverdrup during the 1940/50s on phytoplankton/zooplankton interactions and the role of water column stability for the onset of phytoplankton blooms (Riley, 1942). Why do we speak of an ecological rather than a biogeochemical model? Simply because ecological models do not contain a single chemical element (such as nitrate or phosphate) as a state variable.

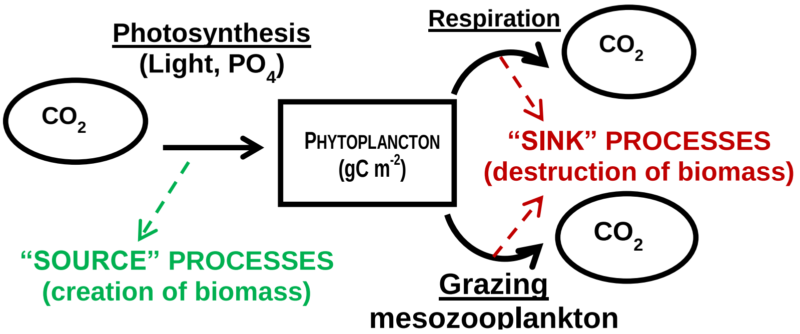


*Figure 7: The ecological model by Riley (1946).*

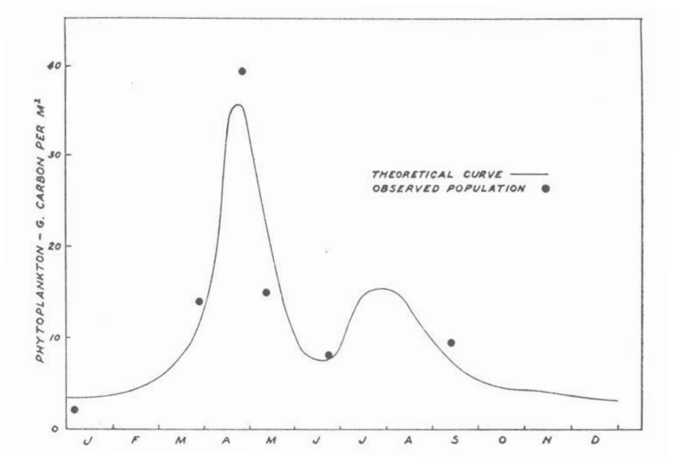


*Figure 8: Comparing model output to data*

This very simple model can reproduce the seasonal cycle of phytoplankton biomass, albeit only by using very large sink terms (respiration and grazing) and limiting the source terms to prevent excess amounts of biomass, especially in summer. The parameters of this model have thus been "tuned" to yield a better match with observations. This can pose a problem with regard to the degree of realism one wishes to maintain, considering that parameters should usually stay within the bounds dictated by observations. For instance, if a certain parameter needs to be set to 10 times the maximum observed value in order for the model to be able to reproduce *in situ* observations, then the model may suffer from a conceptional flaw or bias.

A model that was frequently used by the international scientific community in the context of the JGOFS program was the biogeochemical model by FASHAM et al. (1990). This type of model (**Figure 9**) gave birth to the famous NPZD (Nutrient, Phytoplankton, Zooplankton, Detritus) models. These models became possible due to an improved understanding of the euphotic zone during the 1960s and 70s (importance of zooplankton predation, recognition of nitrogen as limiting element of global primary production, notions of new/regenerated and exported production, microbial loop). In this type of model, there is no notion of specific or functional diversity, nor of stages of development. We speak of a "bulk" model.

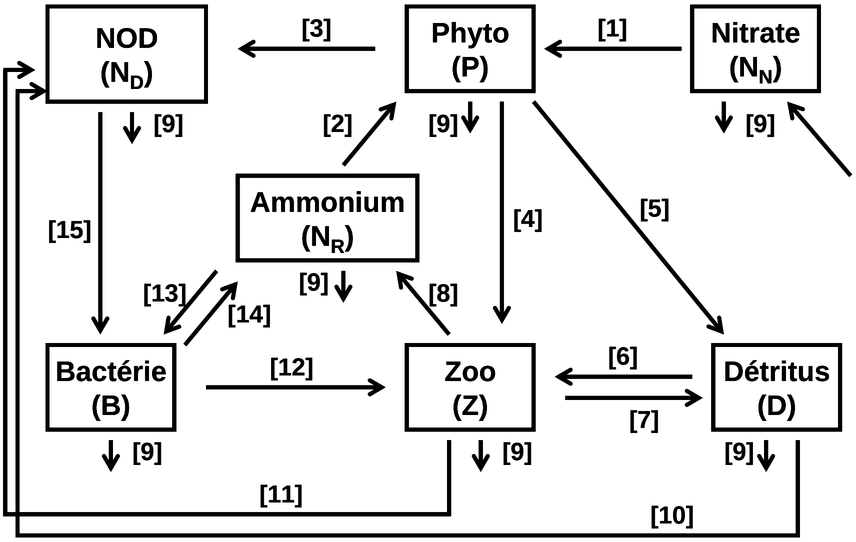


*Figure 9: Representation of the biogeochemical model by Fasham et al. (1990). [1]: Uptake of nitrate ($NO_3$) by phytoplankton, [2]: Uptake of ammonium ($NH_4$) by phytoplankton, [3]: Excretion of dissolved organic nitrogen (DON) by phytoplankton in the form of urea, liquid waste, [4]: Grazing of phytoplankton by zooplankton, [5]: phytoplankton mortality, [6]: Uptake of detritus by zooplankton, [7]: Mortality + faecal pellets by zooplankton, [8]: Excretion of $NH_4$ by zooplankton, [9]: vertical diffusion by turbulence (physical process), [10]: remineralisation of detritus into DON, [11]: Excretion of DON by zooplankton, [12]: Predation of bacteria by zooplankton, [13]: Uptake of $NH_4$ by bacteria, [14]: Excretion of $NH_4$ by bacteria, [15]: Uptake of DON by bacteria*

With knowledge of biogeochemical processes in marine ecosystems continually improving, by the 1990s the concept of nitrogen limiting all primary production was increasingly called into question and a new concept of zones was introduced: the "HNLC" (High Nutrient Low Chlorophyll) zone which is particularly ubiquitous in the Southern and Equatorial Pacific Oceans (where different elements can be limiting: iron, phosphate, and silicate). The biogeochemical models thus has to evolve to take different biogeochemical cycles into account (multi-element models), namely carbon (for the biological pump), nitrogen, phosphorus, silicate, and iron (**Figure 10**). A certain degree of diversity therefore appeared in this type of model due to the subdivision of plankton into compartments according to the type of chemical element they were taking up. There is therefore an additional chemical cycle represented in the model, which only concerns part of the model.

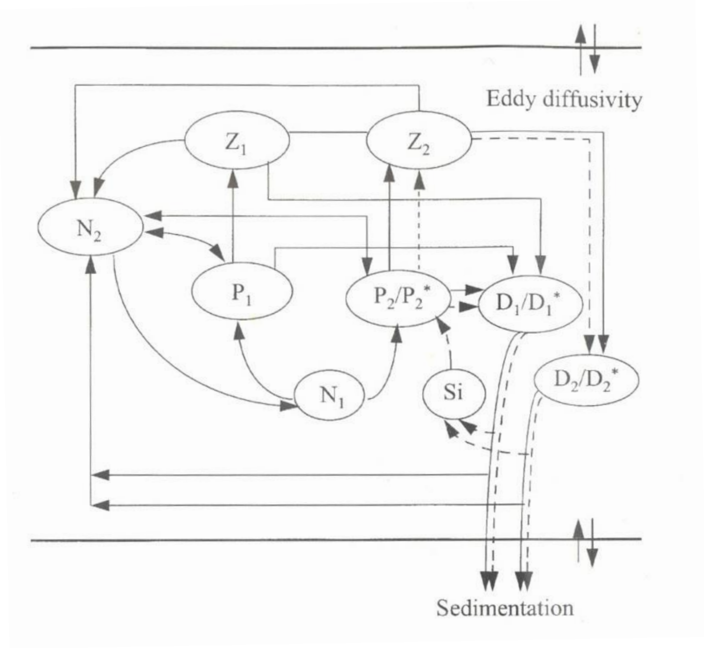


*Figure 10: Block diagram of the biogeochemical model by Pondaven et al. (1999) applied to HNLC zones, representing nitrogen and silicate cycles in 9 different compartments. Dotted arrows: silicate flux; solid arrows: nitrogen flux. The asterisk marks those variables that are also expressed in silicate.*

Over the past decade, the concept of plankton functional groups (Le Quéré et al., 2005) has appeared in biogeochemical oceanography. We even speak of "**functional diversity**". These plankton groups play a key role in controlling the oceanic carbon fluxes; for instance, diatoms for how they export carbon as particulate carbon and biogenic silicate; coccolithophores as they export carbon in the form of calcium carbonate ($CaCO_3$); or *Trichodesmium* for their role in nitrogen fixation. Furthermore, micro-zooplankton has an impact on the amount of carbon in the euphotic zone. One of the most complex models ever constructed and still in use today is the biogeochemical multi-element multi-functional group model of the global ocean (**Figure 11**) by Vichi et al. (2007).

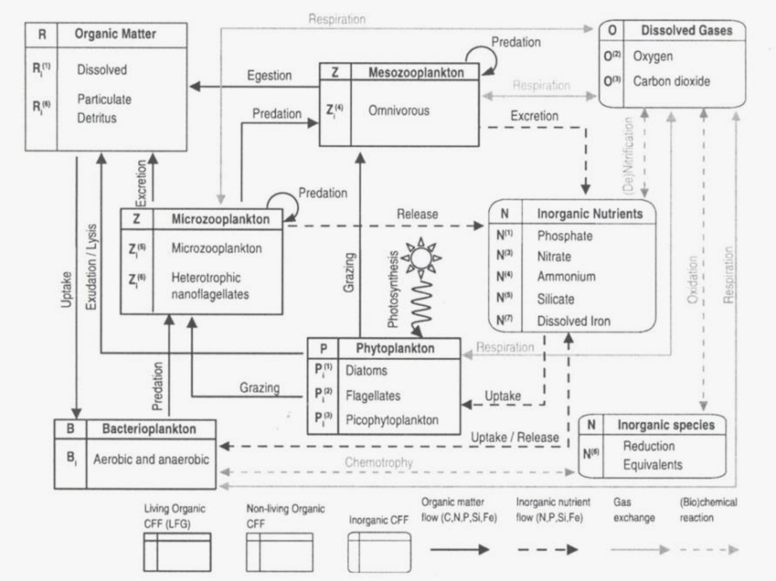


*Figure 11: Schematic of the stat variables and biogeochemical interactions in the BFM (Biogeochemical Fluxes Model) by Vichi et al. (2007). Living organic Chemical Functional Families (CFF).*

The vast majority of LTL models are biomass models. Why? Because *in situ* measurements typically consist of biomass per unit volume rather than the total number of cells which would justify using an IBM approach. Moreover, an IBM approach is only possible if the modelled species is sufficiently well known, especially its physiology; this is rather rare for plankton. IMB models are therefore much less abundant in the literature. Nevertheless, there are some studies on cell-based processes for which the physiology is sufficiently well known such as plankton photosynthesis and nutrient uptake (*e.g.,* ZONNEVELD, 1998 ; CIANELLI et al., 2009 ; Ross & Geider, 2009). More work seems to have been done on zooplankton and larvae (crustaceans, fish, molluscs, etc.) which are metazoans for which observations and case studies are easier to carry out (*e.g.,* CARLOTTI & NIVAL, 1992 ; GUIZIEN et al., 2006 ; EISENHAUER et al., 2009, see **Figure 12 ;** VAUGEOIS et al., 2013, see **Figure 13**).

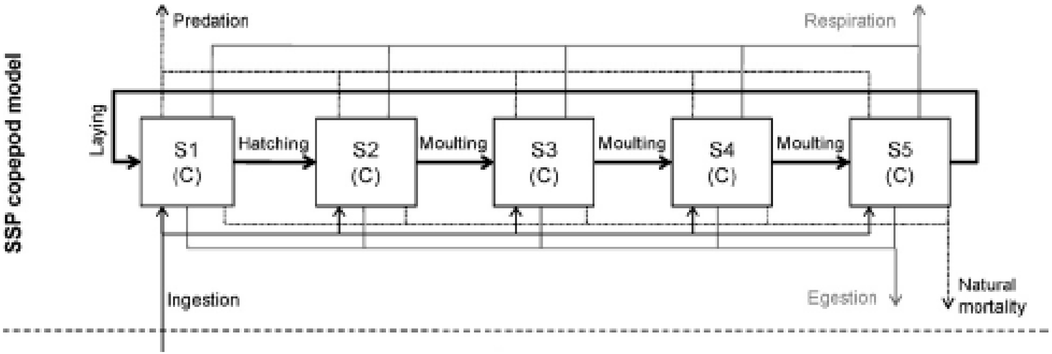


*Figure 12: Copepod IBM representing the different stages of development. S1: eggs and nauplii living on their yolk reserves, S2: nauplii already searching for food, S3 and S4: copepodid, S5: adults.* Fom E*ISENHAUER et al. (2009).*

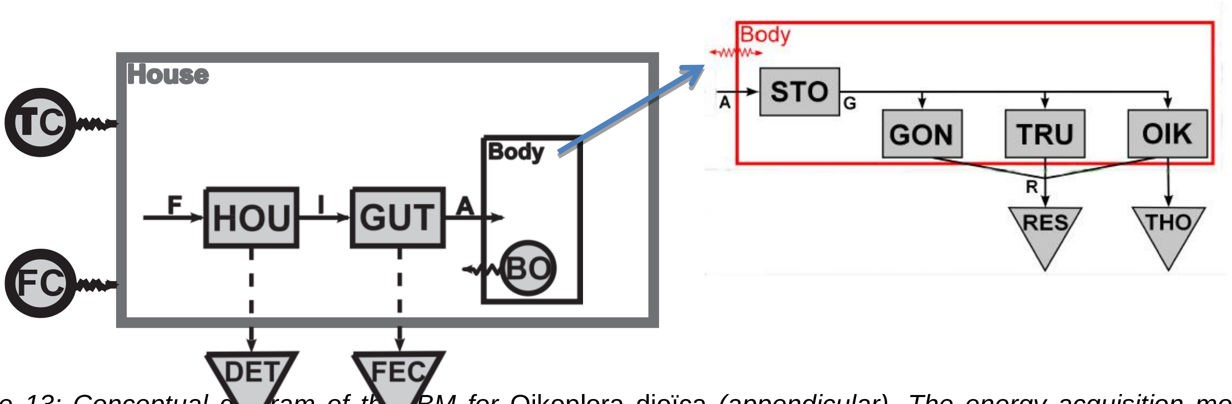


*Figure 13: Conceptual d ram of th BM for* Oikoplora dioïca *(appendicular). The energy acquisition model is forced by temperature (TC) and external nutrient concentration (FC). The model contains state variables (rectangles) and diagnostic variables (triangles). All variables are expressed in terms of carbon biomass: house (HOU), gut (GUT), body (BO), waster accumulated in the house and released into the environment (DET), accumulated faecal pellets (FEC) during the lifetime of the organism. Filtration (F), Ingestion (I), Assimilation (A). For details see* V*AUGEOIS et al. (2013). The state variables for the allocation of energy in the form of carbon (on the right) are the reserves (STO) available for growth, reproduction, and maintenance, the gonads (GON), the trunk (TRU) and oikoplast epithelium (OIK). There are two diagnostic variables: total mass of carbon released through respiration (RES) and in the form of houses (THO) during the organism's lifetime. Growth flux (G), respiration flux (R). For details see* V*AUGEOIS (2014).*

### III.3. <u>Modelling high trophic levels (HTL)</u>

By high trophic levels we mean all types of marine organisms greater than mesozooplankton (i.e. >200 µm). This can of course include fish but also large marine mammals, various crustaceans (e.g., Krill) and molluscs (cephalopods). This can therefore include both plankton and nekton.

Currently, these models are widely used for the management of present and future fish resources and their results are widely used and analyzed by decision-makers both at the local and international level (for the creation of marine reserves, managing commercial fish stocks and setting quotas, etc.). A central question that these models must often find an answer to is:

how many fish can be extracted from the ocean without permanently decimating the resource? The answer is never straightforward or unambiguous because the socio-economic conditions (fishing technologies, fuel prices, degree of organization of fishing professions) of the fishing activity must be taken into consideration. Therefore, to be able to make predictions we must use population models (of abundance) of key HTL species and combine them with socio-economic fishery models, the latter often come with great uncertainties as the human factor comes into play.

HTL stock estimation models come in two broad categories: ***analytical models*** (Gulland, 1974) and ***production*** or ***logistic models*** (Rothschild, 1986).

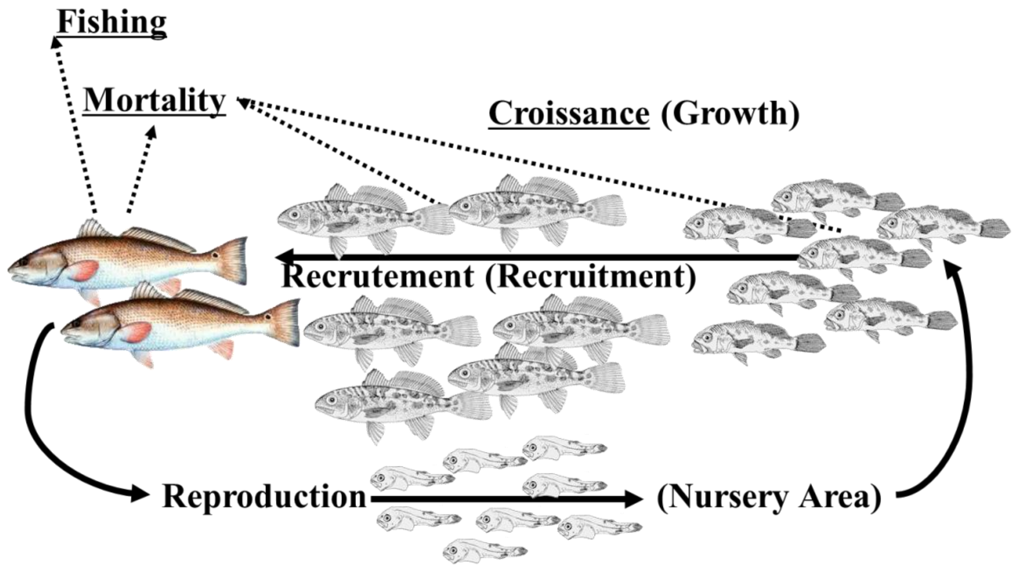


*Figure 14: Processes taken into account in an analytical HTL model of fishes.*

In ***analytical models***, an HTL population is taken as the sum of its individuals (i.e., total number, abundance) and the dynamics are typically controlled by ***three processes*** (**Figure 14**): ***growth***, ***mortality*** and ***recruitment*** (reaching a level of maturity/age class that allows the fish to be caught, recruitment differs for each species: for hake anchovies the recruitment period is 1 year, for instance) from which we need to subtract the losses due to fishing. In these models, the life cycles of HTL species need to be well known and taken into account. The mortality term is usually composed of a fishing-related mortality and a natural mortality (senescence). From the abundance calculated by the model we can obtain the total biomass using the average mass (weight) of each age group.

In analytical models, a fish population with abundance, n, is the sum of the individuals constituting the population and the individual's dynamics are controlled by the aforementioned growth, mortality, and recruitment. The change in abundance over time, $\frac{dn}{dt}$, can thus be written as:

$$\frac{dn}{dt} = G - M + Re\ (-P)$$

This equation can be combined with an equation that describes the change of mass (weight), *w*, of each individual in order to estimate the biomass of each individual in an age group. The change in an individual's mass can be described using an equation of the type $\frac{d}{dt}w = \gamma \cdot w$ with a solution $w(t) = w_0 \cdot \exp(\gamma \cdot t)$ where $w_0$ is the initial mass and $\gamma$ the effective growth rate that depends on the stage of development or the age of the individual. The growth equation for the mass of an individual can also take another form such as the one based on the von Bertalanffy growth function (**Figure 15**): $w(t) = w_\infty(1 - e^{\gamma(t-t_0)})^b$. Where w(t) is the weight at age t, $w_\infty$ is the maximum attainable body mass, $\gamma$ the effective growth rate, $t_0$ the hypothetical age at which the individual has mass zero, and *b* an allometric growth parameter (typically 3). These types of models are combinations of population and individual growth models (the weight is linked to size through $w(t) = a \cdot (L_t)^b$ with $L_t$ the body length at time t, *a* is a scaling constant, and *b* an allometric growth parameter (~3); the body length is usually linked to the age).

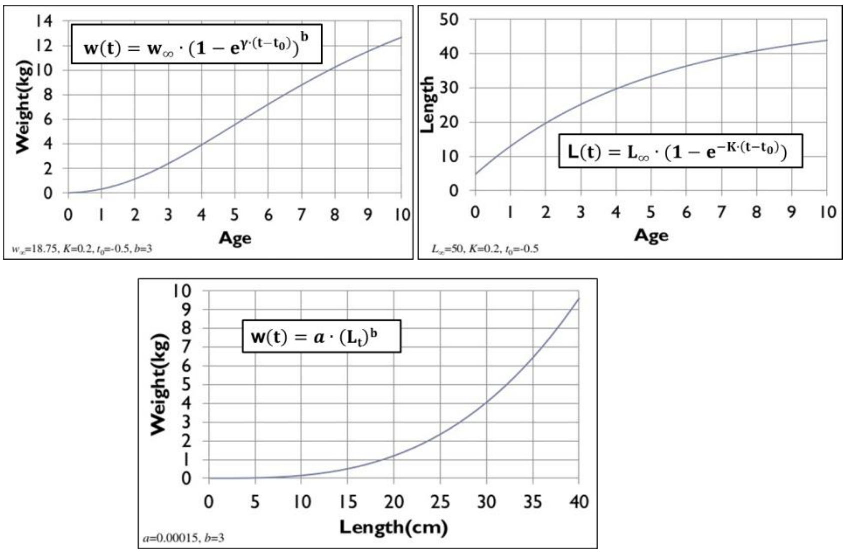


*Figure 15: Relating weight to age (von Bertalanffy), size to age (von Bertalanffy), and weight to size (allometric).*

**Production** (or **logistic**) models treat fish populations as a whole, calculating changes in the total biomass as a function of the current biomass and the fishing effort without taking the population structure (age, weight, size) explicitly into account. The change in biomass, *B*, can be written as:

$$\frac{dB}{dt} = f(B),$$

Where *f*(*B*) could take the following form $f(B) = \alpha \cdot B \cdot (B_0 - B)$ with $\alpha$ a constant. Clearly, the change in biomass will tend toward zero as the biomass itself becomes zero and at a certain equilibrium value $B=B_0$ the population is stable. This model is typically a biomass model.

These models can be further divided into single-species ("individual-based model") and multi-species models (**Figure 16**). Multi-species models can account for trophic interactions between different species, which are usually neglected in single-species models. As we will see towards the end of this course, HTL models largely ignore any links with the lower trophic levels. In particular, environmental conditions and any "bottom-up" effects are neglected (e.g., they use plankton prey densities that are constant in time and space).

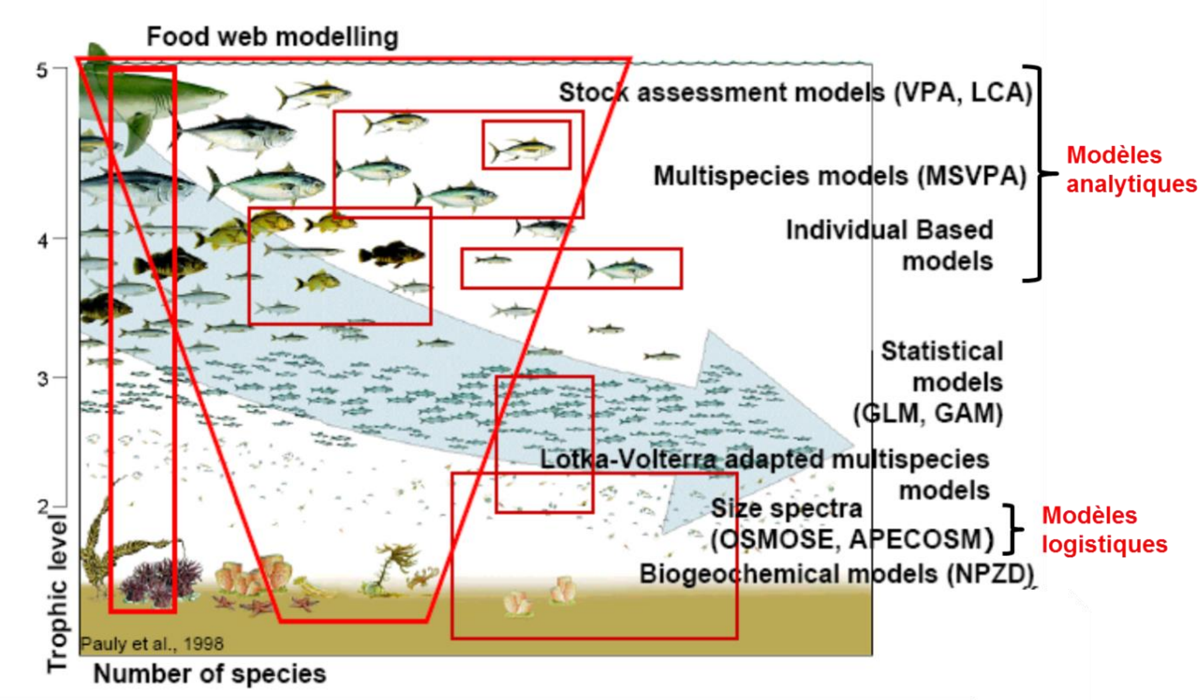


*Figure 16: Different types of HTL ecosystem models depending on the number of species and the trophic level (taken from* S*OLIDORO* & L*IBRALATO, 2008).*

Fish migrations are typically modelled by combining an individual-based approach (IBM) with the output of mean current fields from a hydrodynamic model. The resulting "Lagrangian" trajectories can be calculated from either archived current information or directly using the output from the circulation model. Active movements of the individuals such as swimming, swarming, or ontogenic migrations can therefore be combined with the movements imposed by the main currents. It is difficult to find mathematical formulations of the behavioural response to environmental signals such as light gradients, temperature, salinity, prey, or predator avoidance. The individual-based Lagrangian models consist of two sets of equations: a first series to describe the development of an individual under the given environmental conditions, and a second series to determine the individuals' trajectories by integrating the velocity field of the currents obtained from a circulation model or archived data.

In general, models of fishery resources (i.e., analytical) strongly depend on the data available to characterize the fish stocks (tonnages caught, stomach contents to have an idea of the diet, individual sizes and weights, etc.). This type of model requires much more diverse and comprehensive observational data (HORBOWY, 1996) than biomass production models (i.e., logistic). *In-situ* data is usually obtained from surveys at sea, e.g., using acoustic instruments to detect pelagic species and abundances, or commercial data on the catch per unit effort (CPUE).

Nevertheless, these data are often weakly constrained (often just one sampling per year) and can induce uncertainties due to sub-sampling for example. Data consistency can be improved using statistical methods and by incorporating biological parameters that are independent of catch data. Although fishery resource models (i.e., analytical) essentially omit the lower part of the food web, they still assimilate fishery data containing a lot of implicit information in the observational data (e.g., many fish in one place could mean a significant amount of food there), and it is still necessary that these data exist in the first place.

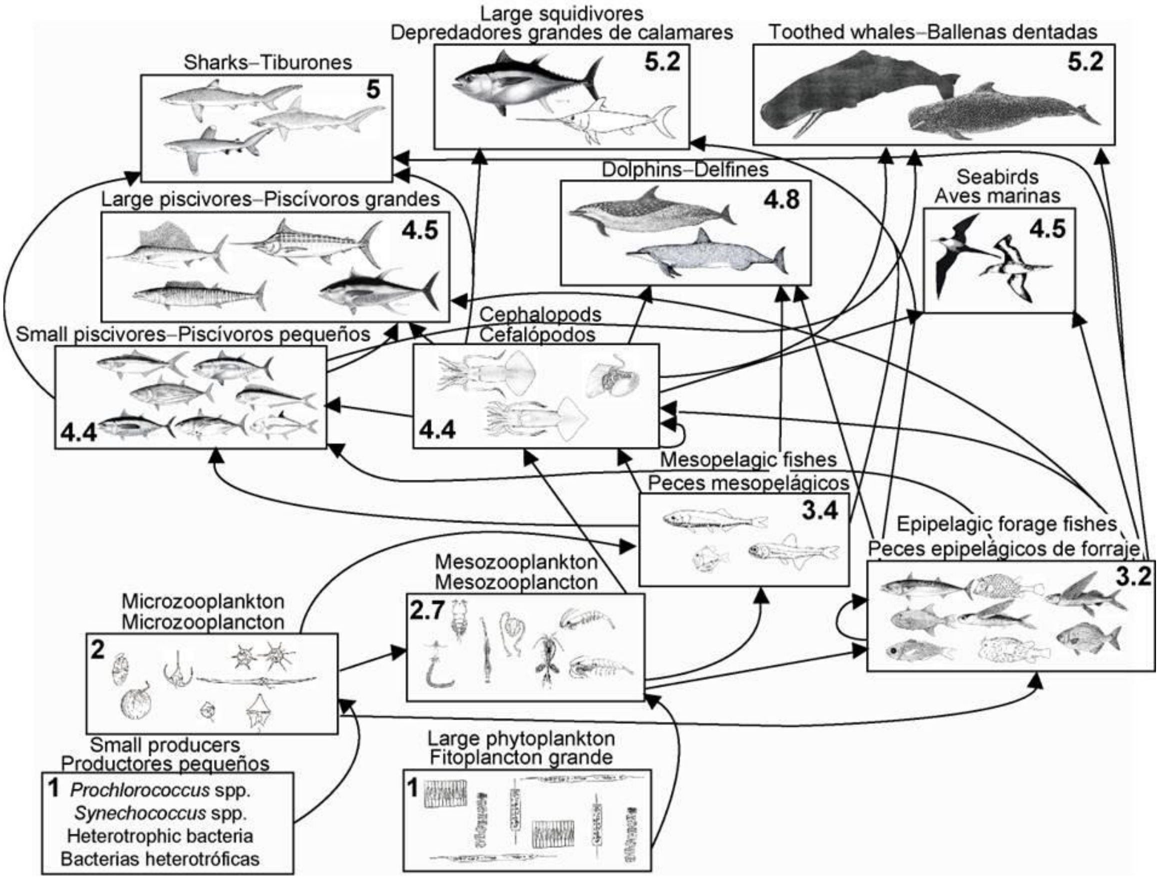


*Figure 17: Example of a “one-way” ecosystem model, the Ecopath model of the pelagic ecosystem in the Eastern Pacific Ocean (Olson and Watters, 2003).*

### III.4. Nature of the linkages between HTL and LTL models

For a long time, one of the main weaknesses of HTL models was them largely ignoring any “bottom-up” effects from LTLs as a resource (see reviews by Hollowed et al., 2000; Shin et al., 2004) or even variations in environmental conditions. Effectively, they represented unidirectional or so-called “one-way” models (**Figure 17**), for instance, employing resource fields that were constant in time and space or ocean currents that never changed strength or direction. In this context, the HTL model is forced by the LTLs and we cannot speak of coupling. These models also did not consider any feedback (top-down effects via predation) on the dynamics of prey such as plankton. For example, in terms of environmental processes, some studies observed changes in the recruitment of some fish species due to a reduction in oxygen in some areas, which was in turn due to a change in the prevailing currents; others saw changes in the dispersal of fish eggs due to changes in prevailing winds and current fields. These physical processes can also affect the size structure of the prey community or their speed of development (they can arrive too early or too late for the developmental stage of their predator => match/mismatch phenomena).

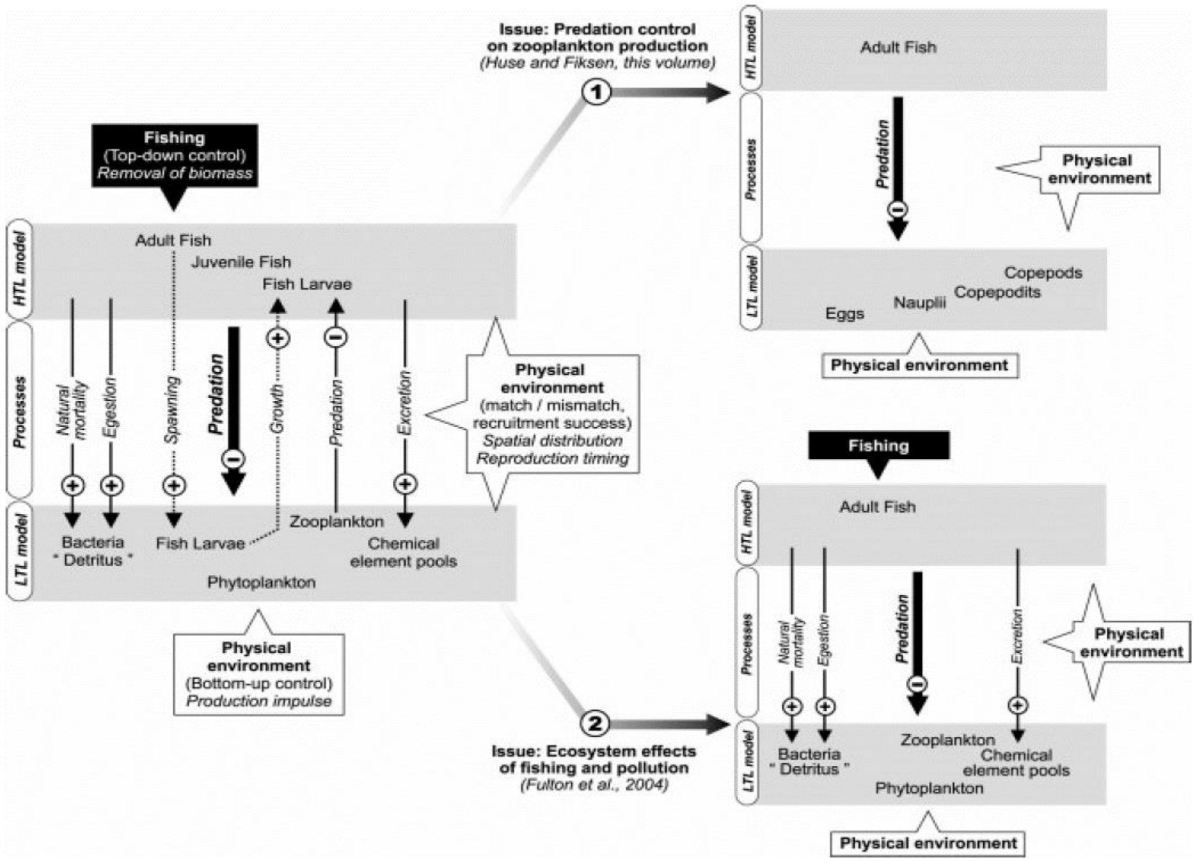


*Figure 18: Schematic diagram of end-to-end models employing two-way coupling (SHIN et al., 2010). Left: complete model showing the different compartments of the LTL and HTL models and the processes taken into account as well as the forcing by the physical environmental. The + and – sings indicate the source and sink terms, respectively. Right: two examples of how an end-to-end model was simplified in different ways to address a particular research question.*

These “one-way” models are rapidly disappearing now as they do not provide good results in terms of future projections and even fail to adequately represent the status quo in HTL stocks. They are being replaced by a new kind of model, the so-called “end-to-end” (SHIN et al., 2010, **Figure 18**) models. These are models that aim to represent the ecosystem in its entirety from the dynamics of micro-organisms and dissolved chemicals (nutrients and also certain pollutants) to the highest trophic levels including even human activities (*e.g.,* ROSE et al., 2010; TRAVERS et al., 2007). Furthermore, it is now common practice to include all sorts of feedbacks between the different model compartments, i.e., interactions are no longer unidirectional or one-way but rather bidirectional (“two-way” coupling). We therefore speak of two-way coupled end-to-end models.

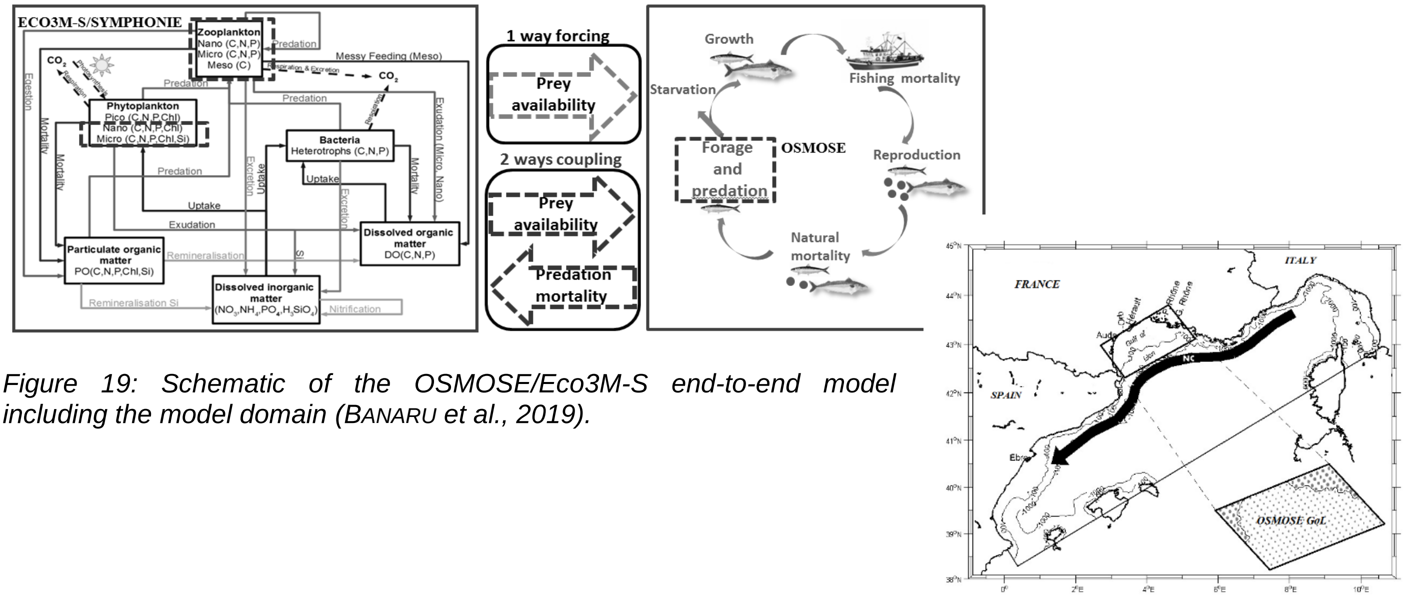


*Figure 19: Schematic of the OSMOSE/Eco3M-S end-to-end model including the model domain (Banaru et al., 2019).*

These types of models are by no means easy to construct, implement, operate, and analyse. Why? While the life cycles of HTL organisms can last several years with migrations over large distances, the relevant time and space scales of environmental variations and of LTL organisms (e.g., plankton) are generally much shorter: from minutes to seasons with strong annual and interannual variations and from 1 m to tens of kilometres.

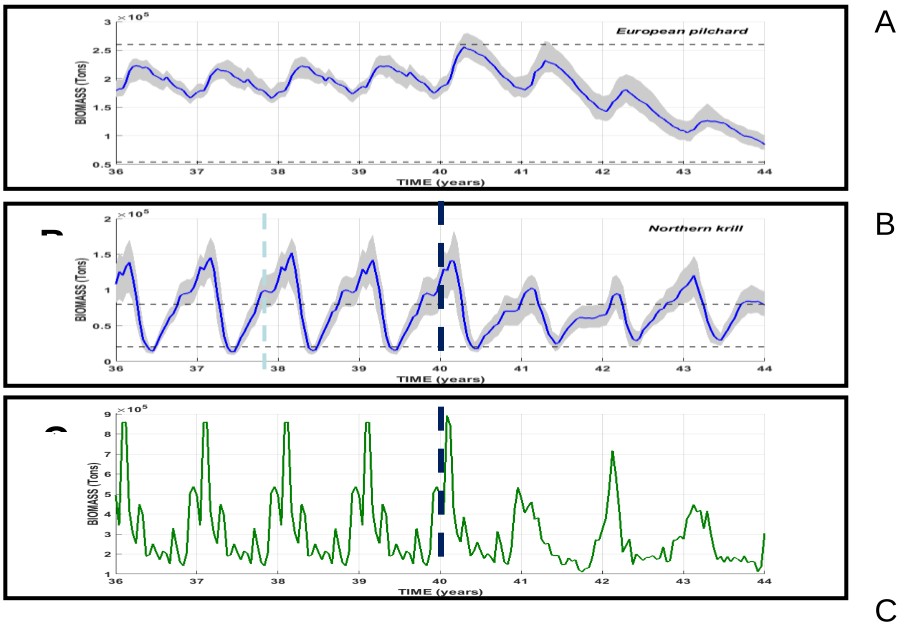


*Figure 20: Output from the OSMOSE/Eco3M-S end-to-end model operated in "one-way" mode (years 36 to 39) and in "two-way" mode (years 40 to 43) showing the biomass for (A) sardines, (B) krill, and (C) microphytoplankton in the Gulf of Lion (Diaz et al., 2019).*

Models that include a "bottom-up" control (prey) and environmental effects on HTL dynamics thus have to account for processes from within very large ranges in spatial and temporal scales including possible memory effects of the ecosystem. The integration of "bottom-up" effects into models of fishery resource management and stock assessment is a difficult task and an field of ongoing research for the years to come.

We end this section with three figures providing examples of end-to-end models for the Gulf of Lion, an active field of research at the MIO. The work uses a coupled hydrodynamic-LTL model (ECO3M-S) and the HTL OSMOSE model (Figures 19-21). The figures show the emerging differences when moving from a one-way forcing to a “two-way” coupling of the HTL and LTL models.

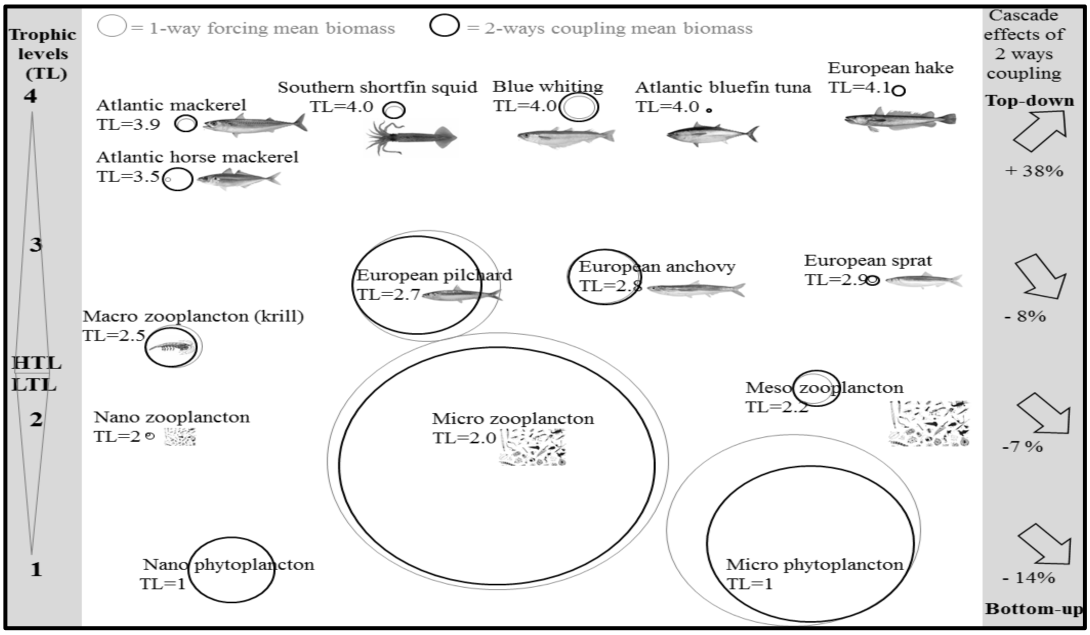


*Figure 21: Illustrating of the effects of trophic cascades on the species biomass in the OSMOSE/Eco3M-S model used in both the “one-way” and “two-way” modes (Diaz et al., 2019). Arrows indicate trends in biomass changes between the two modes while the size of the circles is proportional to the biomass of the species.*

## IV. BASIC CONCEPTS AND PROCESSES FOR THE CONSTRUCTION OF A BIOGEOCHEMICAL MODEL OF A PLANKTON ECOSYSTEM

Biogeochemical models of planktonic ecosystems provide tools to describe, understand, and quantify the material flows within a food web as well as interactions with the atmosphere and sediments. Such models often use what are called functional groups or even groups of species in their own right, but they tend to ignore differences between individuals. Phytoplankton or zooplankton are reproduced using state variables, which, by definition, include all effects resulting from chemical and biological transformations. Ideally, the state variable and the processes should be well defined. However, some processes like cell death are very difficult to quantify. Thus, this type of model can contain parametrisations that are weakly constrained, which poses a problem for the validity of the model outputs. Weakly constrained means that there is often insufficient observational data to properly constrain certain model parameters, i.e., we do not know what a realistic range might be for certain parameters.

## IV.1. Some basic principles for constructing a biomass model

To illustrate the process of model construction, we will start with building simple models that describe certain parts of the pelagic ecosystem. Unlike physical hydrodynamics for which the equations have precise mathematical formulations, the mathematical formulations for planktonic ecosystem models must be derived from observations (i.e., empirically). Ecological principles such as the Redfield Ratio (REDFIELD , 1963), i.e., a fixed molar ratio of the main biogenic elements in living cells, von Liebig's law on limiting factors (DE BAAR, 1994), or size considerations (big eats small) provide a basic framework for constructing the equations. However, these axiomatic principles do not yield any precise mathematical formulation that is required for modelling.

We need to start by identifying the scientific question we would like to address, as this question will determine the type of model and the processes we want to describe with the model. As an example, we will construct a model to simulate the seasonal cycle of phytoplankton at mid-latitudes. The model should be able to quantitatively describe the transfer of inorganic nutrients through the lower trophic level (phytoplankton, zooplankton, bacteria, etc.) and to correctly estimate the changes in biomass in response to changes in external forcing. Once we have identified the questions and goals, we need to determine the variables and processes that should be included in the model and which mathematical formulations to be used to describe them.

A model is characterized by the choice of its variables. State variables are expressed as concentrations or abundance that can be directly compared to *in situ* observations. Concentrations or abundances usually depend on spatial and temporal coordinates and their dynamics are governed by processes that also vary in both time and space and that may depend on other system-specific variables. State variables have a numeric value and a dimension, e.g., mass per unit volume (mmol $m^{-3}$) or a number of individuals per unit volume (number of cells per litre). The processes are generally expressed by rates with an inverse dimension to time, *e.g.*, $day^{-1}$ or $s^{-1}$.

### IV.1.1. Mathematical representation of the nutrient-phytoplankton interaction

We start with a simple pelagic ecosystem model with well-described nutrient dynamics. Primary production, a function of light, allows the growth of algal biomass, which also depends on the uptake of nutrients. Part of the phytoplankton biomass dies and is transformed into detritus. The detritus is then recycled into dissolved nutrients through remineralization processes and becomes available again to phytoplankton. This last step closes the loop and turns this into a closed process. One of the fundamental laws to which biogeochemical models must adhere is the **conservation of mass (“nothing is lost, everything is transformed”,**

**Lavoisier**). The total mass, M, can be expressed as the mass of one of the chemical elements required by phytoplankton and often the Redfield ratios are used to estimate the other constituents. Typically, one chooses for example to express the model in nitrogen or carbon as the main "currency" of the model to quantify the plankton and the detritus. Since all changes in mass in an ecosystem model are controlled entirely by the source and sink terms we can write:

$$\frac{d}{dt}M = sources - puits \tag{1}$$

The use of differential equations means that state variables can be thought of as continuous mathematical functions in time and space. Examples for source and sink terms are the input of external nutrients by a river (source) or the entrapment of nutrients in the sediment (sink). The transfer of nutrients within the food web takes place through processes such as nutrient uptake during primary production or through the transformation of microorganisms, i.e., by mineralization or grazing.

The key problem in building a model is to find adequate mathematical formulations to describe these transformations of matter. Processes such as primary production or mineralization are complex and their mathematical description may require significant simplifications.

To illustrate this procedure, we can start with a simple example of a transformation process characterized by a first order chemical reaction where a substrate **S** will be converted into a product **P** with a constant rate **k** as shown in **Figure 22**.

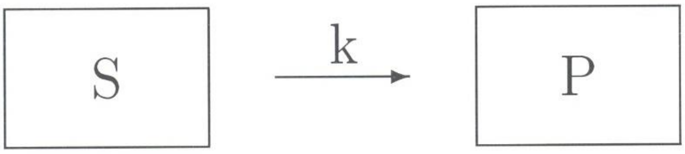


*Figure 22: Conceptual diagram to illustrate a first order chemical reaction.*

Initially, at time t=0, we only have a substrate $S(0)=S_0$ and no biomass $P(0)=0$. By assuming that the concentration of the substrate decreases at the same rate as the product increases, we obtain the following system of equations:

$$\frac{d}{dt}S = -k \cdot S, \quad \frac{d}{dt}P = k \cdot S \tag{2}$$

If we add these equations, we obtain

$$\frac{d}{dt}(S+P) = 0 \tag{3}$$

Eq. (3) expresses the conservation of mass in the absence of external sources or sinks. By integrating Eq. (3) we obtain $S+P=C$, where C is the constant of integration given by the initial condition $S(0)=S_0=C$ and thus $P=S_0-S$.

Integrating Eq. (2) yields $S= S_0\, e^{-kt}$ and $P=S_0\,(1-e^{-kt})$.

This solution describes a chemical process controlled by a rate constant where the substrate is entirely converted into a product. The initial concentration of product is zero and the transformation of substrate into produce is independent of the concentration of product. **Figure 23** (upper panel) shows the solution to this mini-system.

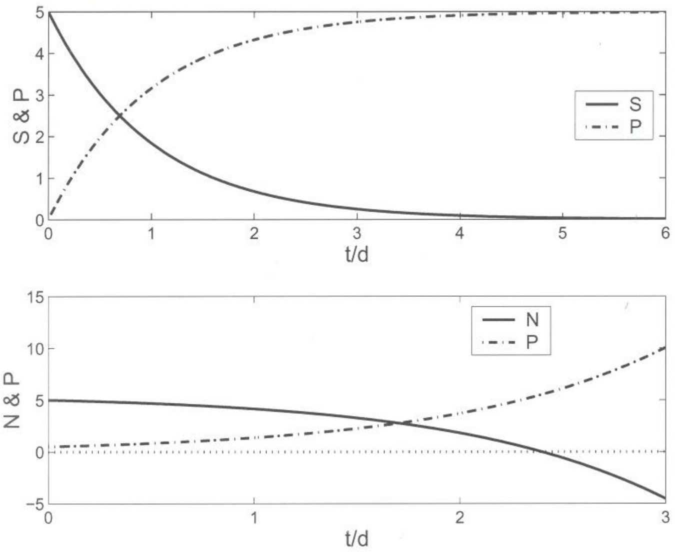


*Figure 23: Top: Evolution of a system where a substrate S is transformed into a product P through a first order chemical reaction. Initial conditions: S0=5 mmol m$^{-3}$, P0=0 mmol m$^{-3}$, and k=1 d$^{-1}$. Bottom: An attempt to model the uptake of a nutrient, N, by a phytoplankton, P, in a fashion that is analogous to a first order chemical reaction. Initial conditions: N0=5 mmol m$^{-3}$, P0=0.5 mmol m$^{-3}$, k=1 d$^{-1}$. Note that the modelled nutrient concentration becomes negative, i.e., this approach is unrealistic.*

The question one might ask is: can such an approach be used to model phytoplankton growth? Primary production depends on light and nutrients. Let us assume that the substrate corresponds to the nutrient, **N**, and the product corresponds to phytoplankton, **P**. We need to take into account that primary production can only occur if there is a non-zero initial population of phytoplankton. Phytoplankton growth thus depends on the existing phytoplankton concentration, P, and on the amount of nutrients that can be taken up as the phytoplankton grows. We can thus formulate the following approach:

$$\frac{d}{dt}P = k \cdot P, \quad \frac{d}{dt}N = -k \cdot P \qquad \text{if the system is conservative} \tag{4}$$

with initial conditions P(0)= $P_0$ and N(0)=$N_0$. The conservation of mass requires that:

$$P + N = P_0 + N_0 \tag{5}$$

which yields the following solutions P= $P_0\,e^{kt}$, N=$N_0$ + $P_0\,(1-e^{kt})$.

This result appears to be quite similar to Eq. (2). Nevertheless, this system of equations becomes unstable because after a certain time, **$\tau$,** all nutrients should be taken up and growth should stop, which is not the case (see **Figure 23**, lower panel). The time, **$\tau$,** after which the concentration of N becomes zero is given by N=0 $\Rightarrow$ $N_0$ + $P_0$=$P_0e^{k\tau}$ which yields $\tau = \frac{1}{k} \cdot \ln\left(1 + \frac{N_0}{P_0}\right)$.

To resolve this problem we can try a different approach where growth depends explicitly on the nutrient concentration (in addition to the phytoplankton concentration), i.e., it will decrease as the nutrient concentration decreases. This would be achieved by the following system of equations:

$$\boldsymbol{\frac{d}{dt}P = k' \cdot N \cdot P, \quad \frac{d}{dt}N = -k' \cdot N \cdot P} \tag{6}$$

Here, *k*' is the rate *k* divided by a reference value of N, say $N_0$. Using the conservation of mass again (Eq. 5), we can write:

$$\frac{d}{dt}P = k' \cdot \left(N_0 + P_0 - P\right) \cdot P, \tag{7}$$

The integration of this equation can be achieved through the separation of variables:

$\frac{dP}{\left(N_0 + P_0 - P\right) \cdot P} = k' \cdot dt$ and though integration by parts ($\int u \cdot v' = [u \cdot v] - \int u' \cdot v$) we get

$$Ln\frac{P}{N_0 + P_0 - P} = \left(N_0 + P_0\right) \cdot \left(k' \cdot t + C\right).$$

The constant of integration, *C*, is given by the initial conditions: $C = \frac{1}{N_0 + P_0} \cdot \ln\left(\frac{P_0}{N_0}\right)$. This gives the following result for *P*:

$P = P_0 \cdot \frac{P_0 + N_0}{P_0 + N_0 \cdot e^{(-k' \cdot (N_0 + P_0)t)}}$ and $N = N_0 \cdot \frac{\left(P_0 + N_0\right) \cdot e^{(-k' \cdot (N_0 + P_0)t)}}{P_0 + N_0 \cdot e^{(-k' \cdot (N_0 + P_0)t)}}$

**Figure 24** shows ta graphical representation of the solution using the following parameter values: $N_0$=5 mmol $m^{-3}$, $P_0$=0,5 mmol $m^{-3}$, k'=k/$N_0$= 0,2 $d^{-1}$ $mmol^{-1}$ $m^3$, and k= 1 $d^{-1}$.

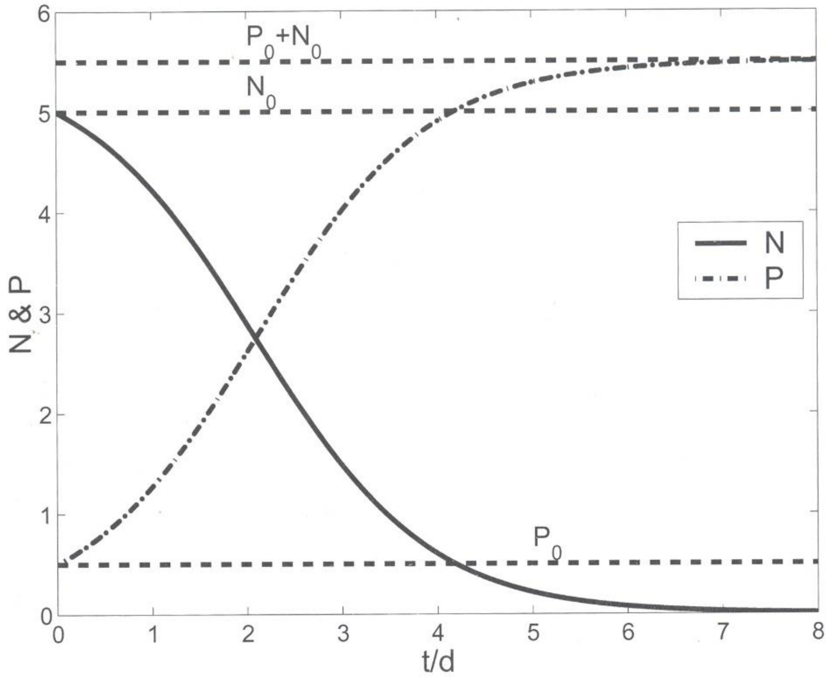


*Figure 24: Temporal evolution of the nutrient and phytoplankton concentration when using a growth rate that depends on the nutrient concentration.*

We note that over time all nutrients are taken up by the phytoplankton: P→$N_0$+$P_0$ and N→0. The numerical solutions to this set of equations are thus stable. Mathematically, this is due to the quadratic term in *P* in Eq. (7). A weak point in Eq. (6) is that the growth rate increases with increasing nutrient concentration, without limit, although laboratory studies clearly show that the growth rate reaches a maximum at some point at which the addition of further nutrients does not result in further increases in growth. We therefore need a more sophisticated approach. Unfortunately, this new approach will result in a set of equations that can no longer we solved analytically but solutions need to be found using specialised numerical methods.

### IV.1.2. Representing nutrient limitation of phytoplankton growth

The factors controlling primary production, namely the availability of light and nutrients, are not constant but vary over time. Hence, the rates such as *k* defined for the above chemical reactions cannot be considered constant and we need to find a more accurate representation. An important concept association to uptake processes is the famous law of the minimum first introduced by von Liebig in the 19th century (de Barr, 1994). The law of the minimum states that plant growth is dictated not by the total resources but by the scarcest resource (carbon, nitrogen, phosphorous, etc.). This principle was first discovered in the field of agricultural science and was used to design fertilisation strategies since the end of the 19th century. A second important point is the fact that carbon, nitrogen, and phosphorous exist in fixed molar (Redfield) ratios of C:N:P=106:16:1 in living marine phytoplankton. This has important implications for models as we can simply represent just one of these elements and will know the abundance of the other two by applying the above Redfield ratios.

Let us know look at how the availability of nutrients affects phytoplankton growth. Let *N* be the nutrient concentration and *P* the phytoplankton biomass that grows proportionally to *P*, then we can write:

$$\frac{d}{dt}P = r_{\max} \cdot f(N) \cdot P,$$

$r_{\max}$ is the maximum growth rate and depends on intrinsic cellular properties of the particular species for a given temperature and light availability. $f(N)$ is a concentration dependent term with $0 < f(N) < 1$, such that if the nutrient concentrations are high we have $f(N) \approx 1$ and a further increase in nutrients will not lead to any additional increase in *P*. In contrast, when the nutrient concentration becomes low, growth should stop and as we have $f(\mathrm{N}) \sim \mathrm{N}^{\upsilon}$ (with $\nu$ a positive integer). Based on lab experiments, Monod (1949) found an empirical relation for this term:

$$f(N) = \frac{N}{k_N + N} \tag{8}$$

with $\mathrm{k_N}$ the half-saturation constant, i.e., $f(\mathrm{N})=0.5$ when $\mathrm{N}=\mathrm{k_N}$. For $\mathrm{N} \gg \mathrm{k_N}$ we have $f(\mathrm{N})=1$ while for $\mathrm{N} \ll \mathrm{k_N}$ we get $f(\mathrm{k_N}) \approx \mathrm{N}/\mathrm{k_N}$. Hence, this Monod formulation resolves the problems we had encountered with Eqs. (4) and (6).

The Monod equation describes the speed of a reaction. It is also known as the Michaëlis-Menten equation (Michaëlis & Menten, 1913) and was derived from experiments on enzymatic reactions.

When we compare the MONOD equation (Eq. 8) with the theory on enzymatic reactions, it is not very evident why nutrient uptake in phytoplankton should follow the same dynamics as enzymatic reactions. Consequently, we return to the two constraints mentioned earlier: growth is stopped once there are no more nutrients and growth is independent of the nutrient concentration above a certain threshold. Hence, any mathematical formulation that meets these two requirements can be used. For instance:

$$f(N) = \frac{N^2}{k_N^2 + N^2} \tag{9}$$

or

$$f(N) = \frac{2}{\pi} \cdot \arctan\left(\frac{N}{k_N}\right), \text{ and } f(N) = 1 - \exp\left(-\frac{N}{k_N}\right).$$

A graphical representation of these functions is shown in **Figure 25**.

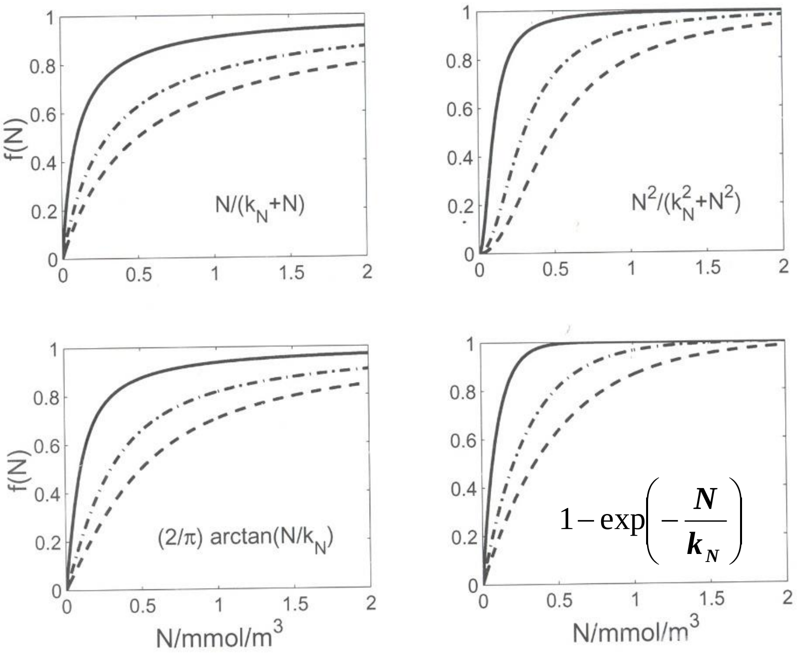


*Figure 25: Four function types that meet the requirements for phytoplankton growth (see text) using half-saturation constants of $k_N$ = 0.1 mmol $m^{-3}$ (solid line), $k_N$ = 0.3 mmol $m^{-3}$ (dash-dotted line), $k_N$ = 0.5 mmol $m^{-3}$ (dashed line).*

We can see that when N=$k_N$ we have *f*($k_N$)=0.6321 in the exponential and 0.5 in the other three functions. Hence, in the exponential $k_N$ cannot be considered as a half-saturation constant in the true sense of the name.

We can now rewrite Eq. (6) using any of the above functions describing nutrient limitation. Using the example of the MONOD function, we get

$$\frac{d}{dt}N = -r_{\max} \cdot \frac{N}{k_N + N} \cdot P, \quad \frac{d}{dt}P = r_{\max} \cdot \frac{N}{k_N + N} \cdot P \tag{10}$$

The dynamics of these equations is shown in **Figure 26**. We can see that the uptake is weaker when using a Monod-type *k*’ than with a constant *k*’. Nevertheless, the results are fairly similar overall. The advantages of having a Monod-type limiting function are two-fold: (i) k does not need to be normalised with some randomly chosen concentration, and (ii) the dimension of $r_{\max}$ is inverse time.

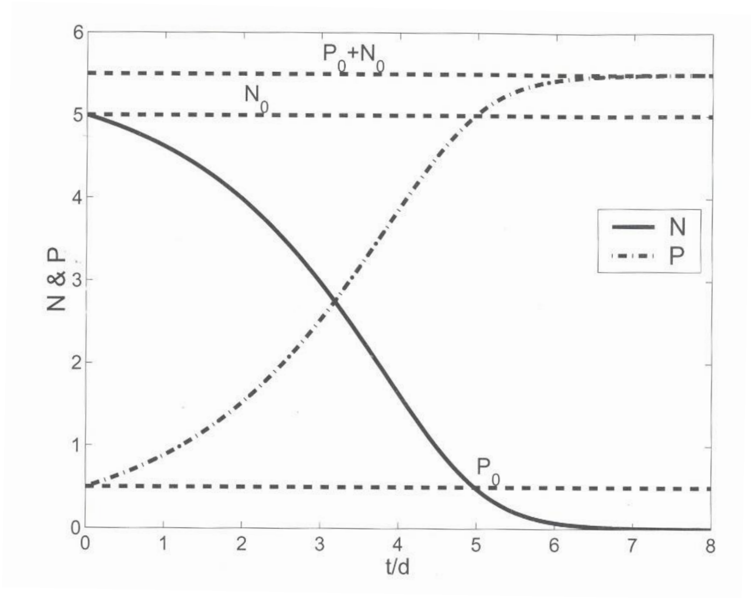


*Figure 26: Growth-nutrient dynamics for a formulation using the Monod equation (Eq. 10) and the following parameter values: $r_{max}$= 0,8 $d^{-1}$ and $k_N$ = 2 mmol $m^{-3}$.*

IV.1.3. Recycling of organic matter

For now, we have considered nutrient uptake by phytoplankton using Eqs. (6) and (10) which describe a process where the nutrients at entirely transferred to the phytoplankton cells. The steady state is reached once the nutrients are depleted. In this section, we introduce a return path for nutrients to go from phytoplankton back into the water column by creating a new variable, *detritus*, and introducing two new processes: (i) phytoplankton mortality (through viral lysis and senescence), and (ii) a rapid recycling of detritus through respiration and remineralization (implicitly). These processes can be combined to create a simple algal primary production model. The simplest model to describe such as system would be an NPD model, which stands for Nutrients, Phytoplankton, and Detritus. Such a model can be used to describe phytoplankton growth in a chemostat (without zooplankton) or if the losses due to zooplankton grazing are parameterised in a higher mortality term. Based on von LIEBIG'S LAW, we can assume that one particular nutrient may be the limiting resource (e.g., nitrogen which is the main limiting nutrient in many marine environments). We therefore express all state variables in terms of nitrogen, especially detritus, which becomes particular organic nitrogen. The structure of such a model is shown in **Figure 27**.

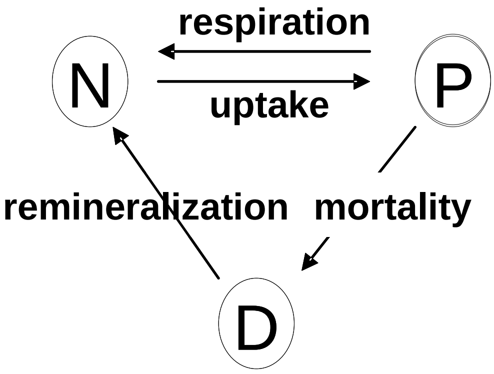


*Figure 27: Conceptual diagram of a simple NPD model.*

The primary production of phytoplankton **P** depends on the amount of light and nutrient uptake, here represented by dissolved inorganic nitrogen (DIN) **N**. The cell metabolism and respiration establish a direct link between phytoplankton and DIN. Through mortality, phytoplankton becomes detritus, **D**, which in turn becomes again DIN via remineralisation processes.

The processes can be described using transfer terms such as $L_{XY}$ or $l_{xy}$, which can be read as a loss from X to Y where the lower case notation in $l$ refers to a constant rate while an upper case letter typically denotes a variable rate that depends on different parameters and/or state variables. In the following example, we assume constant rates and therefore use lower case notation.

We now need to cast the model structure into a set of three equations for the three state variables:

$$\left.\begin{aligned} \frac{d}{dt}N &= -r_{\max}\cdot\frac{N}{k_N+N}\cdot P + l_{PN}\cdot P + l_{DN}\cdot D, \\ \frac{d}{dt}P &= r_{\max}\cdot\frac{N}{k_N+N}\cdot P - l_{PN}\cdot P - l_{PD}\cdot P, \\ \frac{d}{dt}D &= l_{PD}\cdot P - l_{DN}\cdot D, \end{aligned}\right\} \tag{11}$$

The parameters are the maximum uptake rate, $r_{\max}$, which depends on light and temperature, respiration losses, $l_{PN}$, and mortality, $l_{PD}$. $l_{DN}$ is the rate of remineralization. Adding all three equations we obtain:

$$\frac{d}{dt}(N+P+D)=0,$$

which means that the total <u>mass is conserved</u> and the model is called <u>conservative</u>.

When looking for steady state solutions to Eq. (11) which describe the model behaviour on long time scales, we can set $\frac{d}{dt}N=\frac{d}{dt}P=\frac{d}{dt}D=0$.

This yields

$$\left.\begin{aligned} 0 &= -r_{\max}\cdot\frac{N^*}{k_N+N^*}\cdot P^* + l_{PN}\cdot P^* + l_{DN}\cdot D^*, \\ 0 &= r_{\max}\cdot\frac{N^*}{k_N+N^*}\cdot P^* - l_{PN}\cdot P^* - l_{PD}\cdot P^*, \\ 0 &= l_{PD}\cdot P^* - l_{DN}\cdot D^*, \Rightarrow D^* = \frac{l_{PD}\cdot P^*}{l_{DN}} \end{aligned}\right\} \tag{12}$$

A trivial solution is P=0 which his irrelevant here. If we use the 3rd to substitute D in the 1st equation, we find that the first of two equations becomes:

$$r_{\max}\cdot\frac{N^*}{k_N+N^*}-l_{PN}-l_{PD}=0$$

This result suggests that an equilibrium can be reached for a certain value **N*** for which the growth and loss terms cancel out. This rate is given by the following expression:

$N^*=k_N\cdot\frac{l_{PN}+l_{PD}}{r_{\max}-l_{PN}-l_{PD}}$ , then we use the following relation that is always true $P^*+N^*+D^* = N_0$ to find $P^*$ and $D^*$.

If we assume a closed system (*e.g.,* a chemostat) in which the original nitrogen concentration has been reduced from an initial level $N_0$ to a new level $N^*$, then $N_0$-$N^*$ must be present in the P and D compartments. The abundance ratio between P and D at the steady state can be obtained from the 3rd differential equation of the system in Eq. (12)

$$\Rightarrow\frac{P^*}{D^*}=\frac{l_{DN}}{l_{PD}}$$

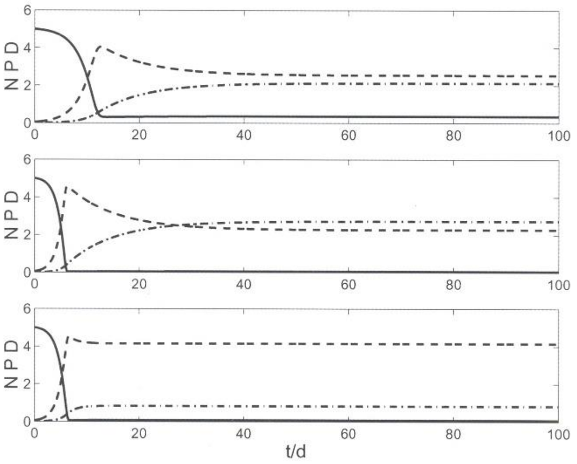


*Figure 28: Nutrient N (solid line), phytoplankton P (dashed line), and detritus D (dash-dotted line) dynamics for different parameter choices. Upper panel: $l_{PN}$=0.5 $d^{-1}$, $l_{PD}$=0.05 $d^{-1}$ and $l_{DN}$=0.06 $d^{-1}$. Middle: $l_{PN}$=0.10 $d^{-1}$, $l_{PD}$=0.06 $d^{-1}$ and $l_{DN}$=0.05 $d^{-1}$. Lower panel: $l_{PN}$=0.10 $d^{-1}$, $l_{PD}$=0.10 $d^{-1}$ and $l_{DN}$=0.5 $d^{-1}$.The steady state for the two last cases is very close to zero (but not zero). In all panels: $r_{max}$= 1 $d^{-1}$ and $k_N$= 0.3 mmol $m^{-3}$. Initial values: $N_0$=5 mmol $m^{-3}$, $P_0$=0.05 mmol $m^{-3}$, $D_0$=0 mmol $m^{-3}$.*

The dynamics of such a model are still rather simple and are illustrated in **Figure 28** for three sets of parameter choices. **Figure 28** confirms that the steady state of the ratios P/D is given by the ratio $l_{DN}/l_{PD}$. The time scale for reaching the steady state depends on the remineralization rate, $l_{DN}$, which represents the bottleneck in this set of equations. While the steady state in the uptake model without a recycling term had phytoplankton at its maximum and the nutrients are zero, by adding the recycling term the steady state is rather different with non-zero and non-maximal values for all state variables. The abundance rations of the different variables are determined by the mortality and remineralization rates. These results also hold for modified uptake function such as $\frac{N?}{\left(k_N^2+N^2\right)}$. In this particular case, the critical nutrient concentration is given by:

$$N^*=\sqrt{k_N\cdot\frac{l_{PN}+l_{PD}}{r_{\max}-l_{PN}-l_{PD}}}$$

### IV.1.4. Zooplankton grazing

The trophic level above phytoplankton is occupied by zooplankton which consumes phytoplankton. Thus, zooplankton grazing represents an important sink term for phytoplankton biomass.

The easiest way to account for this top-down effect is to include the grazing implicitly in the overall phytoplankton mortality. However, changes in zooplankton abundance or dynamics can affect grazing losses and it may be desirable to include this process more explicitly by introducing an additional state variable, namely zooplankton biomass. Now, phytoplankton becomes the limiting resource for zooplankton growth.

If Z represents the zooplankton biomass per unit volume, then zooplankton growth can be described as:

$$\frac{d}{dt}Z \sim g(P)\cdot Z \tag{13}$$

with $g$(P) being the grazing rate which quantifies the ingestion of phytoplankton as a function of prey (phytoplankton) abundance. Similarly to how we addressed nutrient uptake by phytoplankton, we can expect $g$(P) to be a relation that becomes independent of prey abundance when food is highly abundant and proportional to prey abundance when it is scarce. One of the earliest formulations for g(P) stems from Ivlev (Ivlev, 1945) and was derived from a series of experiments on fish feeding. Ivlev found the amount of food consumed by fish increased with the amount of food offered, but only until a certain limit. This prompted him to propose the following expression:

$$g(P) = g_{\max}\cdot\left(1-e^{-I_v\cdot P}\right) \tag{14}$$

with $I_v$ the Ivlev parameter. A priori, there is no specific principle that would dictate the functional form (*i.e.*, the functional response) of such a limiting function, except for the fact that growth and grazing be limited by nutrients and food. We could think of other forms form the Ivlev function like $g(P) = g_{\max}\cdot\left(1-e^{-I_v{}^2\cdot P^2}\right)$ or Monod-type functions $g(P) = g_{\max}\cdot\frac{P}{I_v^{-1}+P}$ (**Figure 29**).

To obtain a complete differential equation for the zooplankton state variable (Eq. 13), we also need to add loss terms due to respiration, $l_{ZN}$, and mortality, $l_{ZD}$. Mortality is comprised of a natural component (e.g., for copepods) but may also include predation by members of higher trophic levels (fish, larvae, etc.). However, an accurate representation of this last process is a rather challenging issue.

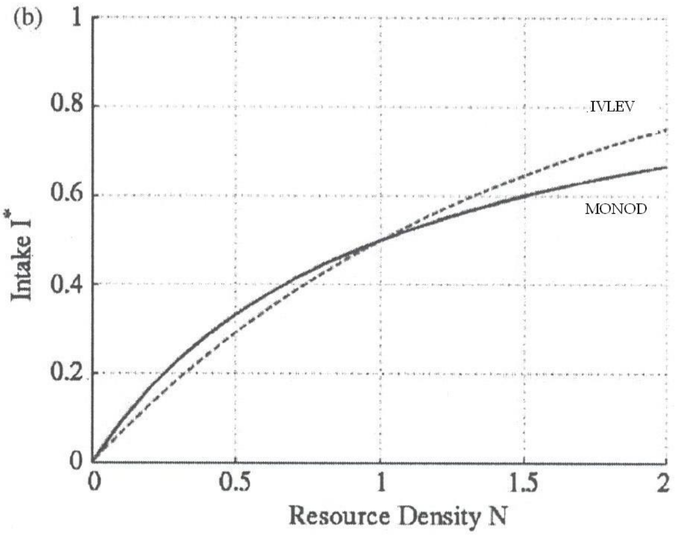


*Figure 29: Comparing the Ivlev and Monod functions for intake (I*) as a function of prey density (N).*

## IV.2. Intrinsic dynamics and stability of size-class based ecosystem models – studying the article by Lima et al. (2002)

In the previous section we discussed some issues and processes that are need be be addresses before starting to model a marine ecosystem. We looked at very simple models of just a few state variables and looked at the dynamics of these variables.

Before tackling some more complex models, it is interesting to study the intrinsic dynamics and stability of these “small” models independently of the physical forcing.

The article by Lima et al. (2002) analysed the dynamics of three common formulations of NPZD type models that employ two different types of functional responses to simulate predation. By functional response, we mean the shape of the mathematical equation that describes predation. The objective of this section is to characterize the stability conditions of this type of model in a changing light and nutrient environment (nitrogen will be the only nutrient considered).

### IV.2.1. General form of the three models in the comparison

The first model is also the simplest one (**Figure 30**) with just one species or size class for each trophic level (NPZD). Then, we first add an additional size class for phytoplankton (NPPZD or $NP_2ZD$) before adding a size class for zooplankton (NPPZZD or $NP_2Z_2D$).

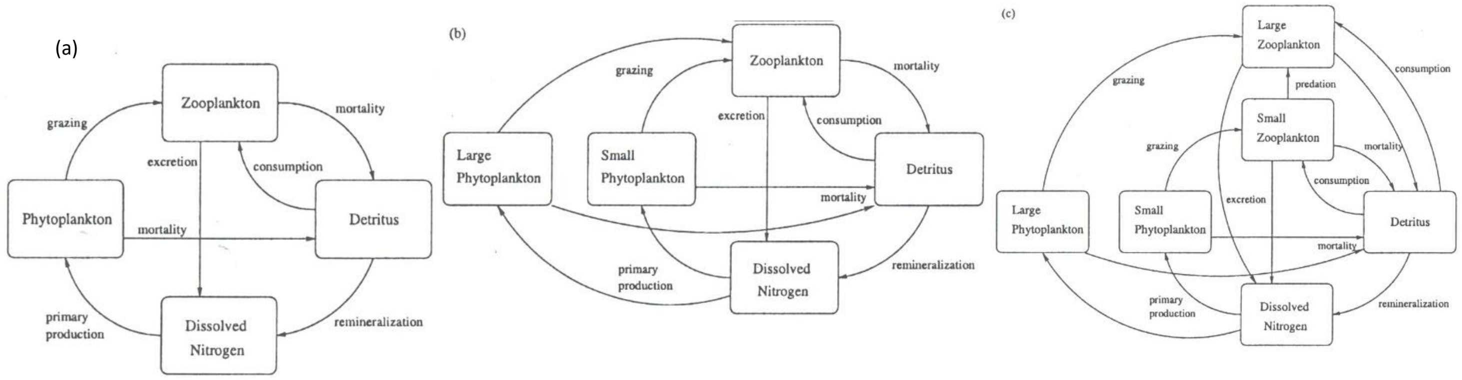


*Figure 30: The three models studied in Lima et al. (2002). (a) NPZD, (b) NPPZD, and (c) NPPZZD.*

In the $NP_2ZD$ model, the one zooplankton group grazes on both the small and large phytoplankton and the detritus while in the $NP_2Z_2D$ version, the small zooplankton eats detritus and small phytoplankton and the large zooplankton consumes small zooplankton, large phytoplankton, and detritus.

### IV.2.2. Differential equations of the temporal evolution of different state variables

- **Phytoplankton**

$$\dot{P}_i = \frac{dP_i}{dt} = \underbrace{U_i(I,N)\cdot P_i}_{1}\underbrace{- g_i \cdot G_i(P_i)\cdot Z_i - s_i \cdot P_i}_{2} \tag{15}$$

Where i=[1,2] refers to the two size classes (1=small and 2=big) or species of phytoplankton/zooplankton. $Z_j$ (Eq. 16) refers to the size classes or to species i-1 when i=2.
The phytoplankton concentration is controlled by growth which is in turn a function of light and nutrient availability (here only N, term 1 in Eq. 15) and by the loss terms (term 2) consisting of zooplankton grazing and natural mortality (senescence).

- **Zooplankton**

$$\dot{Z}_i = \frac{dZ_i}{dt} = \underbrace{a_i \cdot m_i \cdot g_i \cdot G_i(P_i, Z_j, D)\cdot Z_i}_{1}\underbrace{- d_i \cdot Z_i^2}_{2} \tag{16}$$

Zooplankton growth (*term 1*) is modulated by an assimilation efficiency (*$a_i$*), a metabolic efficiency (*$m_i$*), a maximum grazing rate (*$g_i$*), and by the zooplankton concentration itself (*Z*). It also depends on the total availability of food -$G_i(P_i, Z_j, D)$- *i.e.*, phytoplankton, detritus, and, for the case of the NPPZZD model, of small zooplankton. In the two multi-species models (NPPZD and NPPZZD) zooplankton can only feed on phytoplankton of the same size class (index *i*) (**Figure 30**).

The two types of functional responses used to parameterise zooplankton predation ($G_i(P_i, Z_j, D)$ ) are based on Michaelis-Menten-type dynamics:

- The first type (*with fixed preferences*) is given by:

$$G(S) = \sum_{i=1}^{n} G(S_i) = \frac{\sum_{i=1}^{n}(\phi_{S_i}\cdot S_i)}{K_Z + \sum_{i=1}^{n}(\phi_{S_i}\cdot S_i)} \qquad S = (S_1, S_i, \ldots, S_n) \tag{17}$$

with $S_i$ the food source being consumed; $\phi_{S_i}$ (constant) is the preference for food of type $S_i$, and $K_Z$ is the half-saturation constant for zooplankton predation. For instance:

NPZD: $G_Z(P,D) = G(P) + G(D) = \dfrac{\phi_P \cdot P}{K_Z + \phi_P \cdot P + \phi_D \cdot D} + \dfrac{\phi_D \cdot D}{K_Z + \phi_P \cdot P + \phi_D \cdot D}$

NPPZZD: $G_{Z_2}(P_2, Z_1, D) = \dfrac{\phi_{P_2}\cdot P_2 + \phi_{Z_1}\cdot Z_1 + \phi_D \cdot D}{K_Z + \phi_{P_2}\cdot P_2 + \phi_{Z_1}\cdot Z_1 + \phi_D \cdot D}$

- In the second type of functional response, the preferences are no longer constant but depend on the relative availability of different food items (**Figure 31**), and we speak of ***weighted preferences*** (Fasham et al., 1990):

$$\phi'_{S_i} = \frac{\phi_{S_i}\cdot S_i}{\sum_{i=1}^{n}(\phi_{S_i}\cdot S_i)} \tag{18}$$

Hence, in the NPPZZD model, the preference of large zooplankton ($Z_2$) for large phytoplankton ($P_2$) can be expressed as:

$$\phi'_{P_2} = \frac{\phi_{P_2} \cdot P_2}{\phi_{P_2} \cdot P_2 + \phi_{Z_1} \cdot Z_1 + \phi_D \cdot D} \tag{19}$$

with $\phi_{P_2}$, $\phi_{Z_1}$, and $\phi_D$ being the preferences for large phytoplankton, small phytoplankton, and detritus, respectively. If we replace the constant preferences in Eq. (17) with the weighted preferences, we obtain the following parameterisation of zooplankton predation (G) (for the NPPZD model):

$$G(P_1, P_2, D) = \frac{\left(\phi_{P_1} \cdot P_1^2 + \phi_{P_2} \cdot P_2^2 + \phi_D \cdot D^2\right)}{K_Z \cdot \left(\phi_{P_1} \cdot P_1 + \phi_{P_2} \cdot P_2 + \phi_D \cdot D\right) + \phi_{P_1} \cdot P_1^2 + \phi_{P_2} \cdot P_2^2 + \phi_D \cdot D^2} \tag{20}$$

(for other examples see Eqs. 13 and 16 on p. 536 in Lima et al., 2002).

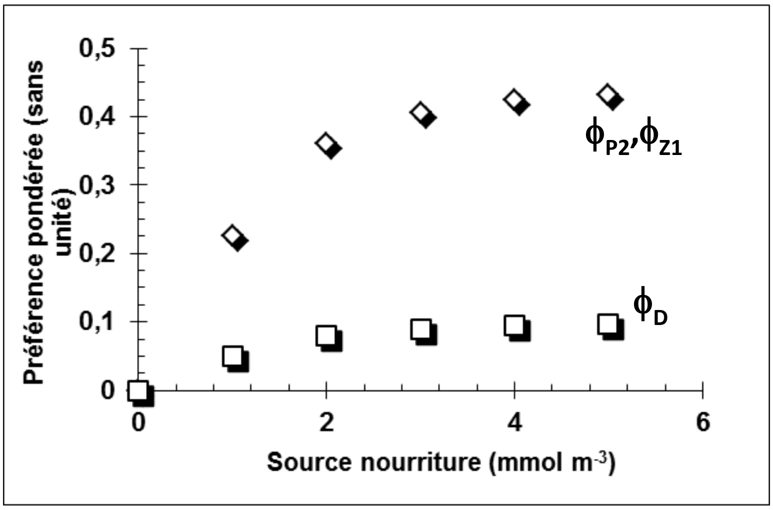


*Figure 31: Evolution of the weighted preferences for large zooplankton as a function of food availability (from* LIMA *et al., 2002).*

The zooplankton loss terms (term 2 in Eq. 16) are grouped together in a non-linear term (quadratic) which is a function of the zooplankton concentration squared. This term provides the closure of the model with respect to the higher trophic levels and helps to stabilise the model by preventing zooplankton concentrations from becoming too high.

- **Detritus**

$$\dot{\boldsymbol{D}} = \frac{\boldsymbol{dD}}{\boldsymbol{dt}} = \sum_i \left[ \underbrace{(1-\boldsymbol{a}_i)\cdot \boldsymbol{g}_i \cdot \boldsymbol{G}_i(\boldsymbol{P}_i, \boldsymbol{Z}_j, \boldsymbol{D})\cdot \boldsymbol{Z}_i}_{1} \underbrace{- \boldsymbol{g}_i \cdot \boldsymbol{G}_i(\boldsymbol{D})\cdot \boldsymbol{Z}_i}_{2} + \underbrace{\boldsymbol{s}_i \cdot \boldsymbol{P}_i}_{3} + \underbrace{\boldsymbol{d}_i \cdot \boldsymbol{Z}_i^2}_{4} \right] - \underbrace{\boldsymbol{e} \cdot \boldsymbol{D}}_{5} \tag{21}$$

The first term represents the contributions be faecal pellets; the second term represents the losses due to grazing; the third term is the contribution by phytoplankton mortality (senescence);

the fourth term results from zooplankton predation; the fifth represents the loss terms via bacterial remineralization (implicit process). Here, we have i ≠ j.

- **Dissolved inorganic nitrogen (DIN)**

$$\dot{N} = \frac{dN}{dt} = \sum_i \left[ \underbrace{a_i \cdot (1 - m_i) \cdot g_i \cdot G_i(P_i, Z_j, D) \cdot Z_i}_{1} - \underbrace{U_i(I, N) \cdot P_i}_{2} \right] + \underbrace{e \cdot D}_{3} \qquad (22)$$

The DIN source terms represent the remineralization of detritus (term 3) and zooplankton excretion, which is proportional to grazing (term 1). The second term is a loss term due to uptake by phytoplankton.

$$N_0 = N + D + \sum_i P_i + \sum_i Z_i \qquad (23)$$

$N_0$ is the total amount of nitrogen in the system, which is considered constant in Lima el al. (2020).

IV.2.3. Intrinsic dynamics of the different models

- Response to variations in light intensity and total nitrogen concentration:

The different models exhibit relatively similar dynamics. All models reach a stable equilibrium for ***moderate to strong light intensities*** and ***low nitrogen concentrations*** (**Figures 4, 7, 11 & 13** in Lima et al., 2002); in the other cases instabilities in the form of oscillations in limit cycle occur.

This begs the question of whether such oscillatory behaviour is real, i.e., have we already observed such a behaviour in the field where nitrogen concentration are high and light availability is low (for instance at the nitracline)? The answer is yes; limit cycle oscillations are not necessarily unrealistic. In fact, oscillations of the chlorophyll concentrations with a periodicity of about 40 days have been observed at the Ocean Weather Station (OWS) Papa in the North Pacific. However, in our NPPZZD model, the oscillation periods are longer and range from 40 to 100 days (**Figure 16** in Lima et al., 2002).

- Effects of increased model complexity on stability:

As the complexity of a given type of functional response (e.g., weighted) increases, the model tends to become unstable over a wider range of light intensities and nitrogen concentrations (**Figures 6, 12, and 14** in Lima et al., 2002). More complex models also take longer to reach a stable equilibrium (**Figures 9 and 16** in Lima et al., 2002). The more interactions there are between model compartments, the more complex the internal dynamics and therefore the longer it takes to reach an equilibrium point:

**NPZD model**: P↑→N↓→Z↑→P↓.

**NPPZZD model**: $P_1\uparrow\rightarrow Z_1\uparrow\rightarrow P_1\downarrow\rightarrow P_2\uparrow\rightarrow Z_2\uparrow\rightarrow P_2\downarrow\rightarrow P_1\uparrow$.

- How the choice of the functional response of predation affects stability:

For a given type of structure (NPPZD, for example), adding a weighted preference parameterization makes it possible to increase the stability of the model for a wider range of light intensities and nitrogen concentrations (e.g., **Figures 11 and 13** in Lima et al. 2002 ). How can such a dynamic be explained? Having a weighted (variable) preference when simulating zooplankton predation is like having a zooplankton compartment of grazers capable of **selecting the most abundant food**. This so-called “switching” mechanism leads to a damping of the oscillations by increasing the rate of loss of the temporarily most abundant prey species, which stabilizes the entire system.

Another consequence of using a functional representation of predation that uses weighted preferences is that several species of phytoplankton are able to coexist (e.g., **Figures 11 and 13** in Lima et al., 2002) which only depend on a single source of nitrogen. Here too, as the predators switch to the most abundant phytoplankton species (“predator switching”) the temporarily less abundant phytoplankter receives a temporary competitive advantage which prevents it from disappearing completely.

- How realistic are the observed oscillations in the multi-species models:

These oscillations between different species lead to the coexistence of several phytoplankton and are observed in multispecies models for high nitrogen concentrations and low light intensities, i.e., environmental conditions that are characteristic of the deep chlorophyll maximum (DCM) zone. These model results suggest that the DCM could be a dynamically unstable area with oscillating abundances of different types of phytoplankton. This dynamic imbalance in species composition could provide a mechanism for species coexistence in the relatively homogeneous environment of the open ocean. This fact that a limited range of resources can support an unexpectedly wide range of species is referred to as the “plankton paradox” (HUTCHINSON, 1961). The combination of physical disturbances (intermittent and seasonal mixing events) and long low-light response times would promote coexistence and persistence of species on seasonal or annual time scales. Observations at the DCM in the North Pacific showed that up to 300 phytoplankton species are able to coexist there (VENRICK, 1988).

- Why is there a limit cycle?

Despite the use of weighted preferences and irrespective of the model structure, the models still exhibit some degree of instability for low light and high nitrogen concentrations. A stable limit cycle is formed in all models from a Hopf bifurcation point. This bifurcation is a critical point where the system’s stability switches and a periodic solution arises around an equilibrium point, in our specific case due to a phase lag between the predator and prey growth rates. In our models, this phase lag is caused by a large and rapid increase in the phytoplankton growth rate relative to the rate of zooplankton growth when nutrient concentrations increase in low light (**Figure 18** in Lima et al., 2002). Zooplankton abundance cannot keep up with the growth in phytoplankton abundance and the system oscillates in a limit cycle.

- Consequences of biodiversity for biomass

The large functional diversity of species in the most complex models allows the biological activity to thrive over a wider range of light and nutrient conditions. Recycling, through zooplankton excretion and the consumption of detritus, is increased in the $NP_2Z_2D$ model. Primary and secondary production will become greater, there will be a sudden increase in nitrogen in the biomass compartments, and the water column will become more oligotrophic for the same light intensities. This result suggests that it will be beneficial to use a complex model if we want to represent an oligotrophic environment (poor in nutrients and biomass) while a slightly simpler model may be better to represent more eutrophic environments (rich in nutrients and high in biomass). This rule of thumb seems to match observations in the ocean fairly well, which show a general increase in phytoplankton species diversity as we move from the poles to low latitudes (BARTON et al., 2010).

## IV.3. Modelling the seasonal variability of the planktonic ecosystem with an NPZD type model in 1D using as example the study by LACROIX and NIVAL (1998)

The study by LACROIX and NIVAL (1998) uses an NPPZD type model to which we add a hydrodynamic model, i.e., a 1D physical model of the water column. The variability of biological variables no longer exclusively depends on the source and sink terms of the biogeochemical processes, as was the case until now, but now they also depend on the vertical advection of water masses and on vertical diffusion. As a result, the variation in the concentration of tracer, *C*, over a short time interval dt ($\frac{\partial[C]}{\partial t}$) can be expressed as:

$$\frac{\partial[C]}{\partial t}+\underbrace{\frac{\partial((\omega+\omega_C)\cdot[C])}{\partial z}}_{1}=\underbrace{\frac{\partial}{\partial z}\left(K_V\cdot\frac{\partial[C]}{\partial z}\right)}_{2}+\underbrace{S([C])-P([C])}_{3}+\underbrace{F([C])}_{4}$$

**$\omega_C$: vertical sinking velocity (due to gravity) of the tracer (this is zero for dissolved tracers),**
**$K_V$: vertical eddy diffusivity.**
**Term 1: vertical advection of the tracer to which the sinking is added,**
**Term 2: vertical diffusion by turbulence,**
**Term 3: sources and sinks of the non-conserved tracer,**
**Term 4: different boundary conditions for each tracer.**

Note: If we had a 3D hydrodynamic model, the above equation would be somewhat different because we would have to consider the horizontal dimensions as well which would yield:

$$\frac{\partial[C]}{\partial t}+\underbrace{\frac{\partial(u\cdot[C])}{\partial x}+\frac{\partial(v\cdot[C])}{\partial y}}_{1'}+\underbrace{\frac{\partial((\omega+\omega_C)\cdot[C])}{\partial z}}_{1}=\underbrace{\frac{\partial}{\partial x}\left(K_H\cdot\frac{\partial[C]}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_H\cdot\frac{\partial[C]}{\partial y}\right)}_{2'}+\underbrace{\frac{\partial}{\partial z}\left(K_V\cdot\frac{\partial[C]}{\partial z}\right)}_{2}+\underbrace{S([C])-P([C])}_{3}+\underbrace{F([C])}_{4}$$

**Term 1': horizontal advection of the tracer,**
**Term 2': horizontal diffusion of the tracer,**
**$K_H$: horizontal turbulent eddy viscosity.**

The 1D hydrodynamic model is forced by the meteorology (solar radiative and non-radiative fluxes) which allows the model to calculate all the physical variables such as temperature, salinity, diffusion coefficients, and current fields (advection) (**Figure 32**).

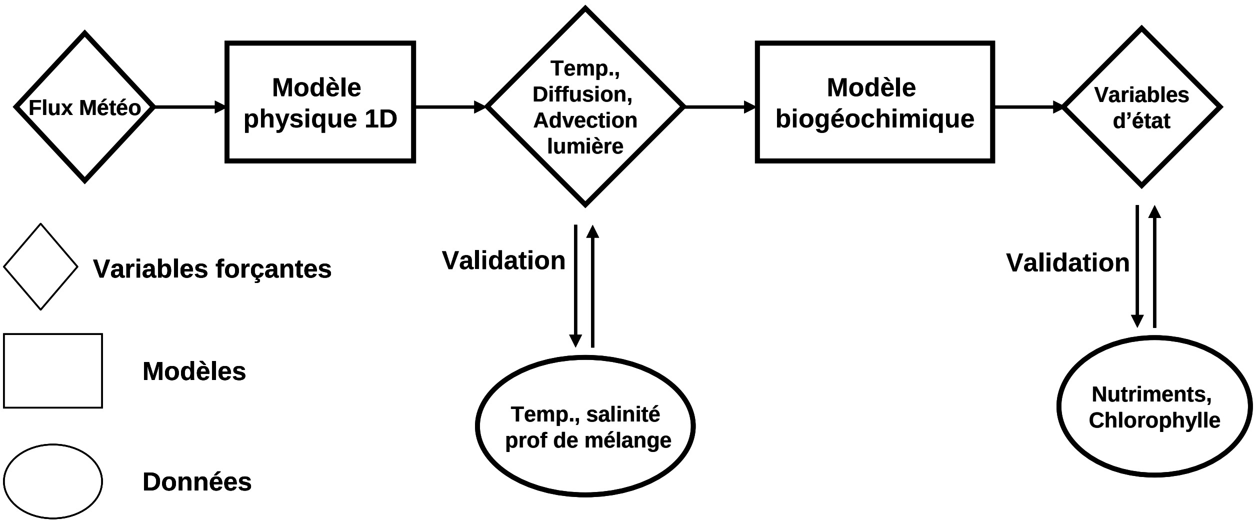


*Figure 32~~-~~: Flow chart illustrating the forcing and coupling between the hydrodynamic model and the model from LACROIX and NIVAL (1998).*

A first validation of the model can be carried out by comparing the model output to field data. The physical model provides the necessary forcing input to solve the equations in the biogeochemical model. For example, if temperature is relevant to primary production, then this temperature is supplied by the physical model. The physical model also calculates any transport of biogeochemical variables (here we have 1D vertical only). The biogeochemical model calculates the sinks and sources of each variable at each time step. As there is no feedback from the biogeochemical state variables back to the physical model, it may be more appropriate to speak of the physical model providing the forcing for the biogeochemistry rather than of a coupling between both models.

The model used in this example is an NPPZD type model that uses nitrogen as its main currency. The article does not present all the equations but only those related to phytoplankton and zooplankton (**Table 4**, p30 in LACROIX and NIVAL 1998). All mathematical formulations in the paper are fairly standard except for the phytoplankton growth dependence on temperature (**Figure 33**).

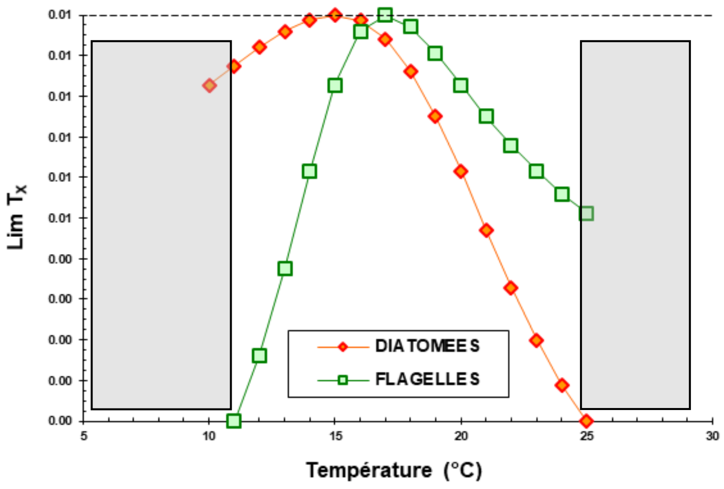


*Figure 33: Dependence of phytoplankton growth on temperature in Lacroix and Nival (1998) model. Temperature regions that are not usually encountered in the Mediterranean have been greyed out.*

Their formulation of the growth dependence on temperature differs between diatoms and flagellates. Flagellates require a slightly higher temperature to achieve maximum growth and will likely dominate the post-bloom period while diatoms are likely to do better during winter and spring. This succession coincides with what we typically observe in the field.

The model requires specifying a total of 45 parameters (**Table 5**, p.31 in LACROIX and NIVAL (1998)), about 35% of which have not been taken from the literature but were set by the authors for their particular simulation which is a rather large percentage.

Another important aspect is how light penetrates through the water column, taking into account not only the absorption of light by water molecules but also by all the other suspended particles of biological and non-biological origin, both living and detrital, and in particular by the chlorophyll molecules of the phytoplankton. Only part of the light spectrum (~43%) is photosynthetically available radiation (PAR), so it is necessary to remove the complementary fraction (~57%) from the total incident irradiance. Part of the incident irradiance is reflected at the water surface ($\alpha$ in Lacroix and Nival (1998), p.34). Considering all these constraints, the light profile shows a rapid exponential decrease with depth (**Figure 34**).

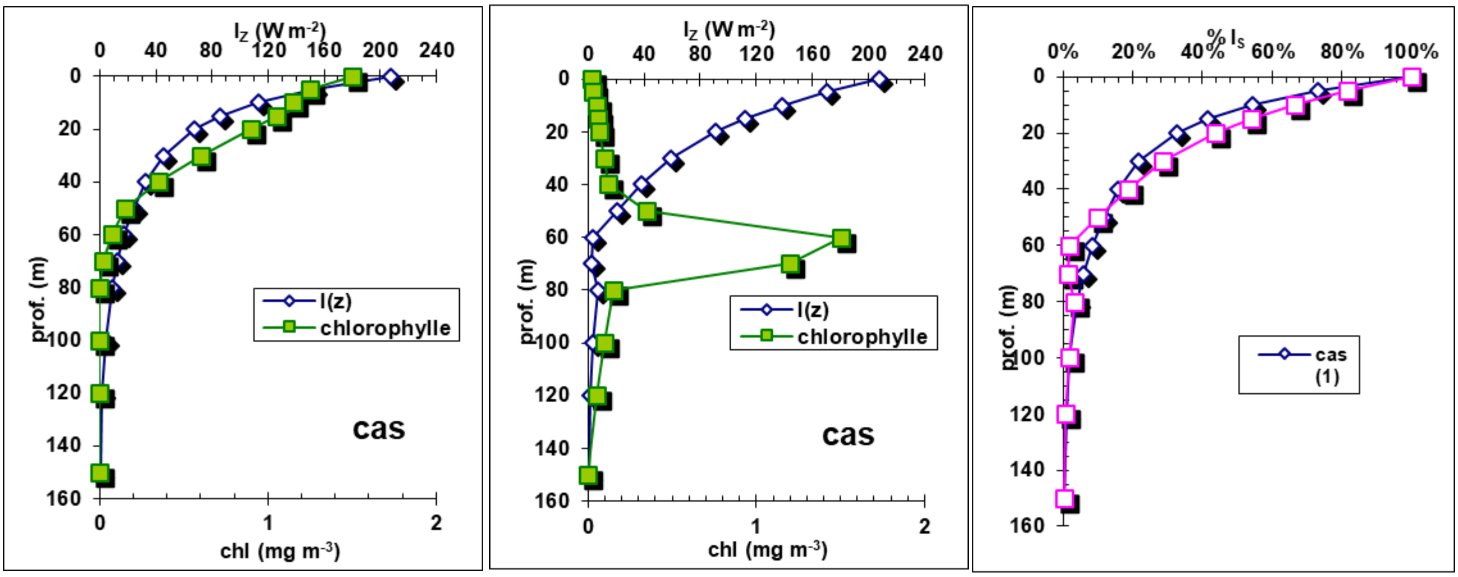


*Figure 34: Vertical profiles of light penetration ($I_Z$) and chlorophyll (chl). The vertical profile of the irradiance percentage (right panel – percentage with respect to the irradiance incident at the surface $I_S$) shows slight differences depending on whether the chl maximum is located at the surface or at depth.*

The initial conditions in the top 200m of the coupled model were taken from *in situ* data collected as part of the FRONTAL campaign. Below 200 m, values from the literature were used which may be problematic as this may introduce a discontinuity and may not match the *in situ* conditions. Certain profiles were assumed homogeneous over the entire water column, which can result in unusable model results at least during the initial “spin-up” time. There is no contribution by the atmosphere or sediments to any biological variables (e.g., no deposition of nutrients) and hence all net fluxes are zero. The model time step was set to one hour and the vertical resolution to 5 m.

For a more detailed analysis and discussion of the results, see Lacroix and Nival (1998).

## IV.4. Performance of NPZD type models

Having presented the typical structures, processes, mathematical formulations as well as a concrete example of an NPZD type model, we must ask ourselves to what extent these models are capable of reproducing field data; i.e., what are the strengths and weaknesses of this type of model?

In general, one of the strengths of these models is that they can represent the spring bloom dynamics at mid-latitudes rather well (**Figure 35**). This is mainly because the spring maximum in plankton is characterized by the rapid growth of just a few species with similar physiological and ecological characteristics that can be represented by a simple one- or two-compartment phytoplankton model. The relatively simple structure of these models facilitates the analysis of the model output with respect to the hydrodynamic forcings and their effects on the biogeochemistry and plankton dynamics of an ecosystem.

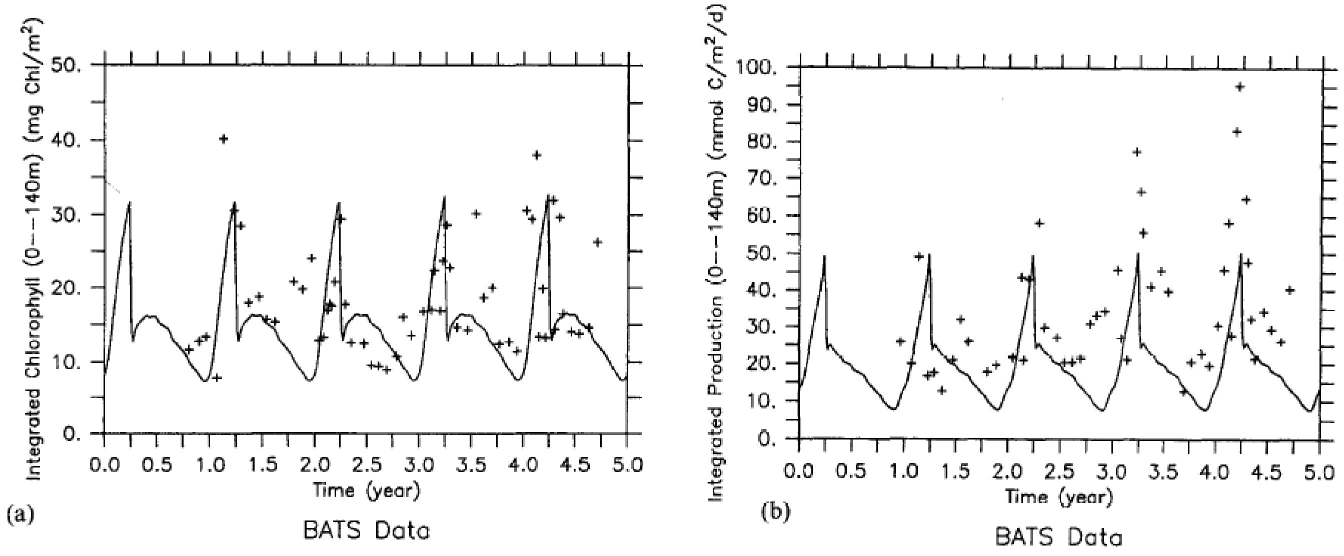


*Figure 35: Comparing observations (symbols )and simulation (solid lines) of (a) chlorophyll and (b) primary production at BATS (Bermuda Atlantic Time-series Study) station between 1988 and 1992 (Doney et al., 1996).*

However, NPZD type models have several weak points. First, their representation of the annual cycle of the main biogeochemical variables is rather poor, particularly of the amounts of phytoplankton after the spring bloom until the beginning of winter. This type of model also fails to reproduce the interannual variability observed in the data, both in standing stocks and material fluxes (**Figures 35 & 36**).

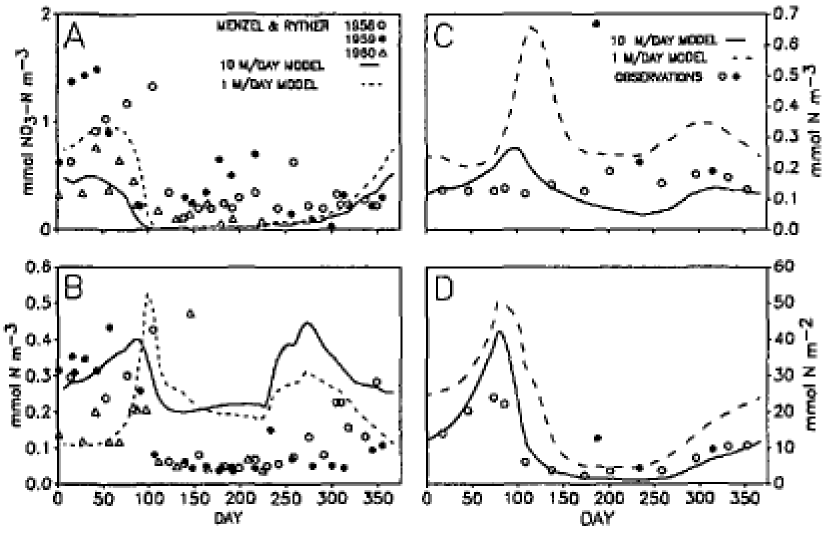


*Figure 36: Comparing the model output to observations from near Bermuda: (A) Nitrate, (B) Chlorophyll in terms of nitrogen, Bacterial biomass (C) per unit volume and (D) integrated. Solid line: sinking velocity of 10 m d$^{-1}$, dashed line: sinking velocity of 1 m d$^{-1}$. From Fasham et al. (1990).*

One last week point of NPZD type models concerns the sensitivity of the model results on the parameter values. The modification of certain parameters can lead to a vastly different model dynamics with regard to the annual cycle of phytoplankton growth (**Figures 36 & 37**). In addition, these parameter values tend to change from model to model. It is therefore always necessary to perform a so-called sensitivity analysis.

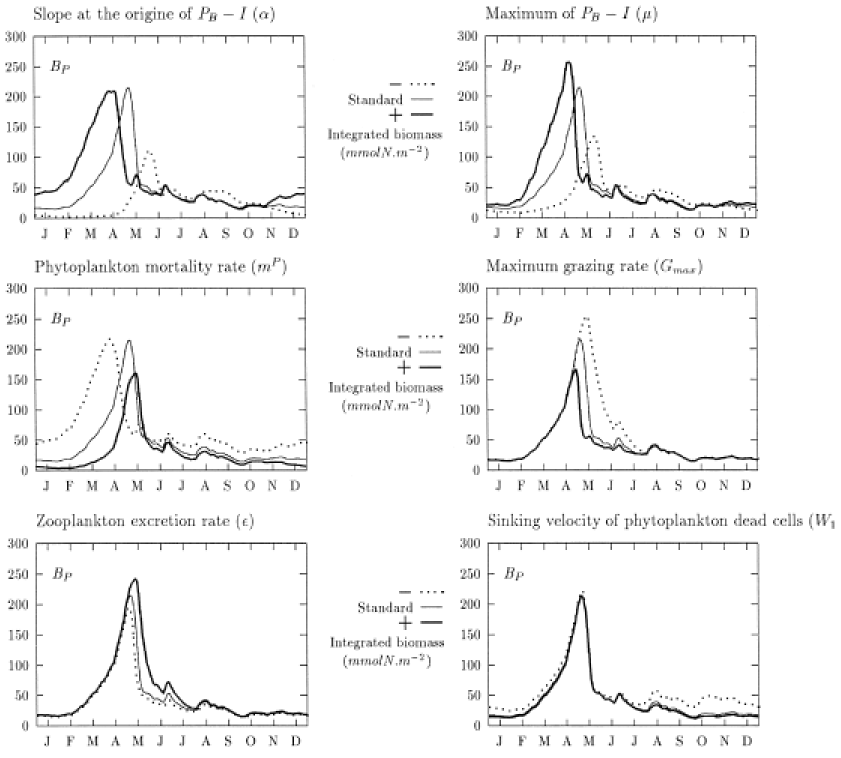
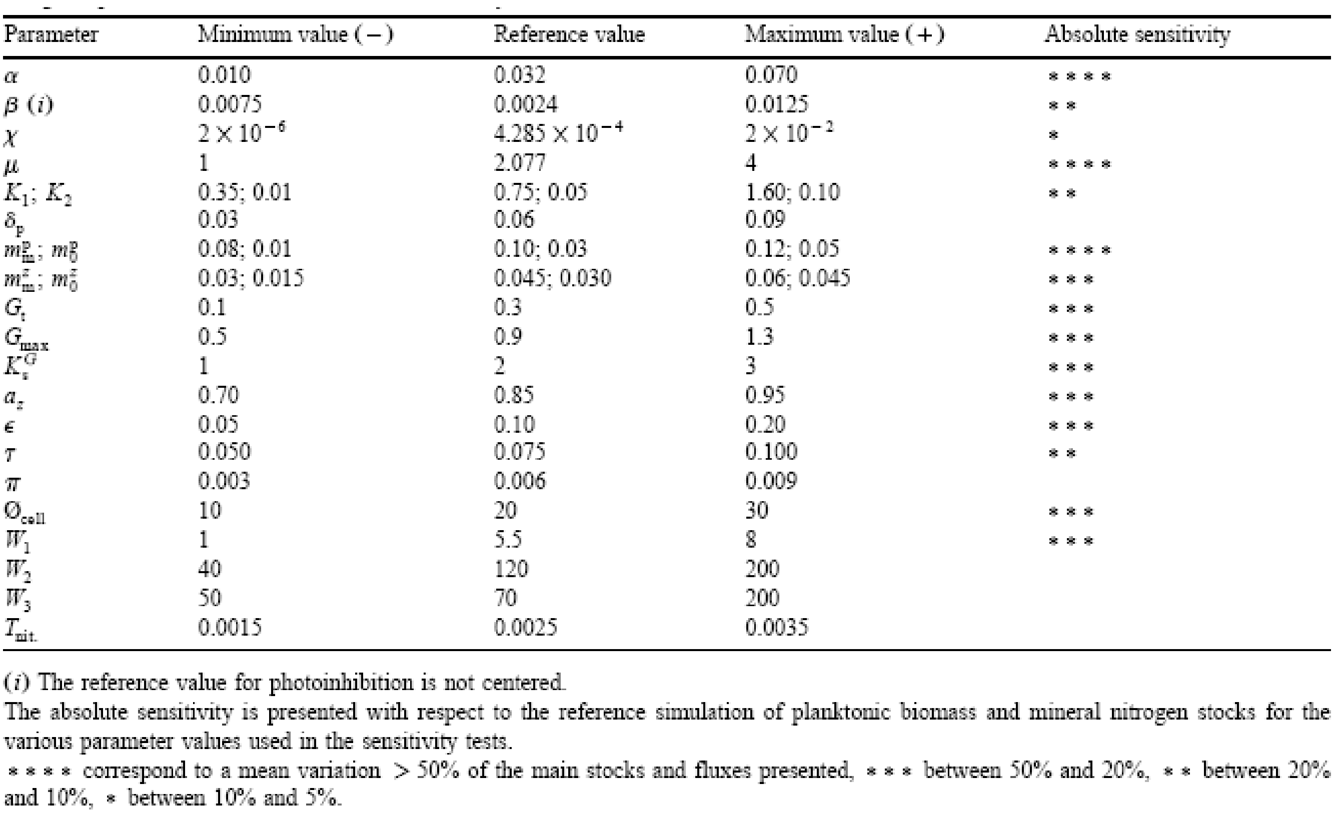


*Figure 37: Demonstrating the effect of changing important parameter values on the annual cycle of integrated phytoplankton biomass. From Druon and Lefèvre (1999).*

These results demonstrate the importance of having parameters whose ranges are not only well constrained from *in situ* observations but who also have an ecological and physiological basis. The latter is not the case for the phytoplankton mortality rate, for instance (**Figure 37**). This is further illustrated with **Table 1** which shows some detailed results of the sensitivity analysis of the NPZD model results and can be used to identify those parameters to which the model shows the highest sensitivity.

*Table 1: Range of parameter values used for the sensitivity analysis (from Druon and Lefèvre, 1999).*



| Parameter | Minimum value ($-$) | Reference value | Maximum value ($+$) | Absolute sensitivity |
|---|---|---|---|---|
| $\alpha$ | 0.010 | 0.032 | 0.070 | $****$ |
| $\beta$ ($i$) | 0.0075 | 0.0024 | 0.0125 | $**$ |
| $\chi$ | $2 \times 10^{-6}$ | $4.285 \times 10^{-4}$ | $2 \times 10^{-2}$ | $*$ |
| $\mu$ | 1 | 2.077 | 4 | $****$ |
| $K_1$; $K_2$ | 0.35; 0.01 | 0.75; 0.05 | 1.60; 0.10 | $**$ |
| $\delta_p$ | 0.03 | 0.06 | 0.09 | |
| $m_m^p$; $m_0^p$ | 0.08; 0.01 | 0.10; 0.03 | 0.12; 0.05 | $****$ |
| $m_m^z$; $m_0^z$ | 0.03; 0.015 | 0.045; 0.030 | 0.06; 0.045 | $***$ |
| $G_t$ | 0.1 | 0.3 | 0.5 | $***$ |
| $G_{max}$ | 0.5 | 0.9 | 1.3 | $***$ |
| $K_s^G$ | 1 | 2 | 3 | $***$ |
| $a_z$ | 0.70 | 0.85 | 0.95 | $***$ |
| $\epsilon$ | 0.05 | 0.10 | 0.20 | $***$ |
| $\tau$ | 0.050 | 0.075 | 0.100 | $**$ |
| $\pi$ | 0.003 | 0.006 | 0.009 | |
| $\O_{cell}$ | 10 | 20 | 30 | $***$ |
| $W_1$ | 1 | 5.5 | 8 | $***$ |
| $W_2$ | 40 | 120 | 200 | |
| $W_3$ | 50 | 70 | 200 | |
| $T_{nit.}$ | 0.0015 | 0.0025 | 0.0035 | |

($i$) The reference value for photoinhibition is not centered.

The absolute sensitivity is presented with respect to the reference simulation of planktonic biomass and mineral nitrogen stocks for the various parameter values used in the sensitivity tests.

$****$ correspond to a mean variation $> 50\%$ of the main stocks and fluxes presented, $***$ between 50% and 20%, $**$ between 20% and 10%, $*$ between 10% and 5%.

## V. TOWARD MORE COMPLEX PHYTOPLANKTON ECOSYSTEM MODELS?

In the previous sections, among other things, we evaluated the capacity of simple planktonic ecosystem models to describe the typical annual cycle of nutrients and plankton in temperate seas. While the models were quite good a reproducing the spring bloom, they had some difficulty in reproducing the remainder of the annual cycle, particularly the post-bloom period. Usually, these simple models use constant parameter values. One way to improve model accuracy could be to use rates that vary over time, which would make it possible to represent the succession of planktonic communities. For example, a higher sedimentation rate in winter and spring mimics the dominance of larger cells such as diatoms, while a lower or even zero sedimentation rate in summer and fall would reflect the dominance of autotrophic flagellates or green microalgae. The advantage of this approach is that we can keep a single generic phytoplankton state variable without having to use several plankton compartments. However, even with this modification it will be difficult to represent a certain level of biodiversity that exists in the ocean, whether near the surface or at depth (e.g., deep chlorophyll maximum). Important processes such as the competition of different species for nutrients and light, which partly determine the biodiversity of plankton, cannot be considered and therefore represented with this approach. The capabilities of these models to improve our understanding of marine ecosystem dynamics and to make predictions about the future remain rather limited. This limitation becomes rather apparent when we try to predict the amounts of carbon sequestration for the next few decades, for instance, and compare these predictions with those from terrestrial ecosystem models (**Figure 38**).

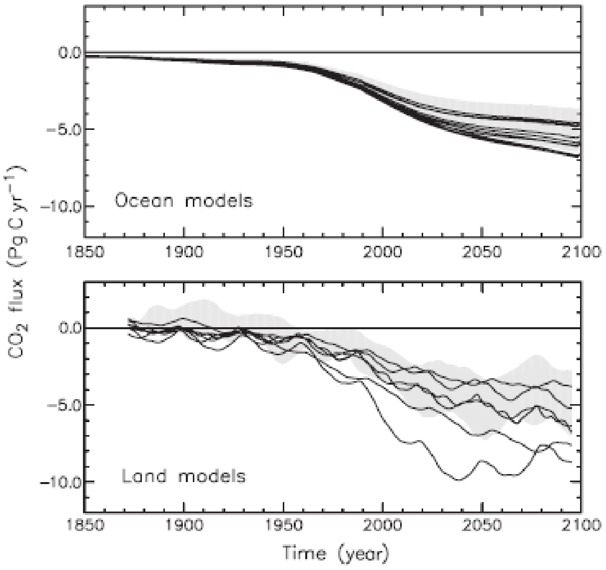


*Figure 38: Projections of oceanic and terrestrial sinks of $CO_2$ estimated by marine biogeochemical models and terrestrial ecosystem models. The different lines represent different scenarios using different atmospheric $CO_2$ concentrations while other climatic variables are kept the same. The shaded area corresponds to scenarios where both the atmospheric $CO_2$ and climate change. From* LE QUÉRÉ *et al. (2005)*

When we look at the projections of the two types of models, we can clearly see that there is a greater variability in the results from the terrestrial ecosystem models compared to oceanic biogeochemical models (OBM). This is because OBMs do not usually include the complexity of the ecological response, which is accounted for in terrestrial models. In the mid-2000s, OBMs had reached what appeared to be an impasse. In addition, it was commonly held at the time that OBMs did not need to be overly complex as much of the biogeochemistry was mainly driven, to a first approximation, by the physics. At the same time, an increasing amount of data on growth, mortality, trophic interactions (predation, etc.), and remineralization of different plankton groups had been accumulating which made it possible to consider the development of a new generation of OBMs that were more based on the organisms' physiology and ecology. These types of models are commonly used now on both global and regional scales and are referred to collectively as Dynamic Green Ocean Models (DGOMs).

The development of DGOMs was inspired by terrestrial models that developed in parallel, the so-called "Dynamic Global Vegetation Models" (DGVMs, CRAMER et al., 2001) as these models had already proven their predictive capabilities, in particular in studies examining the interactions between the climate and the response of terrestrial ecosystems (*e.g.* PRENTICE et al., 2000).

The development of DGOMs called for the definition of so-called plankton function types (PFTs) based on the concept of "functional biodiversity". Several criteria are used to completely define a PFT.

a) A PFT must play a specific biogeochemical role and carry out a particular and important function in the carbon cycle;
b) the PFT must be definable through a series of different physiological, environmental, or nutritional characteristics that determine its biomass and productivity;
c) the behaviour of a PFT must have significant impacts on the performance of other PFTs; for instance, by selectively removing a certain nutrient or via grazing;
d) the PFT must represent a significant part of the biomass at least in a certain region at a certain point in time (e.g., during a season).

Based on these criteria and our current understanding of marine ecosystems about 10 key PFTs can be defined.

1. <u>Pico-heterotrophes (*e.g., heterotrophic bacteria and archaea*) with sizes of up to 1 picometre</u>. This group of organisms remineralizes dissolved and particulate organic matter in the ocean, which limits the export of carbon to greater depths as it converts organic matter into its original inorganic form and allows for the return of $CO_2$ to the atmosphere.
2. <u>Pico-autotrophes (*e.g., pico-eucaryotes, photosynthesizing non-diazotrophic bacteria – Synechococcus, Prochlorococcus*)</u>. With a physical size of about 2µm, this group makes a significant contribution to primary production although a negligible one in terms of carbon export. Members of this group have a high affinity for light and nutrients due to their high

surface-to-volume ratio. They occur in all oceans and make up an important fraction of the planktonic biomass in HNLC zones and oligotrophic regions.

3. Diazotrophs (*e.g.,* Trichodesmium and other unicellular $N_2$-fixing prokaryotes). Members of this group have the physiological capacity to utilize nitrogen in gaseous form ($N_2$), which is rather abundant in the atmosphere, and thereby affect the total quantity of available reactive nitrogen in the water column over relatively long time scales (FALKOWSKI, 1997). $N_2$ fixation requires more energy than the uptake of other (organic or inorganic) forms of nitrogen and cannot take place at low temperatures. Diazotrophs thus have a competitive advantage only in those parts of the ocean that are relatively warm and where nutrient concentrations are low. Although the actual iron demand for these organisms is presently still unknown, it has been suggested that atmospheric input of iron (e.g., deposition of dust from the Sahara) could play an indirect role in the spatial and temporal distribution of these organisms over millennial time scales. The fact that these planktonic organisms also require certain concentrations of phosphorous to exist forms the basis for another hypothesis according to which the distribution of phosphorous may affect the global distribution of nitrogen.

4. Calcifiers (*e.g.,* Coccolithophores). This type of plankton is responsible for more than half of the marine carbonate flux and affects atmospheric $CO_2$ concentrations on a millennial time scale through the process of calcification, including ocean alkalinity and carbonate chemistry. This group also produces the heaviest ballasts observed in sedimenting particles. They can utilize organic phosphorus. However, these organisms are fragile as just one day without light can kill them, which suggests that this group can only exist in regions where the depth of the surface mixing layer does not exceed the euphotic depth. The rate of calcification is greatly reduced when $CO_2$ concentrations in the water are high (low pH). This group could therefore experience a sharp decline in the coming decades due to the increasing ocean acidification. Low zinc concentrations in water would also influence the growth and calcification rates of these organisms.

5. DMS producers (*e.g.*, Phaeocystis and small autotrophic flagellates <20µm). These organisms produce dimethylsulfoniopropionate (DMSP) and convert it to DMS (dimethyl sulphate) using an extracellular enzyme (DMSP-lyase). Thus, these organisms play a key role in the planetary sulphur cycle (precursor compound of clouds and therefore relevance for climate). Other nano- and pico-plankton also produce DMSP but do not have the enzyme, which makes them less efficient at producing DMS. DMS producers have significant phosphorus needs, which excludes them from areas where this nutrient is scarce (in the Mediterranean, for example). They are particularly abundant in coastal areas where they are observed in colonies.

6. Silicifiers (*e.g.,* diatoms). They dominate the microphytoplankton size group (20-200 µm) and are the largest contributors to the spring bloom primary production and biomass in temperate

and Polar Regions. Through direct sedimentation and the predation pathway (excretion of faecal pellets), silicifiers contribute more significantly to the carbon export than smaller plankton. There may also be massive sedimentation events at the end of the spring bloom once the nutrients have become depleted. As the name implies, silicifiers need silicate to construct their cell walls or frustules (composed of opal). They also have higher phosphorus and iron requirements than smaller phytoplankton. In HNLC areas, they respond to iron enrichment as long as silicate remains available. They produce very little DMSP compared to other phytoplankton. The sedimentation of their silicate walls provides a constant flow of opal towards the deep.

7. Mixed-phytoplankton (*e.g.*, Chrysophyceae, autotrophic dinoflagellates). Members of this group come in sizes from 2-200µm and are taxonomically rather diverse and their biogeochemical role is not well defined. In terms of biomass this PFT is rather unimportant as it does not form large blooms in the open ocean. They have a low seasonality and no direct impact on the oceanic biogeochemical cycles of sulphur, silica, or calcium carbonate. However, they serve as food for mesozooplankton.

8. Proto-zooplankton (*e.g.,* ciliates, heterotrophic flagellates). This group consists of heterotrophic unicellular organisms also called protists with sizes between 5 and 200 µm. They preferentially consume small phytoplankton from the nano and pico categories (1-20 µm). Their growth rates are of the same order of magnitude as the phytoplankton upon which they prey. In addition, their food intake rates are similar to the production rates of their prey.

9. Meso-zooplankton (*e.g.,* copepods, larvaceans, amphipods; 200µm to 2mm). They produce large, rapidly settling faecal pellets and are an important food source for fish and their larvae. They preferentially consume large phytoplankton (>20-200µm) such as silicifiers and proto-zooplankton. Their ingestion and reproduction rates are lower than those of proto-zooplankton. They have longer development cycles (egg passage, different larval stages) and lower growth rates.

10. Macro-zooplankton (*e.g.,* euphausiids, salps, pteropods, jellyfish, >2mm). They produce large amounts of faecal pellets that sink even faster than those from the previous PFT. As filter feeders that can consume prey from across a very large size spectrum down to the smallest phytoplankton. These organisms therefore represent an indirect route for the sedimentation of very small organisms. Locally, their growth can be rather rapid which leads to a rather heterogeneous distribution overall that is difficult to predict. At present, the environmental factors that control their biomass, physiology, and general life cycles are poorly understood. Meso- and macro-zooplankton PFTs such as foraminifera and pteropods also produce $CaCO_3$ and contribute about half of the calcium carbonate export flux in the ocean.

In conclusion, this classification is not definitive. It is quite possible that in the future it will be necessary to subdivide these FTPs further to account for some newly discovered process. Of course, the opposite is also possible if the role of a particular PFT should be considered insignificant. The number of PFTs to include in a model also depends on the scientific question to be addressed and on the spatio-temporal scales in which we are interested.

After the description of these PFT, we can ask the following question: is a model containing these PFTs capable of accurately reproducing the mean state and variability in the main fluxes of carbon, oxygen, and DMS in the present ocean. Furthermore, can the model accurately reproduce the observed abundances of the different PFTs?

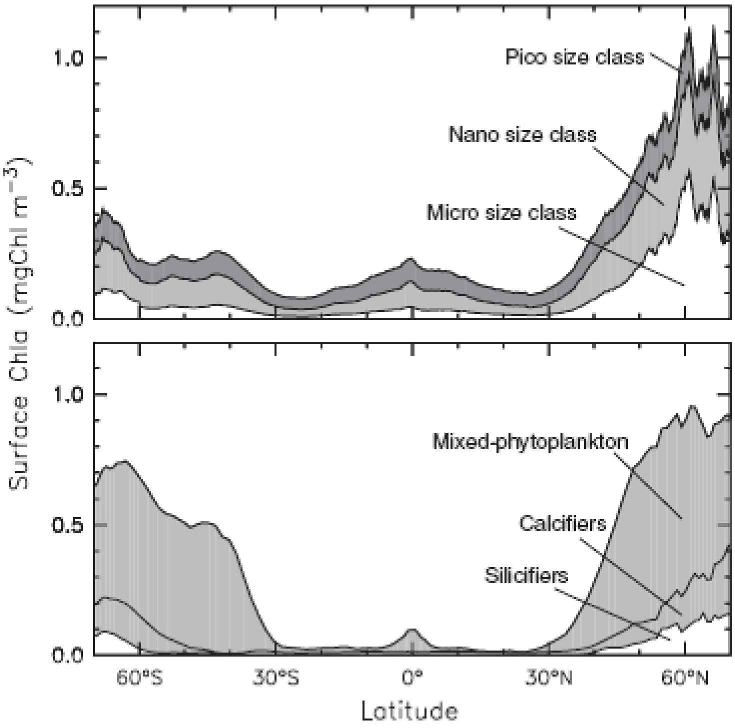
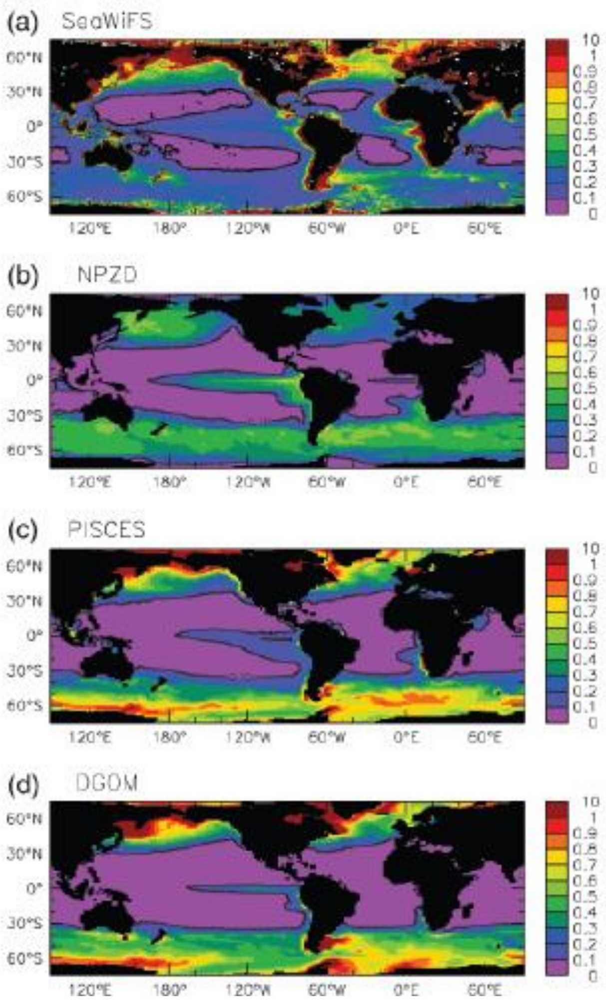


*Figure 39: Top panel: zonal averages of the contribution of different size classes (micro-, nano-, and picoplankton) to the total surface chlorophyll as estimated from analysing SeaWiFs data for the year 2000; bottom panel: contribution of different PFTs (silicifiers, calcifiers, and mixed-phytoplankton) to the surface biomass for the same year, estimated from the output of a DGOM. Taken from Le Quéré et al. (2005).*

If we compare the output from a DGOM to remote sensing data (**Figure 39**), we notice that although they do not match very well quantitatively nor qualitatively, the general trends for different latitudes are well reproduced. In general, the biomass of silicifiers is underestimated while that of mixed-phytoplankton at high latitudes is overestimated.

When considering a DGOM with four PFTs (**Figure 40c**), namely silicifiers, mixed-phytoplankton, proto-, and mesozooplankton, and with the growth of both phytoplankton groups co-limited by the availability of iron, phosphorus, silicon, and light, we can see that the results of this model are already significantly better than with an NPZD model across the global ocean (**Figure 40a-c**). This is mainly due to the explicit representation of the effect of iron fertilization provided by atmospheric inputs from wind. The NPZD models overestimate phytoplankton concentrations in the Southern Ocean and underestimate them at high latitudes in the northern hemisphere. PISCES performs better at high northern latitudes and worse in the Southern Ocean. The overestimation in the Southern Ocean is still present but slightly less marked than with the other models. All models overestimate the extent of the oligotrophic zones in subtropical gyres; a defect that is most marked in the DGOM. As we can see, no model is perfect in all areas.

*Figure 40: Mean annual chlorophyll concentrations (mg m$^{-3}$) from (a) SeaWIFs satellite observations, (b) an NPZD model, (c) the PISCES model with 4 PFTs, and (d) a DGOM with 5 PFTs. Taken from Le Quéré et al. (2005).*



When we add another PFT compartment to the PISCES model (calcifiers in this case), the surface chlorophyll does not change fundamentally (**Figures 40c versus d**) but there are important modifications in the interannual variations of their distribution (**Figures 41c, d**). Still, neither of the two more complex models is capable of reproducing the observed chlorophyll variability. In the SeaWIFS data, the strongest variances occur in areas with intermediate chlorophyll concentrations while in the NPZD and PISCES models the variance of chlorophyll is highest in areas of low chl concentrations and approaches zero in areas with high concentrations. The DGOM behaves slightly differently. It shows a strong variability in the equatorial Pacific where the concentration of chlorophyll *a* is relatively high. An in-depth analysis of the DGOM results shows that the high variability in chlorophyll *a* appears to be linked to the presence of calcifiers that respond much more quickly than other PFTs to changes in phosphorus availability.

In this particular version of the DGOM, calcifiers can be found at latitudes between 40°N and 40°S but they are almost absent at higher latitudes. In reality, calcifiers can be found at higher latitudes up to 70°N/S. The model is set up in a way that zooplankton can prey upon them (among other things), which does not provide the calcifiers with a competitive advantage at high latitude areas.

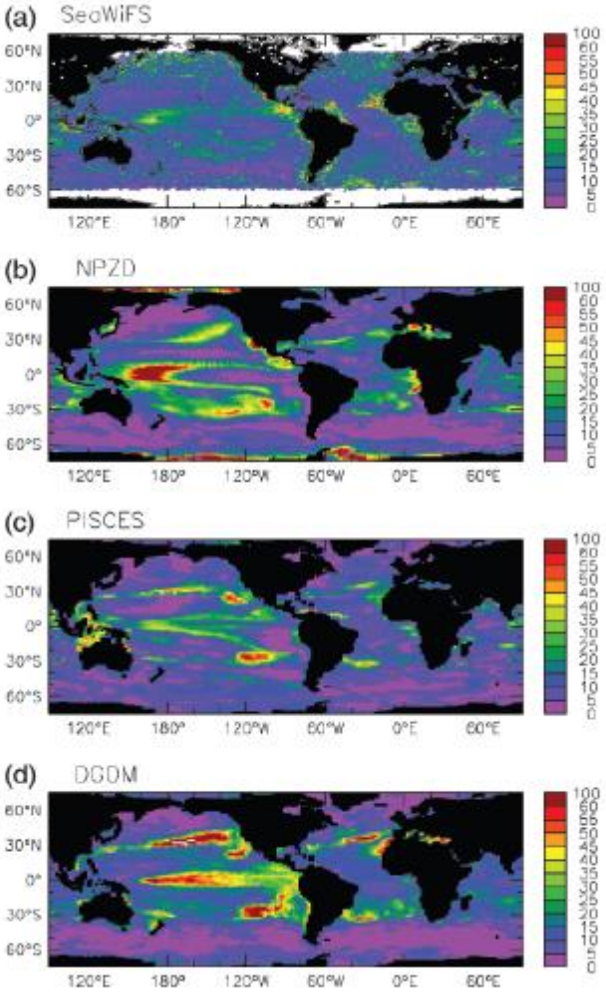


*Figure 41: Interannual variability in chlorophyll* a *(in %) derived from (a) SeaWIFs, (b) and NPZD model, (c) the PISCES model (4 PFTs), (d) a DGOM (5 PFTs). Taken from Le Quéré et al. (2005).*

These organisms have a lower growth rate than other PFTs, a lower affinity for light (they need more light to grow), and a lower tolerance for the absence of light. In this particular model, calcifiers have an advantage in areas where phosphorus and iron concentrations are low, which is not the case in the North Atlantic, for example. These rather poor modelling results demonstrate that our current knowledge of the behaviour/physiology of calcifiers is still incomplete, indicating that we may need to revise the way in which calcifiers are represented in DGOMs, particularly the prey-predator relationships (e.g., defence mechanisms against zooplankton predation).

The sensitivity analyses carried out on various DGOMs show that the choice of the characteristics of each PFT (and thus the parameters) have a significant impact on the resulting biogeochemistry in the model outputs. In global models, surface phytoplankton biomass is mainly controlled by the hydrodynamics of the model; in contrast, the composition of the ecosystem is controlled by the physiological parameters governing growth and loss. The difference in the maximum growth rates between PFTs is a critical parameter for controlling biodiversity in these models. Thus, a proportional change in the maximum growth rate for all PFTs leads only to small changes in the modelled biogeochemical dynamics. However, when these rates are changed in a non-proportional way, the carbon export and all other biogeochemical fields change significantly. Likewise, any change in the grazing preferences of zooplankton has an impact on the particle size distribution and thus on the rate of carbon export.

Therefore, DGOMs also have flaws that still need to be worked out. At present, there are three main directions of research that aim to improve these models:

1) Indirectly: by continuing to analyse the experimental and observational data we need to refine the common characteristics in each PFT. While the characteristics of silicifiers, diazotrophs,

DMS producers, and pico-autotrophs are starting to be fairly well understood, the characteristics of the remaining PFTs are only poorly constrained, mostly due to a lack of observational data. Many more field observations and laboratory experiments are needed to fill this gap in our knowledge. Since the growth conditions (nutrients, light) of phytoplankton can be studied independently of zooplankton, they are relatively well understood. However, the consumption of phytoplankton and detritus by zooplankton is equally important but is much more difficult to measure. Studies of higher trophic levels than phytoplankton deserve a particular focus in the coming years.

2) Collection of *in situ* biomass data for each PFT for comparisons with modelling results. Global databases are being set up for mesozooplankton and bacteria while they already exist for other PFTs. Still, these databases need to extend their geographical coverage. Remote sensing approaches appear to be promising, as the analytical methods to discriminate between different types of autotrophic PFTs in remote sensing data have improved (**Figure 42**).

3) Improve the theoretical understanding of the biogeochemical processes determining the growth and fate of PFTs in the ocean. This long-term effort could help reduce the number of PFTs or the characteristics needed to reproduce their fundamental behaviour/function in marine ecosystems.

In conclusion, it appears that DGOMs are much more versatile than the previous generation of biogeochemical models (NPZD). The greater complexity of DGOMs requires an improved coordination of the research efforts between modellers and observational biologists, geochemists, and biogeochemists, particularly at an international level.

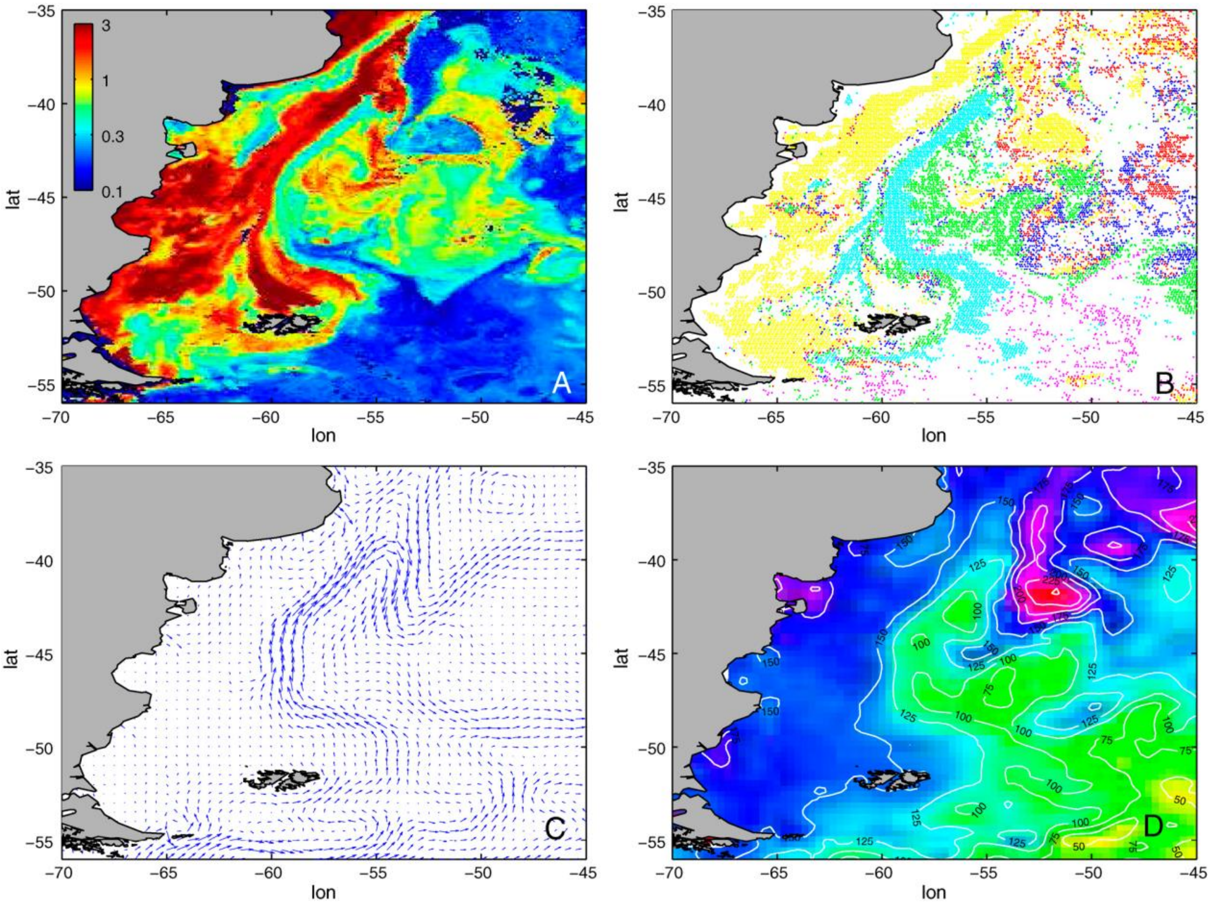


*Figure 42: Spatial distribution of surface chlorophyll from remote sensing observations in the South Atlantic. (A) Total chlorophyll (mg $m^{-3}$); (B) Dominant phytoplankton groups as identified with the PHYSAT algorithm during a spring bloom event (24 November - 1 December 2001). Green pixels indicate diatoms, red are Prochlorococcus, dark blue are Synechococcus, yellow are nanoeukaryotes, magenta are phaeocystis, and cyan represents coccolithophores. (C) Mean circulation, (D) Dynamic sea surface height (elevation in mm above the mean geoid). After D'OVIDIO et al. (2010).*

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