OCEAN BIOGEOCHEMISTRY AND ECOLOGY, MODELING OF

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Introduction

Modeling has emerged in the last few decades as a central approach for the study of biogeochemical and ecological processes in the sea. While this development was facilitated by the fast development of computer power, the main driver is the need to analyze and synthesize the rapidly expanding observations, to formulate and test hypotheses, and to make predictions how ocean ecology and biogeochemistry respond to perturbations. The final aim, prediction, has gained in importance recently as scientists are increasingly asked by society to investigate and assess the impact of past, current, and future human actions on ocean ecology and biogeochemistry.

The impact of the carbon dioxide (CO_2) that humankind has emitted and will continue to emit into the atmosphere for the foreseeable future is currently, perhaps, the dominant question facing the marine biogeochemical/ecological research community. This impact is multifaceted, and includes both direct (such as ocean acidification) and indirect effects that are associated with the CO_2-induced climate change. Of particular concern is the possibility that global climate change will lead to a reduced capacity of the ocean to absorb CO_2 from the atmosphere, so that a larger fraction of the CO_2 emitted into the atmosphere remains there, further enhancing global warming. In such a positive feedback case, the expected climate change for a given CO_2 emission will be larger relative to a case without feedbacks. Marine biogeochemical/ecological models have played a crucial role in elucidating and evaluating these processes, and they are increasingly used for making quantitative predictions with direct implications for climate policy.

There are many other marine biogeochemical and/or ecological problems related to human activities, for which models play a crucial role assessing their importance and magnitude and devising possible solutions. These include, for example, coastal eutrophication, overfishing, and dispersion of invasive species. The use of marine biogeochemical/ecological models is now so pervasive that practically every field of oceanography is on this list.

The aim of this article is to provide an introduction and overview of marine biogeochemical and ecological modeling. Given the breadth of modeling approaches in use today, this overview can by design not be inclusive and authoritative. We rather focus on some basic concepts and provide a few illustrative applications. We start with a broader description of the marine biogeochemical/ecological challenge at hand, and then introduce basic concepts used for biogeochemical/ecological modeling. In the final section, we use a number of examples to illustrate some of the core modeling approaches.

The Marine Ecology and Biogeochemistry Challenge

The complexity of the ocean biogeochemical/ecological problem is daunting, as it involves a complex interplay among biology, physical variability of the oceanic environment, and the interconnected cycles of a large number of bioactive elements, particularly those of carbon, nitrogen, phosphorus, oxygen, silicon, and iron (Figure 1). Furthermore, the ocean is an open system that exchanges mass and many elements with the surrounding realms, such as the atmosphere, the land, and the sediments.

The engine that sets nearly all of these cycles into motion is the photosynthetic fixation of dissolved inorganic carbon and many other nutrient elements into organic matter by phytoplankton in the illuminated upper layers of the ocean (euphotic zone). The net rate of this process (i.e., net primary production) is distributed heterogeneously in the ocean, primarily as a result of the combined limitation of nutrients and light. This results in similar heterogeneity in surface chlorophyll, a direct indicator of the amount of phytoplankton biomass (Figure 2(a)). The large-scale surface nutrient distributions, in turn, reflect the balance between biological removal and the physical processes of upwelling and mixing that transport subsurface nutrient pools upward into the euphotic zone (Figure 2(b)). In addition to the traditional macronutrients (nitrate, phosphate, silicate etc.), growing evidence shows that iron limitation is

Atmosphere
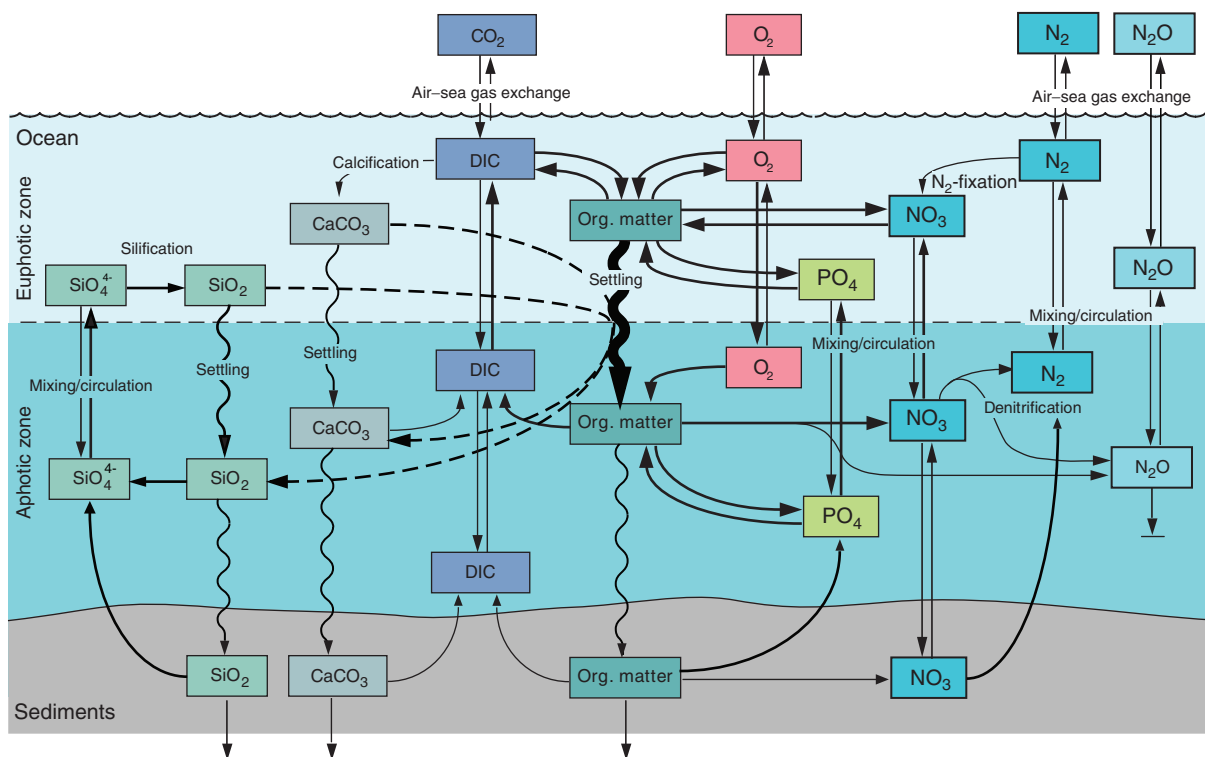
Figure 1   Schematic diagram of a number of key biogeochemical cycles in the ocean and their coupling. Shown are the cycles of carbon, oxygen, phosphorus, nitrogen, and silicon. The main engine of most biogeochemical cycles in the ocean is the biological production of organic matter in the illuminated upper ocean (euphotic zone), part of which sinks down into the ocean's interior and is then degraded back to inorganic constituents. This organic matter cycle involves not only carbon, but also nitrogen, phosphorus, and oxygen, causing a tight linkage between the cycles of these four elements. Since some phytoplankton, such as diatoms and coccolithophorids, produce shells made out of amorphous silicon and solid calcium carbonate, the silicon and $CaCO_3$ cycles also tend to be closely associated with the organic matter cycle. These ocean interior cycles are also connected to the atmosphere through the exchange of a couple of important gases, such as CO_2, oxygen, and nitrous oxide (N_2O). In fact, on timescales longer than a few decades, the ocean is the main controlling agent for the atmospheric CO_2 content.

a key factor governing net primary production in many parts of the ocean away from the main external sources for iron, such as atmospheric dust deposition and continental margin sediments. The photosynthesized organic matter is the basis for a complex food web that involves both a transfer of the organic matter toward higher trophic levels as well as a microbial loop that is responsible for most of the breakdown of this organic matter back to its inorganic constituents.

A fraction of the synthesized organic matter (about 10–20%) escapes degradation in the euphotic zone and sinks down into the dark aphotic zone, where it fuels the growth of microbes and zooplankton that eventually also remineralize most of this organic matter back to its inorganic constituents. The nutrient elements and the dissolved inorganic carbon are then eventually returned back to the surface ocean by ocean circulation and mixing, closing this 'great biogeochemical loop'. This loop is slightly leaky in that a

small fraction of the sinking organic matter fails to get remineralized in the water column and is deposited onto the sediments. Very little organic matter escapes remineralization in the sediments though, so that only a tiny fraction of the organic matter produced in the surface is permanently removed from the ocean by sediment burial. In the long-term steady state, this loss of carbon and other nutrient elements from the ocean is replaced by the input from land by rivers and through the atmosphere.

Several marine phytoplankton and zooplankton groups produce hard shells consisting of either mineral calcium carbonate ($CaCO_3$) or amorphous silica, referred to as 'opal' (SiO_2). The most important producers of $CaCO_3$ are coccolithophorids, while most marine opal stems from diatoms. Both groups are photosynthetic phytoplankton, highlighting the extraordinary importance of this trophic group for marine ecology and biogeochemistry. Upon the death of the mineral-forming organisms, these minerals
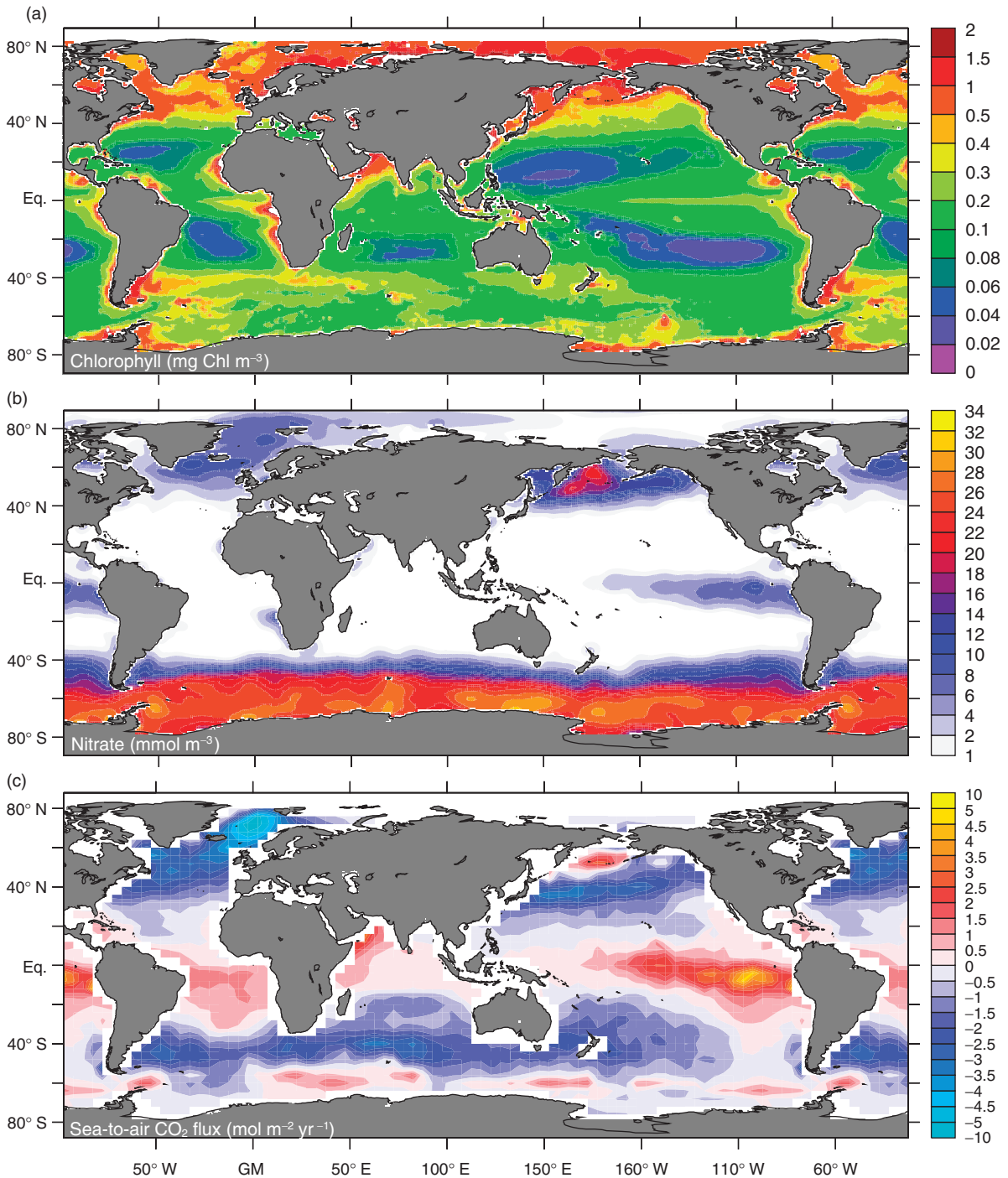
Figure 2   Global maps of the distribution of three key biogeochemical/ecological modeling targets. (a) Annual mean distribution of near-surface chlorophyll (mg Chl m^{-3}) as measured by the *SeaWiFS* satellite. (b) Annual mean surface distribution of nitrate (mmol^{-3}) compiled from *in situ* observations (from the World Ocean Atlas). (c) Annual mean air–sea CO_2 flux (mol m^{-2} yr^{-1}) for a nominal year of 2000 derived from a compilation of *in situ* measurements of the oceanic pCO_2 and a wind-speed gas exchange parametrization. Data provided by *T. Takahashi*, Lamont Doherty Earth Observatory of Columbia University.

also sink into the ocean's interior, thereby often acting as 'ballast' for organic matter.

This great biogeochemical loop also has a strong impact on several gases that are dissolved in seawater and exchange readily with the atmosphere, most importantly CO_2 and oxygen (O_2). Biological processes have opposite effects on these two gases: photosynthesis consumes CO_2 and liberates O_2,

while respiration and bacterial degradation releases CO_2 and consumes O_2. As a result, one tends to find an inverse relationship in the oceanic distribution of these two gases. CO_2 also sets itself apart from O_2 in that it reacts readily with seawater. In fact, due to the high content of alkaline substances in the ocean, this reaction is nearly complete, so that only around 1% of the total dissolved inorganic carbon in the ocean exists in the form of CO_2.

The exchange of CO_2 across the air–sea interface is a prime question facing ocean biogeochemical/ecological research, particularly with regard to the magnitude of the oceanic sink for anthropogenic CO_2. The anthropogenic CO_2 sink occurs on top of the natural air–sea CO_2 fluxes characterized by oceanic uptake in mid-latitudes and some high latitudes, and outgassing in the low latitudes and the Southern Ocean. This distribution of the natural CO_2 flux is the result of an interaction between the exchange of heat between the ocean and the atmosphere, which affects the solubility of CO_2, and the great biogeochemical loop, which causes an uptake of CO_2 from the atmosphere in regions where the downward flux of organic carbon exceeds the upward supply of dissolved inorganic carbon, and an outgassing where the balance is the opposite. This flux has changed considerably over the last two centuries in response to the anthropogenically driven increase in atmospheric CO_2 that pushes additional CO_2 from the atmosphere into the ocean. Nevertheless, the pattern of the resulting contemporary air–sea CO_2 flux (Figure 2(c)) primarily still reflects the flux pattern of the natural CO_2 fluxes, albeit with a global integral flux into the ocean reflecting the oceanic uptake of anthropogenic CO_2.

Given the central role of the great biogeochemical loop, any modeling of marine biogeochemical/ecological processes invariably revolves around the modeling of all the processes that make up this loop. As this loop starts with the photosynthetic production of organic matter by phytoplankton, biogeochemical modeling is always tightly interwoven with the modeling of marine ecology, especially that of the lower trophic levels.

Core questions that challenge marine biogeochemistry and ecology are as follows:

1. What controls the mean concentration and three-dimensional (3-D) distribution of bioreactive elements in the ocean?
2. What controls the air–sea balance of climatically important gases, that is, CO_2, N_2O, and O_2?
3. What controls ocean productivity, the downward export of organic matter, and the transfer of organic matter to higher trophic levels?
4. How do ocean biogeochemistry and ecology change in time in response to climate dynamics and human perturbations?

Modeling represents a powerful approach to studying and addressing these core questions. Modeling is by no means the sole approach. In fact, integrated approaches that combine observational, experimental, and modeling approaches are often necessary to tackle this set of complex problems.

What Is a Biogeochemical/Ecological Model?

At its most fundamental level, a model is an abstract description of how some aspect of nature functions, most often consisting of a set of mathematical expressions. In the biogeochemical/ecological modeling context, a model usually consists of a number of partial differential equations, which describe the time and space evolution of a (limited) number of ecological/biogeochemical state variables. As few of these equations can be solved analytically, they are often solved numerically using a computer, which requires the discretization of these equations, that is, they are converted into difference equations on a predefined spatial and temporal grid.

The Art of Biogeochemical/Ecological Modeling

A model can never fully represent reality. Rather, it aims to represent an aspect of reality in the context of a particular problem. The art of modeling is to find the right level of abstraction, while keeping enough complexity to resolve the problem at hand. That is, marine modelers often follow the strategy of Occam's razor, which states that given two competing explanations, the one that is simpler and makes fewer assumptions is the more likely to be correct. Therefore, a typical model can be used only for a limited set of applications, and great care must be used when a model is applied to a problem for which it was not designed. This is especially true for biogeochemical/ecological models, since their underlying mathematical descriptions are for the most part not based on first principles, but often derived from empirical relationships. In fact, marine biogeochemical/ecological modeling is at present a data-limited activity because we lack data to formulate and parametrize key processes and/or to evaluate the model predictions. Further, significant simplifications are often made to make the problem more tractable. For example, rather than treating

individual organisms or even species, model variables often aggregate entire functional groups into single boxes (e.g., photosynthetic organisms, grazers, and detritus decomposers), which are then simulated as bulk concentrations (e.g., $mol\,C\,m^{-3}$ of phytoplankton).

Despite these limitations, models allow us to ask questions about the ocean inaccessible from data or experiments alone. In particular, models help researchers quantify the interactions among multiple processes, synthesize diverse observations, test hypotheses, extrapolate across time – space scales, and predict past and future behavior. A well-posed model encapsulates our understanding of the ocean in a mathematically consistent form.

Biogeochemical/Ecological Modeling Equations and Approaches

In contrast with their terrestrial counterparts, models of marine biogeochemical/ecological processes must be coupled to a physical circulation model of some sort to take into consideration that nearly all relevant biological and biogeochemical processes occur either in the dissolved or suspended phase, and thus are subject to mixing and transport by ocean currents. Thus, a typical coupled physical–biogeochemical/ecological model consists of a set of time-dependent advection, diffusion, and reaction equations:

$$\frac{\partial C}{\partial t} + \mathrm{Adv}(C) + \mathrm{Diff}(C) = \mathrm{SMS}(C) \qquad [1]$$

where C is the state variable to be modeled, such as the concentration of phytoplankton, nutrients, or dissolved inorganic carbon, often in units of mass per unit volume (e.g., $mol\,m^{-3}$). $\mathrm{Adv}(C)$ and $\mathrm{Diff}(C)$ are the contributions to the temporal change in C by advection and eddy-diffusion (mixing), respectively, derived from the physical model component. The term $\mathrm{SMS}(C)$ refers to the 'sources minus sinks' of C driven by ecological/biogeochemical processes. The SMS term often involves complex interactions among a number of state variables and is provided by the biogeochemical/ecological model component.

Marine biogeochemical/ecological models are diverse, covering a wide range of complexities and applications from simple box models to globally 4-D-(space and time) coupled physical–biogeochemical simulations, and from strict research tools to climate change projections with direct societal implications. Model development and usage are strongly shaped by the motivating scientific or policy problems as well as the dynamics and 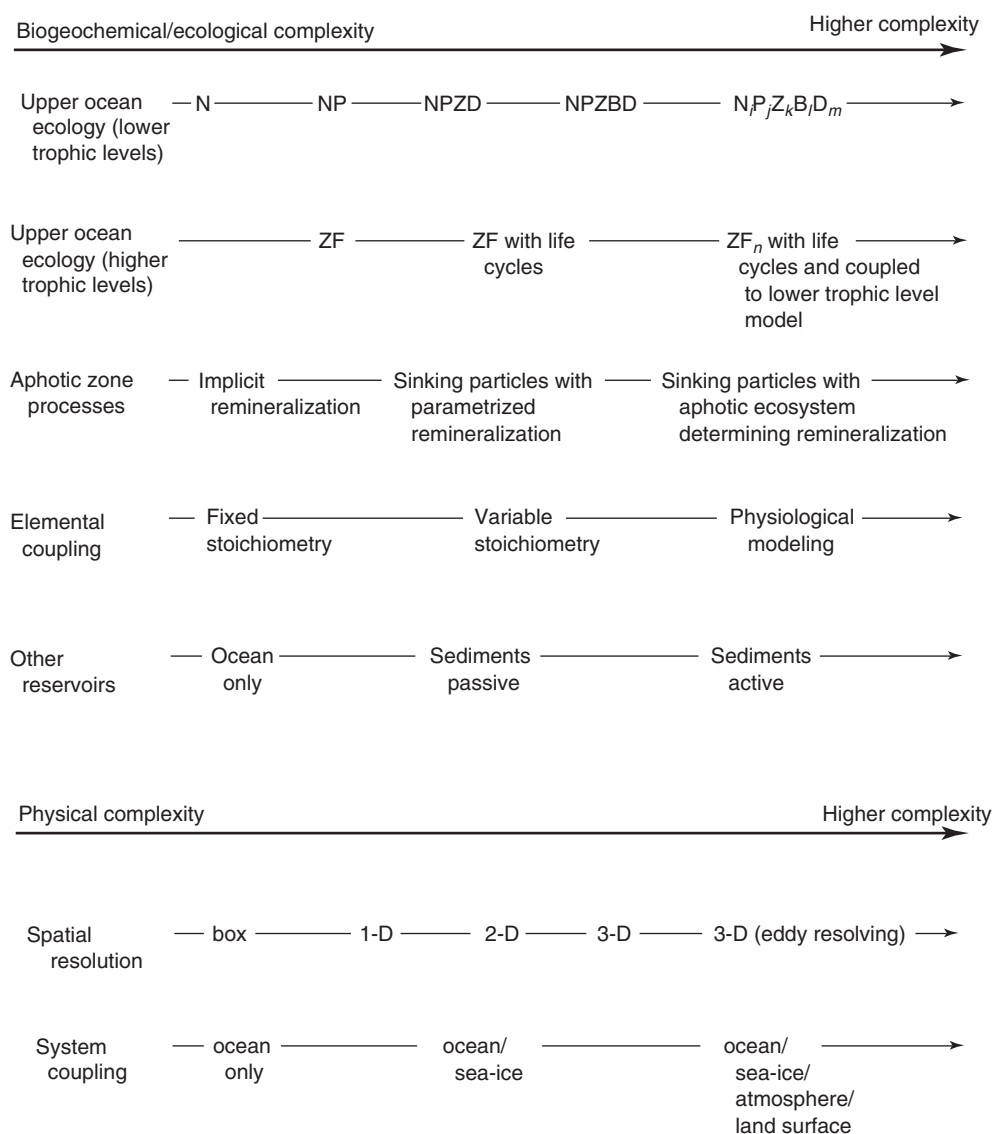time–space scales considered. The complexity of marine biogeochemical/ecological models can be organized along two major axes (Figure 3): the physical complexity, which determines how the left-hand side of [1] is computed, and the biogeochemical/ecological complexity, which determines how the right-hand side of [1] is evaluated.

Due to computational and analytical limitations, there is often a trade-off between the physical and biogeochemical/ecological complexity, so that models of the highest physical complexity are often using relatively simple biogeochemical/ecological models and vice versa (Figure 4). Additional constraints arise from the temporal domain of the integrations. Applications of coupled physical–biogeochemical/ecological models to paleoceanographic questions require integrations of several thousand years. This can only be achieved by reducing both the physical and the biogeochemical/ecological complexity (Figure 4). At the same time, the continuously increasing computational power has permitted researchers to push forward along both complexity axes. Nevertheless, the fundamental tradeoff between physical and biogeochemical/ecological complexity remains.

In addition to the physical and biogeochemical/ecological complexity, models can also be categorized with regard to their interaction with observations. In the case of 'forward models', a set of equations in the form of [1] is integrated forward in time given initial and boundary conditions. A typical forward problem is the prediction of the future state of ocean biogeochemistry and ecology for a certain evolution of the Earth's climate. The solutions of such forward models are the time–space distribution of the state variables as well as the implied fluxes. The expression 'inverse models' refers to a broad palette of modeling approaches, but all of them share the goal of optimally combining observations with knowledge about the workings of a system as embodied in the model. Solutions to such inverse models can be improved estimates of the current state of the system (state estimation), improved estimates of the initial or boundary conditions, or an optimal set of parameters. A typical example of an inverse model is the optimal determination of ecological parameters, such as growth and grazing rates, given, for example, the observed distribution of phytoplankton, zooplankton, and nutrients.

Examples

Given the large diversity of marine biogeochemical/ecological models and approaches, no review can do

Biogeochemical/ecological complexity

Higher complexity

| Upper ocean ecology (lower trophic levels) | N ——— NP ——— NPZD ——— NPZBD ——— $N_iP_jZ_kB_lD_m$ ———→ |

| Upper ocean ecology (higher trophic levels) | ——— ZF ——— ZF with life cycles ——— ZF_n with life cycles and coupled to lower trophic level model ———→ |

| Aphotic zone processes | — Implicit remineralization ——— Sinking particles with parametrized remineralization ——— Sinking particles with aphotic ecosystem determining remineralization ———→ |

| Elemental coupling | — Fixed stoichiometry ——— Variable stoichiometry ——— Physiological modeling ———→ |

| Other reservoirs | — Ocean only ——— Sediments passive ——— Sediments active ———→ |

Physical complexity

Higher complexity

| Spatial resolution | — box ——— 1-D ——— 2-D ——— 3-D ——— 3-D (eddy resolving) ——→ |

| System coupling | — ocean only ——— ocean/ sea-ice ——— ocean/ sea-ice/ atmosphere/ land surface ———→ |

Figure 3 Schematic diagram summarizing the development of complexity in coupled physical–biogeochemical/ecological models. The two major axes of complexity are biogeochemistry/ecology and physics, but each major axis consists of many subaxes that describe the complexity of various subcomponents. Currently existing models fill a large portion of the multidimensional space opened by these axes. In addition, the evolution of models is not always necessarily straight along any given axis, but depends on the nature of the particular problem investigated. N, nutrient; P, phytoplankton; Z, zooplankton; B, bacteria; D, detritus; F, fish.

full justice. We restrict our article here to the discussion of four examples, which span the range of complexities as well as have been important milestones in the evolution of biogeochemical/ecological modeling.

Box Models or What Controls Atmospheric Carbon Dioxide?

Our aim here is to develop a model that explains how the great biogeochemical loop controls atmospheric CO_2. The key to answering this question is a quantitative prediction of the surface ocean concentration of

CO_2, as it is this surface concentration that controls the atmosphere–ocean balance of CO_2. The simplest models used for such a purpose are box models, where the spatial dimension is reduced to a very limited number of discrete boxes. Such box models have played an important role in ocean biogeochemical/ ecological modeling, mostly because their solutions can be readily explored and understood. However, due to the dramatic reduction of complexity, there are also important limitations, whose consequences one must keep in mind when interpreting the results.

Box models can be formally derived from the tracer conservation eq [1] by integrating over
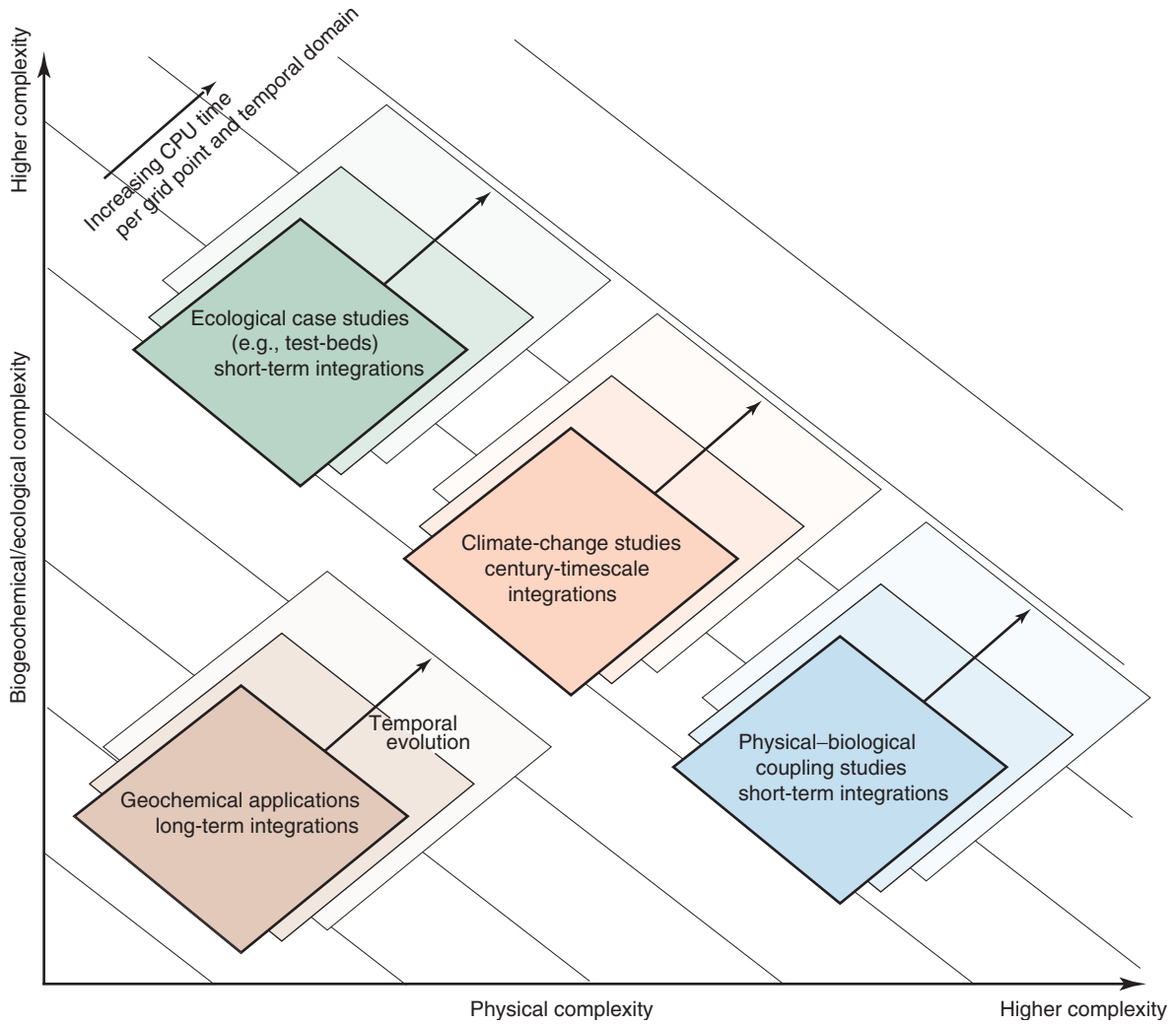
Figure 4 Schematic illustrating the relationship between the physical (abscissa) and the biogeochemical/ecological complexity (ordinate) of different typical applications of coupled physical–biogeochemical/ecological models. Given computational and analytical constraints, there is often a trade-off between the two main complexities. The thin lines in the background indicate the CPU time required for the computation of a problem over a given time period.

the volume of the box, V, and by applying Gauss' (divergence) theorem, which states that the volume integral of a flux is equal to the flux in normal direction across the boundary surfaces, S. The resulting integral form of [1] is:

$$\int \frac{\partial C}{\partial t}\, dV + \oint \left(\mathrm{Adv}_n(C) + \mathrm{Diff}_n(C) \right)\, dS = \int \mathrm{SMS}(C)\, dV \qquad [2]$$

where $\mathrm{Adv}_n(C)$ and $\mathrm{Diff}_n(C)$ are the advective and diffusive transports in the normal direction across S. If we assume that the concentration of tracer C as well as the SMS term within the box are uniform, [2]

can be rewritten as

$$V \cdot \frac{d\overline{C}}{dt} + \sum_i \left(T_{i,\mathrm{out}} \cdot \overline{C} - T_{i,\mathrm{in}} \cdot C_i + v_i(\overline{C} - C_i) \right) = V \cdot \mathrm{SMS}(\overline{C}) \qquad [3]$$

where $\overline{C}$ is the mean concentration within the box. We represented the advective contributions as products of a mass transport, T (dimensions volume time^{-1}), with the respective upstream concentration, separately considering the mass transport into the box and out of the box across each interface i, that is, $T_{i,\mathrm{in}}$ and $T_{i,\mathrm{out}}$. The eddy-diffusion contributions are parametrized as products of a mixing coefficient, v_i (dimension volume time^{-1}), with the gradient

across each interface $(\overline{C} - C_i)$. For simplicity, we subsequently drop the overbar, that is, use C instead of $\overline{C}$.

The simplest box-model representation of the great biogeochemical loop is a two-box model, wherein the ocean is divided into a surface and a deep box, representing the euphotic and aphotic zones, respectively (Figure 5(a)). Mixing and transport between the two boxes is modeled with a mixing term, v. The entire complexity of marine ecology and biogeochemistry in the euphotic zone is reduced to a single term, Φ, which represents the flux of organic matter out of the surface box and into the deep box, where the organic matter is degraded back to inorganic constituents.

Let us consider the deep-box balance for a dissolved inorganic bioreactive element, C_d (such as nitrate, phosphate, or dissolved inorganic carbon):

$$V_d \frac{dC_d}{dt} + v \cdot (C_d - C_s) = \Phi \qquad [4]$$

where V_d is the volume of the deep box and C_s is the dissolved inorganic concentration of the surface box. The steady-state solution of [4], that is, the solution when the time derivative of C_d vanishes $(dC_d/dt = 0)$,

$$v \cdot (C_d - C_s) = \Phi \qquad [5]$$

represents the most fundamental balance of the great biogeochemical loop. It states that the net upward transport of an inorganic bioreactive element by physical mixing is balanced by the downward transport of this element in organic matter. This steady-state balance [5] has several important applications. For example, it permits us to estimate the downward export of organic matter by simply

analyzing the vertical gradient and by estimating the vertical exchange. The balance also states that the magnitude of the vertical gradient in bioreactive elements is proportional to the strength of the downward flux of organic matter and inversely proportional to the mixing coefficient. Since nearly all oceanic inorganic carbon and nutrients reside in the deep box, that is, $V_d \cdot C_d \gg V_s \cdot C_s$, one can assume, to first order, that C_d is largely invariant, so that the transformed balance for the surface ocean concentration

$$C_s = C_d - \frac{\Phi}{v} \qquad [6]$$

reveals that the surface concentration depends primarily on the relative magnitude of the organic matter export to the magnitude of vertical mixing. Hence, [6] provides us with a first answer to our challenge: it states that, for a given amount of ocean mixing, the surface ocean concentration of inorganic carbon, and hence atmospheric CO_2, will decrease with increasing marine export production. Relationship [6] also states that for a given magnitude of marine export production, atmospheric CO_2 will increase with increased mixing.

While very powerful, the two-box model has severe limitations. The most important one is that this model does not consider the fact that the deep ocean exchanges readily only with the high latitudes, which represent only a very small part of the surface ocean. The exchange of the deep ocean with the low latitudes is severly limited because diapcyncal mixing in the ocean is small. Another limitation is that the one-box model does not take into account that the nutrient concentrations in the high latitudes tend to be much higher than in the low latitudes (Figure 2(c)).
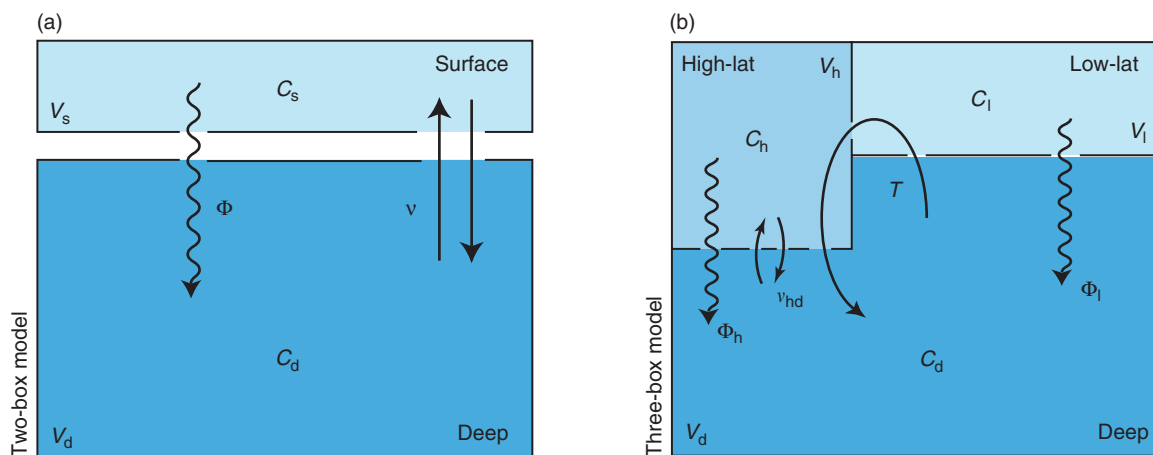
Figure 5 Schematic representation of the great biogeochemical loop in box models: (a) two-box model and (b) three-box model. C, concentrations; V, volume; v, exchange (mixing) coefficient; Φ, organic matter export fluxes; T, advective transport.
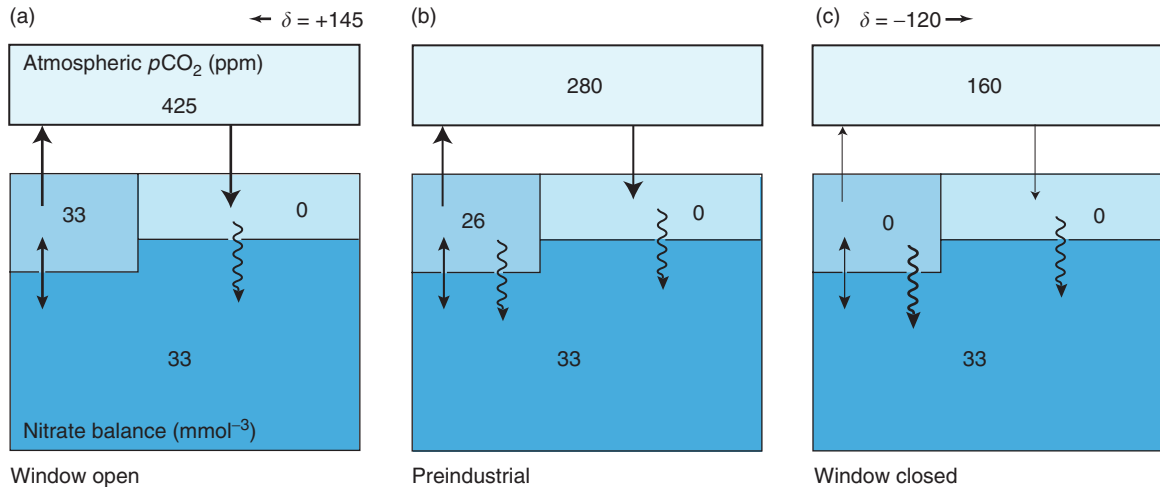
Figure 6 Schematic illustration of the impact of the high-latitude (Southern Ocean) window on atmospheric CO_2. In (a) the high-latitude window is open, high-latitude nitrate is high, and atmospheric CO_2 attains 425 ppm. Panel (b) represents the preindustrial ocean, where the window is half open, nitrate in the high latitudes is at intermediate levels, and atmospheric CO_2 is 280 ppm. In (c), the high-latitude window is closed, high-latitude nitrate is low, and atmospheric CO_2 decreases to about 160 ppm.

An elegant solution is the separation of the surface box into a high-latitude box, h, and a low-latitude box, l (**Figure 5(b)**). Intense mixing is assumed to occur only between the deep and the high-latitude boxes, v_{hd}. A large-scale transport, T, is added to mimic the ocean's global-scale overturning circulation. As before, the complex SMS terms are summarized by Φ_l and Φ_h. In steady state, the surface concentrations are given by

$$
\begin{aligned}
C_l &= C_d - \frac{\Phi_l}{T} \\
C_h &= C_d - \frac{\Phi_h + \Phi_l}{T + v_{hd}}
\end{aligned}
\qquad [7]
$$

which are structurally analogous to [6], but emphasize the different dynamics setting balances in the low and high latitudes. With $v_{hd} \gg T$ and $\Phi_l \approx \Phi_h$, [7] explains immediately why nutrient concentrations tend to be higher in high latitudes than in low latitudes (**Figure 2(b)**). In fact, writing [7] out for both nitrate (NO_3^-) and dissolved inorganic carbon (DIC), and using the observation that surface NO_3^- in the low latitudes is essentially zero (**Figure 2(c)**), the DIC equations are

$$
\begin{aligned}
DIC_l &= DIC_d - r_{C:N} \cdot [NO_3^-]_d \\
DIC_h &= DIC_d - \frac{\Phi_h + r_{C:N} \cdot T \cdot [NO_3^-]_d}{T + v_{hd}}
\end{aligned}
\qquad [8]
$$

where $r_{C:N}$ is the carbon-to-nitrogen ratio of organic matter. Assuming that the deep-ocean nitrate concentration is time invariant, the analysis of [8] reveals that the low-latitude DIC concentration, DIC_l,

is more or less fixed, while the high-latitude DIC concentration, DIC_h, can be readily altered by changes in either the high-latitude export flux, Φ_h, or high-latitude mixing, v_{hd}. Furthermore, if one considers the fact that the rapid communication between the high-latitude ocean and the deep ocean makes the high latitudes the primary window into the oceanic reservoir of inorganic carbon, it becomes clear that it must be the high latitudes that control atmospheric CO_2 on the millenial timescales where the steady-state approximation is justified. This high-latitude dominance in controlling atmospheric CO_2 is illustrated in **Figure 6**, which demonstrates that atmospheric CO_2 can vary between about 160 and 425 ppm by simply opening or closing this high-latitude window. The exact magnitude of the atmospheric CO_2 change depends, to a substantial degree, on the details of the model, but the dominance of high-latitude processes in controlling atmospheric CO_2 is also found in much more complex and spatially explicit models. As a result, a change in the carbon cycle in the high latitudes continues to be the leading explanation for the substantially lower atmospheric CO_2 concentrations during the ice ages.

NP and NPZ Models, or What Simple Ecosystem Models Can Say about Oceanic Productivity

So far, we have represented the ecological, chemical, and physical processes that control the production of organic matter and its subsequent export with a single parameter, Φ. Clearly, in order to assess how marine biology responds to climate change and other perturbations, it is necessary to resolve these

processes in much more detail. Two fundamentally different approaches have been developed to model such ecological processes: concentration-based models and individually based models (IBMs). In the latter, the model's equations represent the growth and losses of individual organisms, and the model then simulates the evolution of a large number of these individuals through space and time. This approach is most commonly used for the modeling of organisms at higher trophic levels, where life cycles play an important role (e.g., models of zooplankton, fish, and marine mammals). In contrast, concentration-based models are almost exclusively used for the modeling of the lower trophic levels, in particular to represent the interaction of light, nutrient, and grazing in controlling the growth of phytoplankton, that is, marine primary production.

The simplest such model considers just one limiting nutrient, N, and one single phytoplankton group, P (see also **Figure 7(a)**):

$$\text{SMS}(P) = V_{\max} \cdot \frac{N}{K_N + N} \cdot P - \lambda_P \cdot P$$
$$\text{SMS}(N) = -V_{\max} \cdot \frac{N}{K_N + N} \cdot P + \mu_P \cdot \lambda_P \cdot P \qquad [9]$$

where the first term on the right-hand side of the phytoplankton eqn [9] is net phytoplankton growth (equal to net primary production) modeled here as a function of a nutrient-saturated growth rate $V_{\max}$, and a hyperbolic dependence on the *in situ* nutrient concentration (Monod-type), with a single parameter, the half-saturation constant, K_N. The second term is the net loss due to senescence, viral infection, and grazing, modeled here as a linear process with a loss rate λ_P. A fraction μ_P of the phytoplankton loss is assumed to be regenerated inside the euphotic zone, while a fraction $(1 - \mu_P)$ is exported to depth (**Figure 7(a)**). These two parametrizations for phytoplankton growth and losses reflect a typical situation for marine ecosystem models in that the growth terms are substantially more elaborate, reflecting the interacting influence of various controlling parameters, whereas the loss processes are highly simplified. This situation also reflects the fact that the processes controlling the growth of marine organisms are often more amenable to experimental studies, while the loss processes are much harder to investigate with careful experiments.

When the SMS terms of [10] are inserted into the full tracer conservation eqn [1], the resulting equations form a set of coupled partial differential equations with a number of interesting consequences in steady state as shown in **Figure 8(a)**. Below a certain nutrient concentration threshold, phytoplankton growth is smaller than its loss term, so that the resulting steady-state solution is $P = 0$, that is, no phytoplankton. Above this threshold, the abundance of phytoplankton (and hence primary production) increases with increasing nutrient supply in a linear manner. Phytoplankton is successful in reducing the dissolved inorganic nutrient concentration to low levels, so that the steady state is characterized by most nutrients residing in organic form in the phytoplankton pool. This NP model reflects a situation where marine productivity is limited by bottom-up processes, that is, the supply of the essential nutrients. Comparison with the nutrient and phytoplankton distribution shown in (**Figure 2(b)**) shows that this model could explain the observations in the subtropical open ocean, where nutrients are indeed drawn down to very low levels. However, the NP model would also predict relatively high P levels to go along with the low nutrient levels, which is clearly not observed (**Figure 2(a)**). In addition, this NP model also fails clearly to explain the high-nutrient regions of the high latitudes. However, we have so far neglected the limitation by light, as well as the impact of zooplankton grazing.

The addition of a zooplankton compartment to the NP model (**Figure 7(b)**) dramatically shifts the nutrient allocation behavior (**Figure 8(b)**). In this case, as the nutrient loading increases, the phytoplankton abundance gets capped at a certain level by zooplankton grazing. Due to the reduced levels of biomass, the phytoplankton is then no longer able to consume all nutrients at high-nutrient loads, so that an increasing fraction of the supplied nutrients remains unused. This top-down limitation situation could therefore, in part, explain why macronutrients in certain regions remain untapped. Most recent research suggests that micronutrient (iron) limitation, in conjunction with zooplankton grazing, plays a more important role in causing these high-nutrient/low chlorophyll regions. Another key limitation is light, which has important consequences for the seasonal and depth evolution of phytoplankton.

Global 3-D Modeling of Ocean Biogeochemistry/Ecology

The coupling of relatively simple NPZ-type models to global coarse-resolution 3-D circulation models has proven to be a challenging task. Perhaps the most important limitation of such NPZ models is the fact that all phytoplankton in the ocean are represented by a single phytoplankton group, which is grazed upon by a single zooplankton group. This means that the tiny phytoplankton that dominate the relatively nutrient-poor central gyres of the ocean, and the

(a)

N–P model

(b)

N–P–Z model
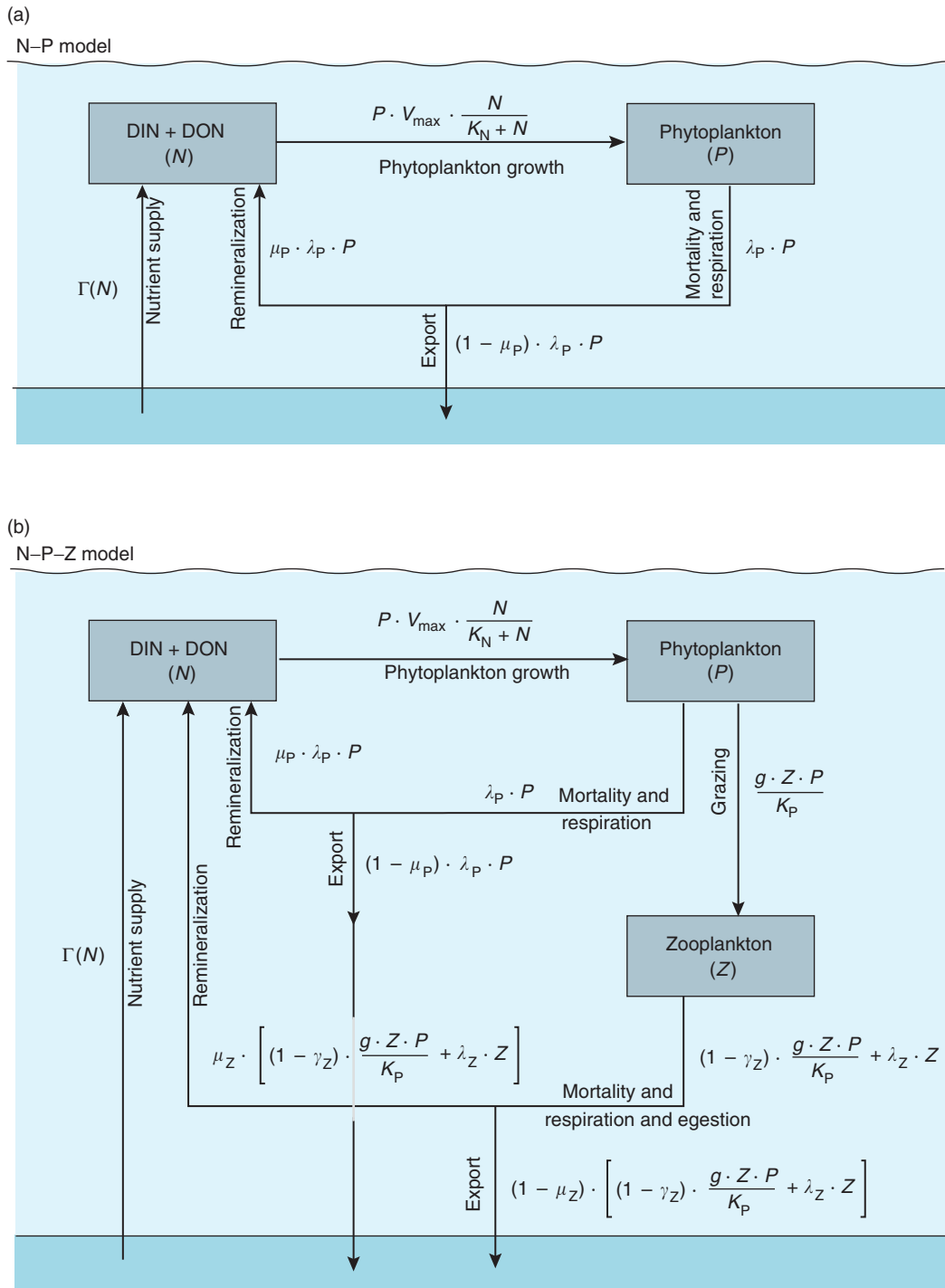
Figure 7 A schematic illustration of (a) a nitrate–phytoplankton model and (b) a nitrate–phytoplankton–zooplankton model. The mathematical expressions associated with each arrow represent typical representations for how the individual processes are parametrized in such models. V_{max}, maximum phytoplankton growth rate; K_N, nutrient half saturation concentration; g, maximum zooplankton growth rate; K_P, half saturation concentration for phytoplankton grazing; γ_Z, zooplankton assimilation efficiency; λ_P, phytoplankton mortality rate; λ_Z, zooplankton mortality rate; μ_P, fraction of dead phytoplankton nitrogen that is remineralized in the euphotic zone; μ_Z, as μ_P, but for zooplankton. Adapted from Sarmiento JL and Gruber N (2006) *Ocean Biogeochemical Dynamics*, 526pp. Princeton, NJ: Princeton University Press.
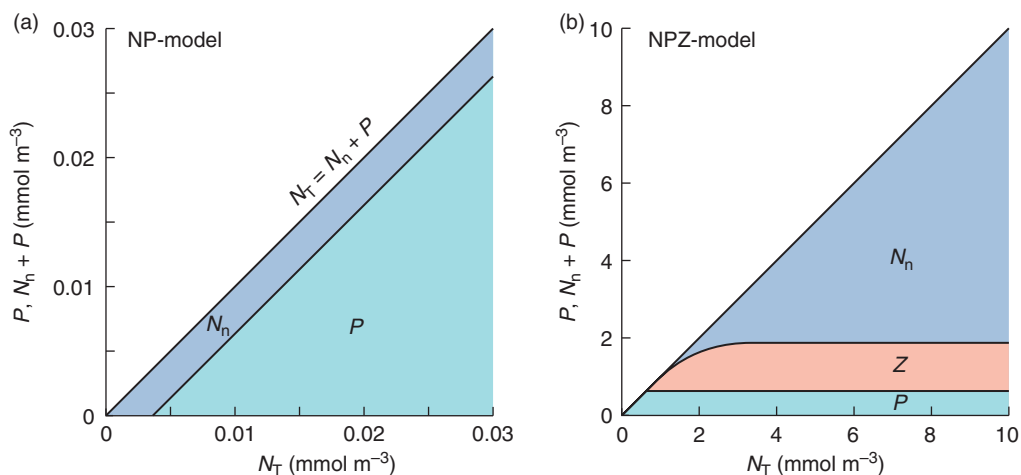
Figure 8 Nitrogen in phytoplankton (P), zooplankton (Z), and nitrate (N_n) as a function of total nitrogen. (a) Results from a two-component model that just includes N and P. (b) Results from a three-component model that is akin to that shown in **Figure 7(b)**. The vertical axis is concentration in each of the components plotted as the cumulative amount. Adapted from Sarmiento JL and Gruber N (2006) *Ocean Biogeochemical Dynamics*, 526pp. Princeton, NJ: Princeton University Press.

large phytoplankton that dominate the highly productive upwellling regions are represented with a single group, whose growth characteristics cannot simultaneously represent both. An additional challenge of the large-scale coupling problem is the interaction of oceanic circulation/mixing with the marine ecological and biogeochemical processes. Often, small deficiencies in the physical model get amplified by the ecological/biogeochemical model, so that the resulting fields of phytoplankton abundance may diverge strongly from observations.

The latter problem is addressed by improving critical aspects of the physical model, such as upper ocean mixing, atmospheric forcing, resolution, and numerical tracer transport algorithms, while the first problem is addressed by the consideration of distinct plankton functional groups. These functional groups distinguish themselves by their different size, nutrient requirement, biogeochemical role, and several other characteristics, but not necessarily by their taxa. Currently existing models typically consider the following phytoplankton functional groups: small phytoplankton (nano- and picoplankton), silicifying phytoplankton (diatoms), calcifying phytoplankton (coccolithophorids), N_2-fixing phytoplankton, large (nonsilicifying) phytoplankton (e.g., dinoflagellates and phaeocystis), with the choice of which group to include being driven by the particular question at hand. The partial differential equations for the different phytoplankton functional groups are essentially the same and follow a structure similar to [9], but are differentiated by varying growth parameters, nutrient/light requirements, and susceptibility to grazing. At present, most applications include between five and 10

phytoplankton functional groups. Some recent studies have been exploring the use of several dozen functional groups, whose parameters are generated stochastically with some simple set of rules that are then winnowed via competition for resources among the functional groups. Since the different phytoplankton functional groups are also grazed differentially, different types of zooplankton generally need to be considered as well, though fully developed models with diverse zooplankton functional groups are just emerging. An alternative is to use a single zooplankton group, but with changing grazing/growth characteristics depending on its main food source. A main advantage of models that build on the concept of plankton functional groups is their ability to switch between different phytoplankton community structures and to simulate their differential impact on marine biogeochemical processes. For example, the nutrient poor subtropical gyres tend to be dominated by nano- and picoplankton, whose biomass tends to be tightly capped by grazing by very small zooplankton. This prevents the group forming blooms, even under nutrient-rich conditions. By contrast, larger phytoplankton, such as diatoms, can often escape grazing control (at least temporarily) and form extensive blooms. Such phytoplankton community shifts are essential for controlling the export of organic matter toward the abyss, since the export ratio, that is, the fraction of net primary production that is exported, tends to increase substantially in blooms.

Results from the coupling of such a multiple functional phytoplankton ecosystem model and of a relatively simple biogeochemical model to a global 3-D circulation model show substantial success in

representing the basic features of chlorophyll, air–sea CO_2 flux, and surface nutrient concentration (Figure 9) seen in the observations (Figure 2). The comparison also shows some clear deficiencies, such as the lack of the representation of the highly elevated chlorophyll concentrations associated with many continental boundaries. This deficiency is

mostly a result of the lack of horizontal resolution. This could be overcome, theoretically, by increasing the resolution of the global models to the eddy-resolving scale needed to properly represent such boundary regions (c. 5–10 km or so, rather than the several hundred kilometer resolution currently used for most global-scale biogeochemical/ecological
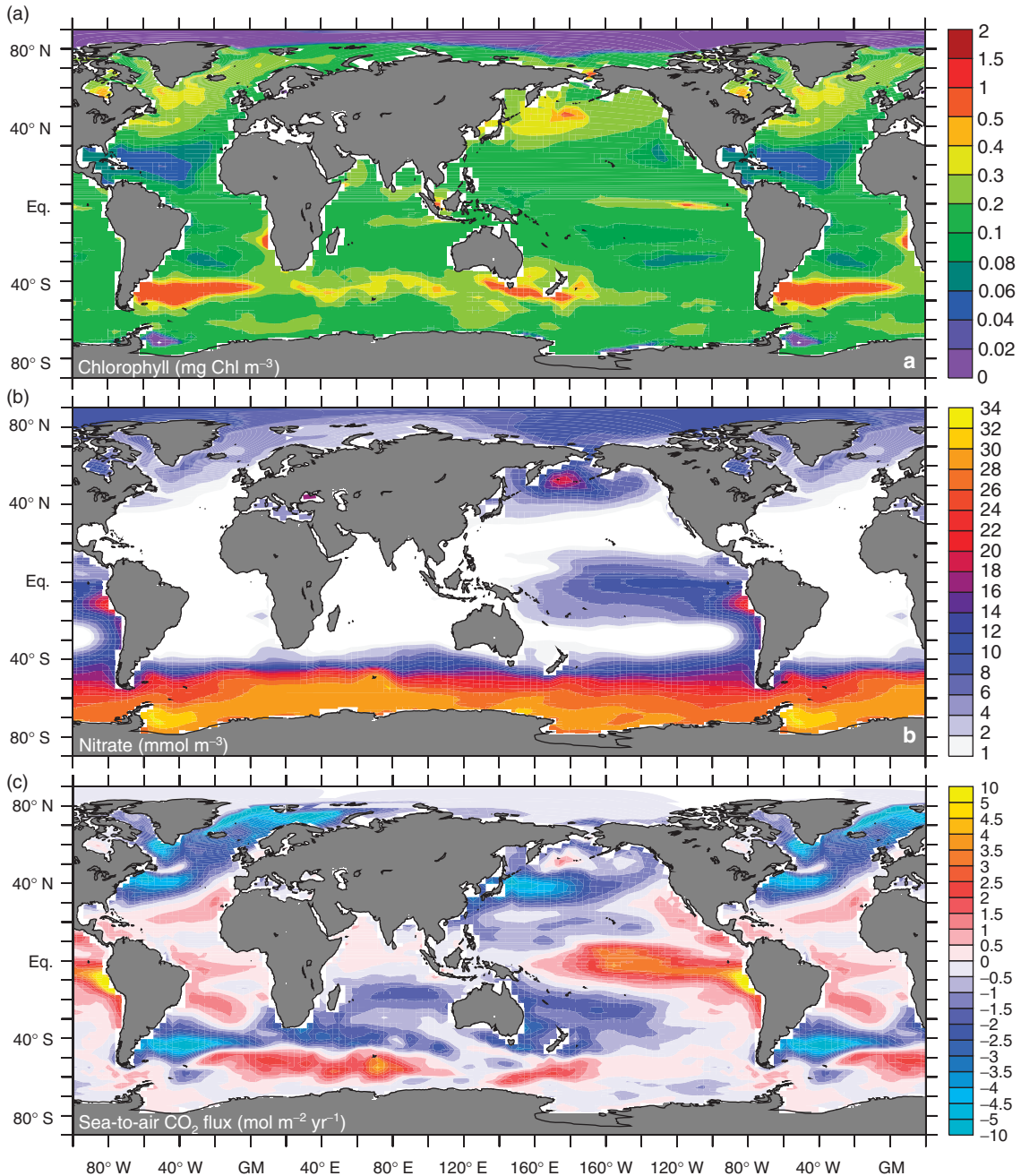
Figure 9 Global maps of model simulated key biogeochemical/ecological targets (cf. Figure 2) from the National Center for Atmospheric Research (NCAR) Community Climate System Model (CCSM): (a) annual mean distribution of near-surface chlorophyll (mg Chl m^{-3}); (b) annual mean surface distribution of nitrate (mmol^{-3}); and (c) annual mean air–sea CO_2 flux (mol m^{-2} yr^{-1}) for the period 1990 until 2000. All model results stem from a simulation, in which a multiple functional phytoplankton group model was coupled to a global 3-D ocean circulation model. Results provided by S.C. Doney and I. Lima, WHOI.
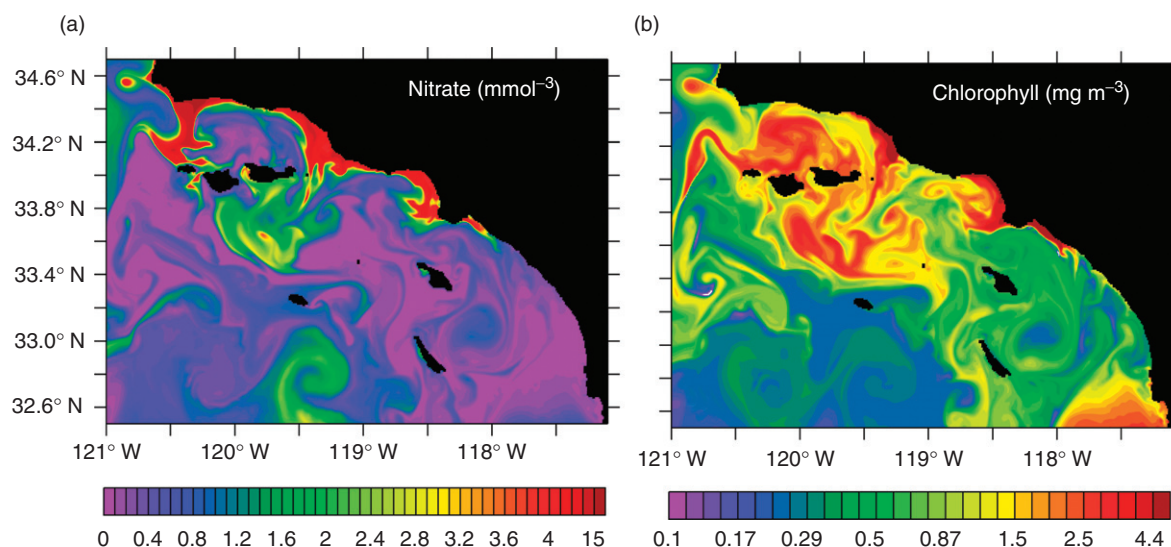
Figure 10 Snapshots of (a) surface nitrate and (b) surface chlorophyll as simulated by a 1-km, that is, eddy-resolving, regional model for the Southern California Bight. The snapshots represent typical conditions in response to a spring-time upwelling event in this region. The model consists of a multiple phytoplankton functional group model that has been coupled to the Regional Ocean Modeling System (ROMS). Results provided by H. Frenzel, UCLA.

simulations). This is currently feasible for only very short periods, so that limited domain models are often used instead.

Eddy-resolving Regional Models

Limited domain models, as shown in **Figure 10** for the Southern California Bight, that is, the southernmost region of the West Coast of the US, can be run at much higher resolutions over extended periods, permitting the investigation of the processes occurring at the kilometer scale. The most important such processes are meso- and submesoscale eddies and other manifestations of turbulence, which are ubiquitous features of the ocean. The coupling of the same ecosystem/biogeochemical model used for the global model shown in **Figure 9** to a 1-km resolution model of the Southern California Bight reveals the spatial richness and sharp gradients that are commonly observed (**Figure 10**) and that emerge from the intense interactions of the physical and biogeochemical/ecological processes at the eddy scale. Since such mesoscale processes are unlikely to be resolved at the global scale for a while, a current challenge is to find parametrizations that incorporate the net impact of these processes without actually resolving them explicitly.

Future Directions

The modeling of marine biogeochemical/ecological processes is a new and rapidly evolving field, so that

predictions of future developments are uncertain. Nevertheless, it is reasonable to expect that models will continue to evolve along the major axes of complexity, including, for example, the consideration of higher trophic levels (**Figure 4**). One also envisions that marine biogeochemical/ecological models will be increasingly coupled to other systems. A good example are Earth System Models that attempt to represent the entire climate system of the Earth including the global carbon cycle. In those models, the marine biogeochemical/ecological models are just a small part, but interact with all other components, possibly leading to complex behavior including feedbacks and limit cycles. Another major anticipated development is the increasing use of inverse modeling approaches to optimally make use of the increasing flow of observations.

Glossary

advection   The transport of a quantity in a vector field, such as ocean circulation.

anthropogenic carbon   The additional carbon that has been released to the environment over the last several centuries by human activities including fossil-fuel combustion, agriculture, forestry, and biomass burning.

biogeochemical loop, great   A set of key processes that control the distribution of bioreactive elements in the ocean. The loop starts with the photosynthetic production of organic matter in the light-illuminated upper ocean, a fraction of which

is exported to depth mostly by sinking of particles. During their sinking in the dark deeper layers of the ocean, this organic matter is consumed by bacteria and zooplankton that transform it back to its inorganic constituents while consuming oxidized components in the water (mostly oxygen). The great biogeochemical loop is closed by the physical transport and mixing of these inorganic bioreactive elements back to the near-surface ocean, where the process starts again. This great biogeochemical loop also impacts the distribution of many other elements, particularly those that are particle reactive, such as thorium.

coccolithophorids A group of phytoplankton belonging to the haptophytes. They are distinguished by their formation of small mineral calcium carbonate plates called coccoliths, which contribute to the majority of marine calcium carbonate production. An example of a globally significant coccolithophore is *Emiliania huxleyi*.

diatoms A group of phytoplankton belonging to the class Bacillariophyceae. They are one of the most common types of phytoplankton and distinguish themselves through their production of a cell wall made of amorphous silica, called opal. These walls show a wide diversity in form, but usually consist of two symmetrical sides with a split between them.

diffusion The transport of a quantity by Brownian motion (molecular diffusion) or turbulence (eddy diffusion). The latter is actually some form of advection, but since its net effect is akin to diffusion, it is often represented as a diffusive process.

export production The part of the organic matter formed in the surface layer by photosynthesis that is transported out of the surface layer and into the interior of the ocean by particle sinking, mixing, and circulation, or active transport by organisms.

models, concentration based Models, in which the biological state variables are given as numbers per unit volume, that is, concentration. This approach is often used when physical dispersion plays an important role in determining the biological and biogeochemical impact of these state variables. Concentration-based models are most often used to represent lower trophic levels in the ocean.

models, forward Models, in which time is integrated forward to compute the temporal evolution of the distribution of state variables in response to a set of initial and boundary conditions.

models, individually based Models, in which the biological state variables represent individual organisms or a small group of individual organisms. This approach is often used when life cycles play a major role in the development of these organisms, such as is the case for most marine organisms at higher trophic levels.

models, inverse Models that aim to optimally combine observations with knowledge about the workings of a system as embodied in the model. Solutions to such inverse models can be improved estimates of the current state of the system (state estimation), improved estimates of the initial or boundary conditions, or an optimal set of parameters. A typical example of an inverse model is the optimal determination of ecological parameters, such as growth and grazing rates, given, for example, the observed distribution of phytoplankton, zooplankton, and nutrients.

net primary production Rate of net fixation of inorganic carbon into organic carbon by autotrophic phytoplankton. This net rate is the difference between the gross uptake of inorganic carbon during photosynthesis and autotrophic respiration.

organisms, autotrophic An autotroph (from the Greek *autos* = self and *trophe* = nutrition) is an organism that produces organic compounds from carbon dioxide as a carbon source, using either light or reactions of inorganic chemical compounds, as a source of energy. An autotroph is known as a producer in a food chain.

organisms, heterotrophic A heterotroph (Greek *heterone* = (an)other and *trophe* = nutrition) is an organism that requires organic substrates to get its carbon for growth and development. A heterotroph is known as a consumer in the food chain.

plankton Organisms whose swimming speed is smaller than the typical speed of ocean currents, so that they cannot resist currents and are hence unable to determine their horizontal position. This is in contrast to nekton organisms that can swim against the ambient flow of the water environment and control their position (e.g., squid, fish, krill, and marine mammals).

plankton, phytoplankton Phytoplankton are the (photo)autotrophic components of the plankton. Phytoplankton are pro- or eukaryotic algae that live near the water surface where there is sufficient light to support photosynthesis. Among the more important groups are the diatoms, cyanobacteria, dinoflagellates, and coccolithophorids.

plankton, zooplankton Zooplankton are heterotrophic plankton that feed on other plankton. Dominant groups include small protozoans or metazoans (e.g., crustaceans and other animals).

See also

Biogeochemical Data Assimilation. Carbon Cycle. Carbon Dioxide (CO₂) Cycle. Forward Problem in Numerical Models. Inverse Modeling of Tracers and Nutrients. Mesoscale Eddies. Nitrogen Cycle. Ocean Carbon System, Modeling of. Ocean Circulation. Phosphorus Cycle.

Further Reading

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