OCEAN CARBON SYSTEM, MODELING OF

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Introduction

Oceanic transient tracers such as radiocarbon and tritium are important tools for carbon cycle research because they provide estimates of timescale and absolute rates. The marine carbon cycle is governed by both ocean biology and physics. Carbon observations are often framed therefore in terms of simple, idealized ocean circulation models. Model advection and diffusion rates are typically calibrated against transient tracer data. Such models are straightforward to construct and computationally inexpensive and are thus conducive to hypothesis testing and extensive exploration of parameter space. They are used commonly to examine specific biogeochemical process, quantify the uptake of anthropogenic carbon and study the carbon cycle responses to climate change. Idealized models have potential drawbacks, however, and part of the art of numerical modeling is deciding on the appropriate model(s) for the particular question at hand.

Carbon plays a unique role in the Earth's environment, bridging between the physical and biogeochemical systems. Carbon dioxide (CO_2), a minor constituent in the atmosphere, is a so-called greenhouse gas that helps to modulate the planet's climate and temperature. Given sunlight and nutrients, plants and some microorganisms convert CO_2 via photosynthesis into organic carbon, serving as the building blocks and energy source for most of the world's biota. The concentration of CO_2 in the atmosphere is affected by the net balance of photosynthesis and the reverse reaction respiration on land and in the ocean. Changes in ocean circulation and temperature can also change CO_2 levels because carbon dioxide is quite soluble in sea water. In fact, the total amount of dissolved inorganic carbon (DIC) in the ocean is about fifty times larger than the atmospheric inventory. The air–sea exchange of carbon is governed by the gas transfer velocity and the surface water partial pressure of CO_2 (pCO$_2$), which increases with warmer temperatures, higher DIC and lower alkalinity levels. The natural carbon cycle has undergone large fluctuations in the past, the most striking during glacial periods when atmospheric CO_2 levels were about 30% lower than preindustrial values. The ocean must have been involved in such a large redistribution of carbon, but the exact mechanism is still not agreed upon.

Human activities including fossil fuel burning and land-use practices (e.g., deforestation, biomass burning) are altering the natural carbon cycle. Currently about 9 Pg carbon per year (1 Pg $= 10^{15}$ g) are emitted into the atmosphere, and direct measurements show that the atmospheric CO_2 concentration is indeed growing rapidly with time. Elevated atmospheric CO_2 levels are projected to heat the Earth's surface, and the evidence for climate warming is mounting. Only about 40% of the released anthropogenic carbon remains in the atmosphere, the remainder is taken up in about equal portions (or 2 Pg carbon per year) by land and ocean sinks (**Figure 1**). The future magnitude of these sinks is not well known, however, and is one of the major uncertainties in climate simulations.

Solving this problem is complicated because human impacts appear as relatively small perturbations on a large natural background. In the ocean, the reservoir of organic carbon locked up as living organisms, mostly plankton, is only about 3 Pg carbon. The marine biota in the sunlit surface ocean are quite productive though, producing roughly 50 Pg of new organic carbon per year. Most of this material is recycled near the ocean surface by zooplankton grazing or microbial consumption. A small fraction, something like 10–20% on average, is exported to the deep ocean as sinking particles or as dissolved organic matter moving with the ocean circulation. Bacteria and other organisms in the deep ocean feed on this source of organic matter from above, releasing DIC and associated nutrients back into the water, a process termed remineralization. The export flux from the surface ocean is a key factor driving the marine biogeochemical cycles of carbon, oxygen, nitrogen, phosphorus, silicon, and trace metals such as iron.

The surface export and subsurface remineralization of organic matter are difficult to measure directly. Biogeochemical rates, therefore, are often inferred based on the large-scale distributions of DIC, alkalinity, inorganic nutrients (nitrate, phosphate and silicate), and dissolved oxygen. The elemental stoichiometry of marine organic matter, referred to as the Redfield ratio, is with some

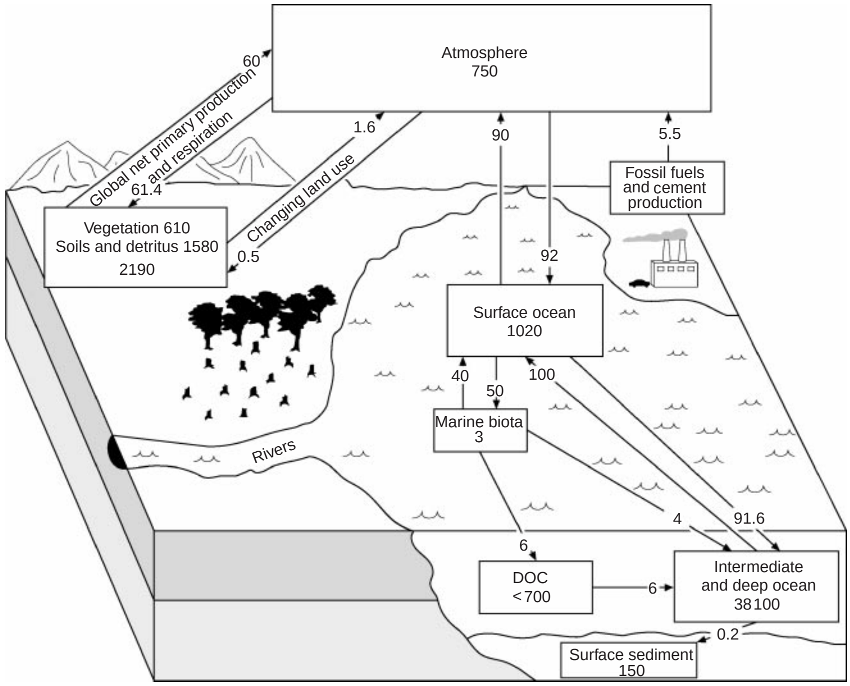

Figure 1 Schematic of global carbon cycle for the 1980s including natural background and human perturbations. Carbon inventories are in Pg carbon (1 Pg = 10^{15} g) and fluxes are in Pg carbon per year. DOC, dissolved organic carbon. (Adapted with permision from Schimel *et al.* 1995.)

interesting exceptions relatively constant in the ocean, simplifying the problem of interrelating the various biogeochemical fields. Geochemical distributions have the advantage that they integrate over much of the localized time/space variability in the ocean and can be used to extrapolate to region and basin scales. Property fields, though, reflect a combination of the net biogeochemical uptake and release as well as physical circulation and turbulent mixing. Additional information is required to separate these signals and can come from a mix of dynamical constraints, numerical models and ocean process tracers.

The latter two approaches are related because natural and artificial tracers are used to calibrate or evaluate ocean models. A key aspect of these tracers is that they provide independent information on time-scale, either because they decay or are produced at some known rate, for example due to radioactivity, or because they are released into the ocean with a known time history. The different chemical tracers can be roughly divided into two classes. Circulation tracers such as radiocarbon, tritium-^{3}He, and the chlorofluorocarbons are not strongly impacted by biogeochemical cycling and are used primarily to quantify physical advection and mixing rates. These tracers are the major focus here. The distribution of other tracer species is more closely governed by biology and chemistry, for example the thorium isotope series, which is used to study export production, particle scavenging, vertical transport, and remineralization rates.

Ocean Tracers and Dynamics: A one-dimensional (1-D) Example

Natural radiocarbon (^{14}C), a radioactive isotope of carbon, is a prototypical example of a (mostly) passive ocean circulation tracer. Radiocarbon is produced by cosmic rays in the upper atmosphere and enters the surface ocean as radiolabeled carbon dioxide ($^{14}CO_2$) via air–sea gas exchange. The ^{14}C DIC concentrations in the ocean decrease away from the surface, reflecting the passage of time since the water was last exposed to the atmosphere. Some radiolabeled carbon is transported to the deep ocean in sinking particulate organic matter, which can be largely corrected for in the analysis. The ^{14}C deficits relative to the surface water can be converted into age estimates for ocean deep waters using the radioactive decay half-life (5730 years). Natural radiocarbon is most effective for describing the slow thermohaline overturning circulation of the deep ocean, which has timescales of roughly a few hundred to a thousand years.

The main thermocline of the ocean, from the surface down to about 1 km or so, has more rapid ventilation timescales, from a few years to a few decades. Tracers useful in this regard are chlorofluorocarbons, tritium and its decay product ^{3}He, and bomb-radiocarbon, which along with tritium was released into the atmosphere in large quantities in the 1950s and 1960s by atmospheric nuclear weapons testing.

When properly formulated, the combination of ocean process tracers and numerical models provides powerful tools for studying ocean biogeochemistry. At their most basic level, models are simply a mathematical statement quantifying the rates of the essential physical and biogeochemical processes. For example, advection–diffusion models are structured around coupled sets of differential equations:

$$\frac{\partial C}{\partial t} = -u \cdot \nabla C + \nabla K \nabla C + J \qquad [1]$$

describing the time rate of change of a generic species C. The first and second terms on the right hand side of the equation stand for the local divergence due to physical advection and turbulent mixing, respectively. All of the details of the biogeochemistry are hidden in the net source/sink term J, which for radiocarbon would include net input from particle remineralization (R) and radioactive loss ($-\lambda^{14}C$).

One of the first applications of ocean radiocarbon data was as a constraint on the vertical diffusivity, upwelling and oxygen consumption rates in the deep waters below the main thermocline. As illustrated in **Figure 2**, the oxygen and radiocarbon concentrations in the North Pacific show a minimum at mid-depth and then increase toward the ocean seabed. This reflects particle remineralization in the water column and the inflow and gradual upwelling of more recently ventilated bottom waters from the Southern Ocean. Mathematically, the vertical profiles for radiocarbon, oxygen (O_2), and a conservative tracer salinity (S) can be posed as steady-state, 1-D balances:

$$0 = K_z \frac{d^2S}{dz^2} - w\frac{dS}{dz} \qquad [2]$$

$$0 = K_z \frac{d^2O_2}{dz^2} - w\frac{dO_2}{dz} + R_{O_2} \qquad [3]$$

$$0 = K_z \frac{d^2\,{}^{14}C}{dz^2} - w\frac{d^{14}C}{dz} + {}^{14}C:O_2 R_{O_2} - \lambda^{14}C \qquad [4]$$

K_z and w are the vertical diffusivity and upwelling rates, and $^{14}C:O_2$ is a conversion factor.

Looking carefully at eqn [2], one sees that the solution depends on the ratio K_z/w but not K_z or w separately. Similarly the equation for oxygen gives us information on the relative rates of upwelling and remineralization. It is only by the inclusion of radiocarbon, with its independent clock due to

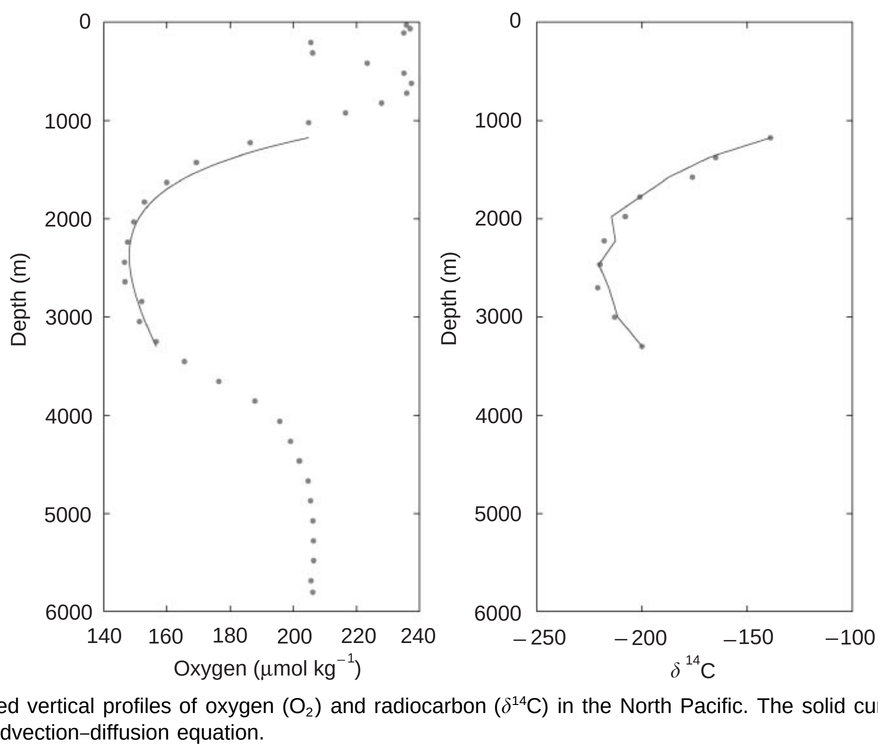

Figure 2 Observed vertical profiles of oxygen (O_2) and radiocarbon ($\delta^{14}C$) in the North Pacific. The solid curves are the model solution of a 1-D advection–diffusion equation.

radioactive decay, that we can solve for the absolute physical and biological rates. The solutions to eqns [2]–[4] can be derived analytically, and as shown in **Figure 2** parameter values of $w = 2.3 \times 10^{-5}\,\mathrm{cm\,s^{-1}}$, $K_z = 1.3\,\mathrm{cm^2/s^2}$, and $R_{O_2} = 0.13 \times 10^{-6}$ mol $\mathrm{kg^{-1}\,y^{-1}}$ fit the data reasonably well. The 1-D model derived vertical diffusivity is about an order of magnitude larger than estimates from deliberate tracer release experiments and microscale turbulence measurements in the upper thermocline. However, they may be consistent with recent observations of enhanced deep-water vertical mixing over regions of rough bottom topography.

Idealized Ocean Circulation Models

The 1-D example shows the basic principles behind the application of tracer data to the ocean carbon cycle, but the complexity (if not always the sophistication) of the models and analysis has grown with time. Ocean carbon models can be roughly divided into idealized models (multi-box, 1-D and 2-D advection-diffusion models) and 3-D general circulation models (GCMs). Although the distinction can be blurry at times, idealized models are characterized typically by reduced dimensionality and/or kinematic rather than dynamic physics. That is the circulation and mixing are specified rather than computed by the model and are often adjusted to best match the transient tracer data.

Global Box Models

An example of a simple, high latitude outcrop box model is shown in **Figure 3(A,B)**. The boxes represent the atmosphere, the high and low latitude surface ocean and the deep interior. In the model, the ocean thermohaline circulation is represented by one-way flow with high latitude sinking, low latitude upwelling, and poleward surface return flow. Horizontal and vertical mixing are included by two-way exchange of water between each pair of boxes. The physical parameters are constrained so that model natural radiocarbon values roughly match observations. Note that the ^{14}C concentration in the deep water is significantly depleted relative to the surface boxes and amounts to a mean deep-water ventilation age of about 1150 years.

The model circulation also transports phosphate, inorganic carbon, and alkalinity. Biological production, particle export and remineralization are simulated by the uptake of these species in the surface boxes and release in the deep box. The model allows for air–sea fluxes of CO_2 between the surface boxes and the atmosphere. The low latitude nutrient concentrations are set near zero as observed. The surface nutrients in the high latitude box are allowed to vary and are never completely depleted in the simulation of modern conditions. Similar regions of 'high-nutrient, low-chlorophyll' concentrations are observed in the subpolar North Pacific and Southern Oceans and are thought to be maintained by a combination of light and iron limitation as well as zooplankton grazing. The nutrient and DIC concentrations in the deep box are higher than either of the surface boxes reflecting the remineralization of sinking organic particles.

The 3-box ocean outcrop model predicts that atmospheric CO_2 is controlled primarily by the degree

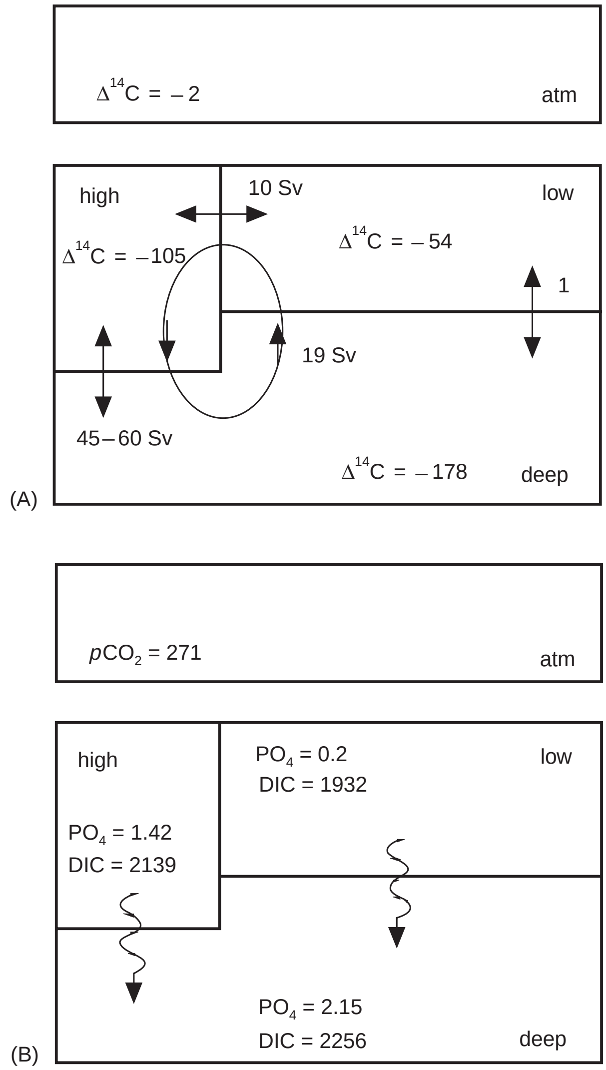

Figure 3 Results from a simple three-box ocean carbon cycle model. (A) shows the physical circulation and modeled radiocarbon ($\Delta^{14}C$) values. (B) shows the model biogeochemical fields, ocean dissolved inorganic carbon (DIC) and phosphate (PO_4) and atmospheric pCO_2. (Adapted with permission from Toggweiler and Sarmiento (1985).)

of nutrient utilization in high latitude surface regions. Because marine production and remineralization occur with approximately fixed carbon to nutrient ratios, the elevated nutrients in the deep box are associated with an equivalent increase in DIC and pCO_2. Large adjustments in the partitioning of carbon between the ocean and atmosphere can occur only where this close coupling of the carbon and nutrient cycles breaks down. When subsurface water is brought to the surface at low latitude, production draws the nutrients down to near zero and removes to first order all of the excess seawater DIC and pCO_2. Modifications in the upward nutrient flux to the low latitudes have relatively little impact on the model atmospheric CO_2 as long as the surface nutrient concentrations stay near zero.

At high latitudes, however, the nutrients and excess DIC are only partially utilized, resulting in higher surface water pCO_2 and over decades to centuries higher atmospheric CO_2 concentrations. Depending on the polar biological efficiency, the model atmosphere effectively sees more or less of the high DIC concentrations (and pCO_2 levels) of the deep ocean. Thus changes in ocean biology and physics can have a correspondingly large impact on atmospheric CO_2. On longer timescales approaching a few millennia, these variations are damped to some extent by adjustments of the marine calcium carbonate cycle and ocean alkalinity.

The three-box outcrop model is a rather crude representation of the ocean, and a series of geographical refinements have been pursued. Additional boxes can be added to differentiate the individual ocean basins (e.g., Atlantic, Pacific, Indian), regions (e.g., tropics, subtropics), and depths (e.g., thermocline, intermediate, deep, and bottom waters) leading to a class of models with a half-dozen to a few dozen boxes. The larger number of unknown advective flows and turbulent exchange parameters, however, complicates the tuning procedure. Other model designs take advantage of the vertical structure in the tracer and biogeochemical profile data. The deep box(es) is discretized in the vertical, essentially creating a continuous interior akin to a 1-D advection–diffusion model. This type of model is often used for anthropogenic CO_2 uptake calculations, where it is important to differentiate between the decadal ventilation timescales of the thermocline and the centennial timescales of the deep water.

Intermediate Complexity and Inverse Models

In terms of global models, the next step up in sophistication from box models is intermediate complexity models. These models typically have higher resolution and/or include more physical dynamics but fall well short of being full GCMs. Perhaps the most common examples for ocean carbon cycle research are zonal average basin models. The dynamical equations are similar to a GCM but are integrated in 2-D rather than in 3-D, the third east–west dimension removed by averaging zonally across the basin. In some versions multiple basins are connected by an east–west Southern Ocean channel. The zonal average models often have a fair representation of the shallow wind-driven Ekman and deep thermohaline overturning circulations but obviously lack western boundary currents and gyre circulations. Tracer data remain an important element in tuning some of the mixing coefficients and surface boundary conditions and evaluating the model solutions.

Based on resolution, many inverse models can also be categorized as intermediate complexity, but their mode of operation differs considerably from the models considered so far. In an inverse model, the circulation field and biogeochemical net source/sink (the J terms in the notation above) are solved for using the observed large-scale hydrographic and tracer distributions as constraints. Additional dynamic information may also be incorporated such as the geostrophic velocity field, general water mass properties, or float and mooring velocities.

Inverse calculations are typically posed as a large set of simultaneous linear equations, which are then solved using standard linear algebra methods. The inverse techniques are most commonly applied to steady-state tracers, though some exploration of transient tracers has been carried out. The beauty of the inverse approach is that it tries to produce dynamically consistent physical and/or biogeochemical solutions that match the data within some assigned error. The solutions are often underdetermined in practice, however, which indicates that a range of possible solutions exist. From a biogeochemical perspective, the inverse circulation models provide estimates of the net source/sink patterns, which can then be related to potential mechanisms.

Thermocline Models

Ocean process tracers and idealized models have also been used extensively to study the ventilation of the main thermocline. The main thermocline includes the upper one kilometer of the ocean where the temperature and potential density vertical gradients are particularly steep. Thermocline ventilation refers to the downward transport of surface water

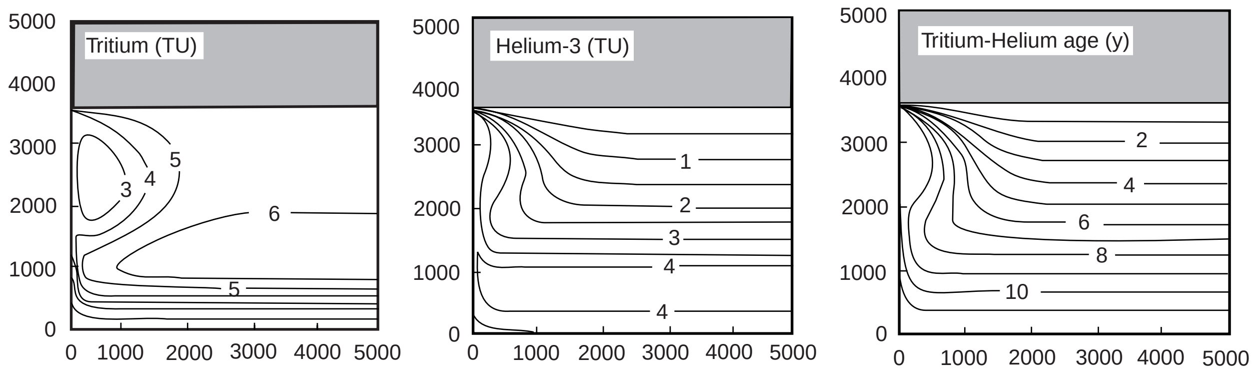

Figure 4 Tracer results from a two-dimensional gyre model. The model represents the circulation on a constant density surface (isopycnal) in the main thermocline that outcrops along the northern boundary (shaded region). Thermocline ventilation is indicated by the gradual increase of tritium-^{3}He ages around the clockwise flowing gyre circulation. (Reproduced with permission from Musgrave (1990).)

recently exposed to the atmosphere, replenishing the oxygen and other properties of the subsurface interior. Based on the vertical profiles of tritium and ^{3}He as well as simple 1-D and box models, researchers in the early 1980s showed that ventilation of the main thermocline in the subtropical gyres occurs predominately as a horizontal process along surfaces of constant density rather than by local vertical mixing. Later work on basin-scale bomb-tritium distributions confirmed this result and suggested the total magnitude of subtropical ventilation is large, comparable to the total wind driven gyre circulation.

Two dimensional gyre-scale tracer models have been fruitfully applied to observed isopycnal tritium-^{3}He and chlorofluorocarbons patterns. As shown in **Figure 4**, recently ventilated water (near-zero tracer age) enters the thermocline in the north and is swept around the clockwise circulation of the gyre. Comparisons of model tracer patterns and property–property relationships constrain the absolute ventilation rate and the relative effects of isopycnal advection versus turbulent mixing by depth and region.

Thermocline tracer observations are also used to estimate water parcel age, from which biogeochemical rate can be derived. For example, remineralization produces an apparent oxygen deficit relative to atmospheric solubility. Combining the oxygen deficit with an age estimate, one can compute the rate of oxygen utilization. Similar geochemical approaches have been or can be applied to a host of problems: nitrogen fixation, denitrification, dissolved organic matter remineralization, and nutrient resupply to the upper ocean. The biogeochemical application of 2-D gyre models has not been pursued in as much detail. This form of modeling, however, is particularly useful for describing regional patterns and in the areas where simple tracer age approaches breakdown.

Summary and Discussion

Designed around a particular question or hypothesis, conceptual models attempt to capture the basic elements of the problem while remaining amenable to straightforward analysis and interpretation. They are easy to construct and computationally inexpensive, requiring only a desktop PC rather than a supercomputer. When well formulated, idealized models provide a practical method to analyze ocean physical and biogeochemical dynamics and in some cases to quantitatively constrain specific rates. Their application is closely tied to ocean tracer observations, which are generally required for physical calibration and evaluation. Idealized models remain a valuable tool for estimating the oceanic uptake of anthropogenic carbon and the long timescale responses (centuries to millennia) of the natural carbon cycle. Also, some of the more memorable and lasting advances in tracer oceanography are directly linked to simple conceptual models. Examples include constraints on the deep-water large-scale vertical diffusivity and demonstration of the dominance of lateral over vertical ventilation of the subtropical main thermocline.

By their very nature, however, idealized models neglect many important aspects of ocean dynamics. The alternative is full 3-D ocean GCMs, which incorporate more realistic spatial and temporal geometry and a much fuller suite of physics. The cost of course is greater complexity, a more limited number of simulations, and a higher probability of crucial regional errors in the base solutions, which may compromise direct, quantitative model-data comparisons. Ocean GCMs, particularly coarseresolution global versions, are also sensitive to the subgrid scale parameterizations used to account for unresolved processes such as mesoscale eddy mixing, surface and bottom boundary layer dynamics and air–sea and ocean–ice interactions. Ocean GCM solutions, however, should be exploited to address exactly those problems which are intractable for simpler conceptual and reduced dimensional models. For example, two key assumptions of the 1-D advection–diffusion model presented in **Figure 2** are that the upwelling occurs uniformly in the horizontal and vertical and that mid-depth horizontal advection is not significant. Ocean GCMs and tracer data, by contrast, show a rich three-dimensional circulation pattern in the deep Pacific.

The behavior of idealized models and GCMs can diverge, and it is not always clear that complexity necessarily leads to more accurate results. A debate is underway regarding the relative importance of high and low latitude ocean regions in maintaining atmospheric CO_2 levels. Almost all the current 3-D GCM-based carbon models show a stronger sensitivity to changes in the low latitudes than do box models. It is likely that the aggregation and oversimplification of the box models is at fault, but the issue is not yet fully resolved. In the end, the choice of which model to use depends on the scientific problem and the judgment of the researcher. Probably the best advice is to explore solutions from a hierarchy of models and to thoroughly evaluate the skill of the models against a range of tracers and other dynamical measures. Just because a model does a good job reproducing the distribution of one tracer field does not mean that it can be applied indiscriminately to another variable, especially if the underlying dynamics or timescales differ.

Models can be quite alluring in the sense that they provide concrete answers to questions that are often difficult or nearly impossible to address from sparsely sampled field data. However, one should not forget that numerical models are simply a set of tools for doing science. They are no better than the foundations upon which they are built and should not be carried out in isolation from observations of the real ocean. For ocean carbon cycle models, the two key elements are the ocean physical circulation and the biogeochemical processes. Even the best biogeochemical model will perform poorly in an ill-constructed physical model. Conversely, if the underlying biogeochemical mechanisms are poorly known, a model may be able to correctly reproduce the distributions of biogeochemical tracers but for the wrong reasons. Mechanistic-based models are critical in order to understand and predict natural variability and the response of ocean biogeochemistry to perturbations such as climate change.

See also

Biogeochemical Data Assimilation. Carbon Cycle. Carbon Dioxide (CO_2) Cycle. CFCs in the Ocean. Dispersion and Diffusion in the Deep Ocean. Forward Problem in Numerical Models. Ocean Circulation. Nitrogen Cycle. Phosphorus Cycle. Radiocarbon. Thermohaline Circulation. Tracers and Large Scale Models. Tritium–Helium Dating.

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