

Global Ocean Carbon Cycle Modeling

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Abstract

One of the central objectives of the Joint Global Ocean Flux Study (JGOFS) is to use data from the extensive field effort to improve and evaluate numerical ocean carbon cycle models, models that will subsequently be used to better understand the present ocean state and predict past and potential future responses to anthropogenic perturbations and climate change. Historically, ocean biological and chemical modelling has evolved along a three related, though often distinct, paths: anthropogenic CO₂ transient tracer uptake; biogeochemical cycles; and ecosystem dynamics. An important trend is the unification of these three approaches, leading ultimately to a coherent modeling framework linking ocean physics, biology and chemistry over a range of time and space scales. Substantial improvements are underway on the current suite of numerical models to incorporate the major shifts in biogeochemical paradigms resulting from recent field studies. Marine biogeochemical modeling is inherently data driven, and the JGOFS field data sets (time-series, process studies, and global survey) together with the emerging satellite products are invaluable in two ways: the basis for new and improved, mechanistically based parameterizations of specific biogeochemical processes; and the resource for testing the overall skill of integrated system models through detailed model-data comparisons. Here we present a selective overview of the current state, future directions and major challenges for basin to global ocean carbon cycle modelling, drawing on examples primarily from the NCAR program. Several themes are highlighted including multi-element cycling and community structure, large-scale physical circulation, mesoscale space and time variability, mass exchange between the open ocean and the atmosphere, land, and coastal ocean, climate variability, and model-data evaluation and data assimilation.

1 Introduction

One of the central objectives of the Joint Global Ocean Flux Study (JGOFS) is to use data from the extensive field effort to improve and evaluate numerical ocean carbon cycle models. Substantial improvements are required in the current suite of numerical models if we are to better understand the present ocean biogeochemical state and predict potential future responses to anthropogenic perturbations. Significant progress has been made in this regard, and even greater strides are expected over the next decade as the synthesis of the JGOFS data sets are completed and disseminated to the scientific community. The goals of this chapter are to outline the role of modelling in ocean carbon cycle research, review the status of basin to global-scale modelling, and highlight major problems, challenges, and future directions.

Marine biogeochemical models are quite diverse, covering a wide range of complexities and applications from simple box models to global 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. A common theme, however, is that models allow us to ask questions about the ocean we could not address using data alone. In particular, models help researchers quantify the interactions among multiple processes, synthesize diverse observations, test hypotheses, extrapolate across time and space scales, and predict future behavior.

A well posed model encapsulates our understanding of the ocean in a mathematically consistent form. Many, though not all, models can be cast in general form as a coupled set of time-dependent advection, diffusion, reaction equations:

$$\frac{\partial X}{\partial t} + \vec{u} \cdot \nabla X - \nabla \cdot (K \nabla X) = \text{sources/sinks} \quad (1)$$

where X refers to a set of prognostic or predicted variables (e.g. temperature, phytoplankton biomass, dissolved inorganic carbon). The second and third terms on the left hand side of the equation describe the physical processes of advection and mixing, respectively. All of the chemical and biological interactions are subsumed into the final source/sink term(s) on the right hand side, which often involve complex interactions among a number of prognostic variables. In addition, the model may require external boundary conditions (e.g. solar radiation, wind stress, dust deposition) and for time varying problems initial conditions. The model equations are then solved numerically by integrating forward in time for X .

Numerical models cannot capture all of the complexity of the real world. Part of the art of modelling is to abstract the essence of a particular problem, balancing model complexity with insight. Many processes must be either parameterized in a simple fashion or neglected altogether. For example, the biophysical details of photosynthesis, though quite well known, may not necessarily be crucial and certainly not sufficient for simulating the seasonal bloom in the North Atlantic. On the other hand, a number of key processes (e.g. phytoplankton mortality, the controls on community structure) are not well characterized and are often used as model tuning parameters.

As opposed to much of ocean physics, fundamental relationships either are not known or may not exist at all for much of marine biogeochemistry. Therefore, ocean biogeochemical modeling is inherently data driven. The JGOFS field data are invaluable in this regard, providing the basis for highlighting model deficiencies, developing improved parameterizations, and evaluating overall model performance. The desire for increasing model realism and sophistication must be tempered by the realization that models can quickly outstrip the ability to parameterize the appropriate processes or evaluate the overall simulation. Inverse methods and data assimilation will certainly help in this regard, but the true benefits will only be gained when the underlying models rest on sound, mechanistic basis.

Broadly speaking, much of current ocean carbon cycle modelling can be condensed into a few overarching scientific questions that match well with the other individual chapters of this book. These include: What are the physical and biological controls on primary, new and export production? What are the roles of multiple limiting nutrients, mesoscale variability and trophic structure? How are organic and inorganic carbon transported, transformed and remineralized below the surface layer? How much anthropogenic carbon does the ocean take up and where? How does ocean biogeochemistry respond to climate variability and are there feedbacks on climate change?

Ocean carbon modeling is a diverse and growing field and can not be covered comprehensively in a single chapter. Rather, we present an overview of the current state and major issues involving ocean biogeochemical and ecosystem modeling drawing mostly on specific examples from the NCAR modelling program.

Historically, global ocean biological and chemical modelling has evolved along three related, though often distinct, paths. First, a number of early efforts were directed toward improving oceanic anthropogenic carbon uptake estimates, building on simple box models and coarse resolution ocean physical general circulation models (GCMs). Transient tracer simulations (radiocarbon, tritium, chlorofluorocarbons) developed in conjunction as a way to assess model physical circulation and mixing. Second, biogeochemical carbon cycle models, while often relying on the same physical model frameworks, were developed to improve our understanding of the dynamics controlling large-scale biogeochemical fields (e.g. surface $p\text{CO}_2$, subsurface nutrient, oxygen and dissolved inorganic carbon distributions) and their responses to climate variability and secular change (e.g. glacial–interglacial transition and greenhouse warming). The treatment of biological processes in this class of models has been rather rudimentary in most cases. Third, marine ecosystem models have been focused much more on the details of biological interactions within the upper ocean, tracking the controls on upper ocean primary and export production as well as the flow of mass and energy through the marine food web. These models often are created for specific biogeographical regions commonly based on local surface or 1-D time-series data sets. More recently, ecosystem models are being extended to basin and global scale. One of the most important trends in the field is the unification of these three approaches, leading ultimately to a coherent modeling framework linking ocean physics, biology and chemistry over a range of time and space scales.

2 Anthropogenic Carbon Uptake, Transient Tracers, and Physics

An initial and ongoing focus of ocean biogeochemical modelling research is to quantify the rate at which the ocean takes up transient tracers and excess anthropogenic CO_2 . The water column and upper few meters of marine sediments contain the largest mobile, natural reservoir of carbon on time-scales of 10^2 to 10^5 years. With about 50 times more carbon than that stored in the atmosphere (Figure 1) (Siegenthaler and Sarmiento, 1993), the ocean will serve as the ultimate sink for about 90% of human fossil fuel emissions (Archer et al., 1998). Anthropogenic carbon uptake is often computed as a passive perturbation to the natural dissolved inorganic carbon (DIC) field (Sarmiento et al., 1992), a fairly reasonable assumption for the pre-industrial to the present time period. Carbon uptake, therefore, would be simply a matter of ocean physics, primarily determined by the ventilation time-scales exposing deep water to the surface and, to a much lesser degree, air-sea gas exchange. The invasion into the ocean of transient tracers such as radiocarbon, tritium, and the chlorofluorocarbons provide a direct, often quite dramatic illustration of ocean ventilation and are commonly used either to calibrate/evaluate ocean physical models or as proxies for anthropogenic CO_2 uptake.

Early attempts to calculate ocean CO_2 uptake in the 1970's and 1980's relied heavily on ocean box and 1-D advection diffusion models of varying complexity (e.g. Oeschger et al., 1975; Siegenthaler and Joos, 1992). This class of models represents in a fairly crude, schematic form the basics of ocean thermocline ventilation and thermohaline circulation. The crucial model advection and mixing parameters are typically set by calibrating simulated transient tracer distributions (tritium, natural and bomb radiocarbon) to observations. More recently, such models have mostly been sup-

planted by full 3-D general circulation models for the anthropogenic CO₂ question. But because they are simple to construct (and interpret) and computationally inexpensive, box models and a related derivative the 2-D, zonally averaged basin model (Stocker et al., 1994) continue to be used today for a number of applications requiring long temporal integrations including paleoceanography (Toggweiler, 1999; Stephens and Keeling, 2000) and climate change (Joos et al., 1999). Some caution is advised, however, as recent studies (Broecker et al., 1999; Archer et al., 2000) clearly demonstrate that box model predictions for key carbon cycle attributes can differ considerably from the corresponding GCM results.

Ocean general circulation model studies of anthropogenic carbon uptake date back to the work of Maier-Reimer and Hasselmann (1987) and Sarmiento et al. (1992), and the number of model estimates (and modelling groups) for CO₂ uptake has increased significantly over the 1990's. For example, more than a dozen international groups are participating in the IGBP/GAIM Ocean Carbon Model Intercomparison Project (OCMIP; <http://www.ipsl.jussieu.fr/OCMIP/>). These numerical experiments are closely tied to and greatly benefit from efforts to evaluate ocean GCMs using hydrographic (Large et al., 1997; Gent et al. 1998) and transient tracer data (Toggweiler et al., 1989a; 1989b; Maier-Reimer, 1993; England, 1995; Heinze et al., 1998; England, 2000). More recently, empirically based methods have been developed for estimating anthropogenic carbon distributions directly from ocean carbon and hydrographic observations (Gruber et al., 1996; Gruber, 1998; Wanninkhof et al., 1999; Watson this volume). With the completion of the high quality, JGOFS/WOCE global CO₂ survey (Wallace, 1995; 2001), a baseline can be constructed for the world ocean for the pre-industrial DIC field and the anthropogenic carbon perturbation as of the mid-1990's, an invaluable measure for testing numerical model skill and monitoring future evolution.

As an example, the large-scale patterns of anthropogenic CO₂ air-sea flux and integrated water column inventory from the NCAR CSM Ocean Model (Large et al., 1997; Gent et al., 1998) are shown in Figure 2. The regions of highest anthropogenic carbon uptake—equatorial upwelling bands, western boundary currents, high latitude intermediate and deep water formation regions—are associated with the transport of older subsurface waters to the air-sea interface (Doney, 1999). Although the maximum specific uptake rates are found in the subpolar North Atlantic, the area is relatively small, and the integrated uptake of the Southern Ocean and Equatorial band are larger. The anthropogenic DIC water column anomaly is stored primarily in the thermocline and intermediate waters of the subtropical convergence zones and the lower limb of the North Atlantic thermohaline circulation as illustrated by the second panel of Figure 2 and Figure 3, a depth versus latitude comparison of field data derived and model simulated anthropogenic DIC. The two meridional sections follow the thermohaline overturning circulation from the northern North Atlantic to the Southern Ocean and then back to the northern North Pacific. The model simulates in a reasonable fashion the patterns from empirical estimate except perhaps in the subpolar and intermediate depth North Atlantic, which may reflect problems with the model formation of North Atlantic Deep Water (Large et al., 1997).

At present, most numerical models predict a similar net uptake of anthropogenic CO₂ for the 1990's of approximately 2 Pg C yr⁻¹ (1 Pg C equals 10¹⁵g C) (Orr et al., 2001), a result supported by atmospheric biogeochemical monitoring and a variety of other techniques (Schimel et al., 1995; Keeling et al., 1996; Rayner et al., 1999). The models, however, show considerable regional differences particularly in the Southern Ocean (Orr et al., 2001). The agreement of the NCAR model and empirical basin inventories is quite good (Table 1), suggesting that at least at this scale the NCAR model transport is relatively skillful.

While based on a more complete description of ocean physics, the coarse resolution, global GCMs used for these carbon studies still require significant parameterization of sub-gridscale phenomenon such as deep water formation, surface and bottom boundary layer physics, and mixing rates along and across density surfaces (isopycnal and diapycnal diffusion). The ongoing OCMIP effort is comparing about a dozen current generation global ocean carbon models among themselves and against ocean observations. Completed analysis of OCMIP Phase 1 and early results from Phase 2 demonstrate significant differences among the models in the physical circulation (Doney and Lindsay, in prep.) and simulated chlorofluorocarbon (Dutay et al., 2001), radiocarbon, and current and projected future anthropogenic CO₂ fields (Orr et al., 2001). The largest model-model differences and model-data discrepancies are found in the Southern Ocean, reflecting differences in the relative strength and spatial patterns Antarctic Mode (Intermediate) Waters and Antarctic Bottom Water (AABW) (Dutay et al., 2001). Models using horizontal mixing rather than an isopycnal scheme (e.g. Gent and McWilliams, 1980) tend to overestimate convective mixing in the region of the Antarctic Circumpolar Current (Danabasoglu et al., 1994). Not surprisingly, the formation of AABW appears quite sensitive to the under-ice, surface freshwater fluxes in the deep water formation zones (Doney and Hecht, 2001); uncoupled ocean models appear to have weak AABW formation while many of the coupled ocean-sea ice models tend to have way to much bottom water production.

These known deficiencies in ocean GCM physics hamper quantitative model-data comparisons of biogeochemical and ecosystem dynamical models as well. Uncertainties in the physical flow field, particularly vertical velocity (Harrison, 1996), mixing and convection, affect a variety of biogeochemical processes—nutrient supply, boundary layer stability and mean light levels, downward transport of transient tracers, anthropogenic carbon and semi-labile dissolved organic matter—and thus obscure the validation of tracer and biogeochemical components. The refinement of global ocean GCMs is an on-going process, and substantial progress will likely arise from improved treatments of surface boundary forcing and subgrid-scale physics, not simply higher resolution (McWilliams, 1996; Haidvogel and Beckmann, 1999). Transient tracers and biogeochemistry can contribute in this regard by providing additional, often orthogonal constraints on model performance to traditional physical measures (Gnanadesikan and Toggweiler, 1999). The incorporation of active biology tests new facets of the physical solutions, especially the surface air-sea fluxes and boundary layer dynamics (Large et al., 1994; Doney, 1996; Doney et al., 1998) and their interaction with the interior mesoscale field (Gent and McWilliams, 1990).

3 Global Biogeochemical Cycles

The net anthropogenic ocean carbon uptake occurs on top of the large background DIC inventory and ocean gradients, air-sea fluxes, biological transformations, and internal transports driven by the natural carbon cycle (Figure 1). Beginning with a series of global biogeochemical simulations in the early 1990s (Bacastow and Maier-Reimer, 1990; Maier-Reimer, 1993; Najjar et al., 1993), numerical models have played key roles in estimating basin and global-scale patterns and rates of biogeochemical processes (e.g. export production, remineralization). The primary measure for evaluating such models has been the large-scale fields of inorganic nutrients, oxygen, and DIC (Levitus et al., 1993; Conkright et al., 1998; Wallace, 2001). As more robust global estimates of biogeochemical rates (e.g. new production, Laws et al., 2001) are developed from the JGOFS field data and satellite remote sensing, they too are being included model-data comparisons (Gnanade-

sikan et al., 2001). Numerical biogeochemical models are also valuable tools for exploring specific hypotheses (e.g. iron fertilization; Joos et al., 1991), estimating interannual variability (Le Quéré et al., 2001), and projecting future responses to climate change (Sarmiento et al., 1998).

With a few exceptions (Six and Maier Reimer, 1996), the treatment of biology in these global biogeochemical models to date has been rather rudimentary. This is exhibited in Figure 4 by a schematic of the biotic carbon model from OCMIP Phase 2 (Najjar et al., in prep.). The OCMIP model consists of five prognostic variables, a limiting nutrient PO_4 , dissolved inorganic carbon DIC, total alkalinity TALK, semi-labile dissolved organic matter DOM, and dissolved oxygen. Upper ocean production (0–75m) is calculated by restoring excess model PO_4 toward a monthly nutrient climatology (Louanchi and Najjar, 2000). The production is split with 1/3 going into rapidly sinking particles and the remainder into the DOM pool. The sinking particles are remineralized in the subsurface consumption zone ($> 75\text{m}$) using an empirical particle flux depth curve similar in form (though with different numerical parameters; Yamanaka and Tajika, 1996) to that found by Martin et al. (1987) from sediment trap data. The DOM decays back to phosphate and DIC using first order kinetics with a 6 month time-scale throughout the water column. Most of the DOM is remineralized within the surface production zone but a fraction is mixed or subducted downward prior to decay and thus contributes to overall export production. Surface CaCO_3 production is set at a uniform 7% of organic matter production, and all of the CaCO_3 is export as sinking particles which are remineralized with a deeper length-scale relative to organic matter. The relative uptake and release rates of PO_4 , DIC, and O_2 from the organic pools are set by fixed, so-called Redfield elemental ratios, and CO_2 and O_2 are exchanged with the atmosphere via surface air-sea gas fluxes computed using the quadratic wind-speed gas exchange relationship of Wanninkhof (1992).

Despite its simplicity, the OCMIP model captures to a degree many of the large-scale ocean biogeochemical patterns found in nature. The model zonally averaged, total new production (particle export plus net DOM production) is compared in Figure 5a with recent new/export production estimates from Laws et al. (2001) (satellite primary production and ecosystem model based f-ratios) and Moore et al. (2001a; 2001b) (global ecosystem model; see below for more details). The NCAR model estimate has been recomputed at 150m rather than 75m as specified in the OCMIP formulation to be more consistent with data based and the other model estimates. The global integrated new production estimates from the GCM (9.6 Pg C at 150m), satellite diagnostic calculation (12.6 Pg C), and ecosystem model (11.9 Pg C) are comparable but with significant regional differences. The Moore et al. and Laws et al. curves have similar patterns with high values in the Northern Hemisphere temperate and subpolar latitudes, low levels in the tropics and subtropics and slightly elevated rates in the Southern Ocean around 40°S . The GCM results are considerably larger in the equatorial upwelling band and lower in the subtropics, reflecting in part net production, horizontal export and subsequent remineralization of organic matter. The Laws et al. (2001) estimates are based on two components: satellite derived primary production rates from CZCS ocean color data and Behrenfeld and Falkowski (1997) algorithm and a functional relationship of f-ratio to temperature and primary production from an ecosystem model. As discussed by Gnanadesikan et al. (2001), the Laws et al. (2001) values in the equatorial region are sensitive to assumptions about the maximum growth rates as a function of temperature (and implicitly nutrients), and alternative formulations can give higher values (though still lower than their GCM).

A significant fraction of the GCM export production at mid- to high latitudes is driven by net DOM production followed by downward transport (global integral at 150m of 2.4 Pg C) (Figure 5a and 5b). This has been observed in the field at a number of locations (Carlson et al., 1994; Hansell and Carlson, 1998), and is thought to be an important mechanism north of the Antarctic

Polar Front supporting a significant fraction of the organic matter remineralization in the upper thermocline (Doval and Hansell, 2000). Because the semi-labile DOM in the model is advected by the horizontal currents, the local sum of new production and remineralization do not always balance leading to net convergence/divergence of nutrients and DIC as seen in some ocean inversion transport estimates and horizontal inputs of organic nutrients into subtropical areas from remote source regions (Rintoul and Wunsch, 1991). Another factor to consider when looking at the model production estimates and model-data comparisons is the sensitivity of new production to the depth surface chosen for the vertical integral. The cumulative (surface to depth) new production drops off significantly with depth below 75m in the model because of the assumed rapid decrease in the sinking particle flux and relatively shallow penetration of DOM governed mostly by seasonal convection (Figure 5b). For most field studies, the vertical mixing and advection terms are difficult to quantify, and the new production is computed typical at either the base of the euphotic zone (100m to 125m) or the shallowest sediment trap (~150m).

Another important measure of model skill is the surface water $p\text{CO}_2$ field (Sarmiento et al., 2001), which can be compared to extensive underway $p\text{CO}_2$ observations (e.g. Takahashi et al., 1997; 1999) and atmospheric CO_2 data sets (Keeling et al., 1996; Rayner et al., 1999). The model surface water $p\text{CO}_2$ field is the thermodynamic driving force for air-sea gas exchange and is governed by biological DIC drawdown, physical transport, surface temperature (and salinity), and air-sea fluxes. Figure 6 shows the annual mean air-sea $\Delta p\text{CO}_2$ field from the model for 1990 (pre-industrial equilibrium plus anthropogenic perturbation) and the Takahashi et al. (1997) climatology. The large-scale patterns are similar with CO_2 outgassing from the equatorial regions, where cold DIC rich water is brought to the surface by upwelling, and CO_2 uptake in the western boundary currents, Antarctic Circumpolar Current, and North Atlantic deep water formation zones. The most striking regional model-data difference is the predicted larger (smaller) uptake in the Southern Ocean (North Atlantic) from the Takahashi et al. (1997) and the indication of net outgassing right along the Antarctic coast. Interestingly, the model Southern Ocean results are more in line with recent atmospheric inversion results from TRANSCOM3 (S. Denning, per. comm., 2000).

The model subsurface nutrient, DIC and oxygen fields can also be compared with observations, in this case the historical hydrographic data sets and JGOFS/WOCE global CO_2 survey. The pre-industrial DIC results are shown in the same format as for anthropogenic DIC (Figure 3), meridional sections in the Atlantic and Pacific (Figure 7). The model surface to deep water DIC vertical gradient, which is comparable to the observations, results from contributions of about 2/3rds from the biological export (“biological pump”) and 1/3rd from the physics (“solubility pump”). The horizontal gradients in the deep-water are determined by a mix of the thermohaline circulation and the subsurface particle remineralization rate, and the NCAR-OCMIP model captures most of the broad features. Several of the key model-data differences can be ascribed, at least partly, to problems with the model physics (e.g. too shallow outflow of North Atlantic Deep Water, Large et al., 1997; overly weak production of Antarctic bottom water, Doney and Hecht, 2001). The WOCE/JGOFS carbon survey and historical data sets can also be used to estimate the horizontal transport of biogeochemical species within the ocean (e.g. Brewer et al., 1989; Rintoul and Wunsch, 1991; Broecker and Peng, 1992; Holfort et al., 1998; Wallace, 2001), providing another constraint for ocean biogeochemical models (Murnane et al. 1999; Gruber et al., 2001; Sarmiento et al. 2001).

4 Ecosystem Dynamics

If the simple OCMIP biogeochemical model captures the zeroth-order state of the ocean carbon cycle then what are the important areas for progress? An obvious deficiency of the OCMIP straw-man is the lack of explicit, prognostic biological dynamics to drive surface production, export and remineralization. By linking to a fixed surface nutrient climatology, we have avoided specifying the details of how the surface nutrient field is controlled (e.g. grazing, iron fertilization, mesoscale eddies) or how it might evolve under altered forcing. While useful for the purposes of OCMIP, clearly a more mechanistic approach is desired for many applications. For example, looking toward the next several centuries, future changes in ocean circulation and biogeochemistry may lead to large alterations in the background carbon cycle that could strongly impact projected ocean carbon sequestration (Denman et al., 1996; Sarmiento et al., 1998; Doney and Sarmiento, 1999; Boyd and Doney, this volume). Realistic projections will require coupled ecosystem–biogeochemical models that include the main processes thought to be sensitive to climate change (e.g. atmospheric dust, nitrogen fixation, community structure).

As an example of a typical marine ecosystem, consider the schematic shown in Figure 8. The model developed for vertical 1-D simulations of the Sargasso Sea by Doney et al. (1996) incorporates five prognostic variables: phytoplankton, zooplankton, nutrient, detritus and chlorophyll (a so called PZND model). As is common, the model aggregates populations and species of organisms into broadly defined trophic compartments. The equations are based on the flow of a single limiting currency, in this case the concentration of nitrogen (mol N/m^3), among compartments rather than individual organisms. The various source/sink terms (e.g. photosynthesis, zooplankton grazing, detrital remineralization) are calculated using standard, though not always well agreed upon, sets of empirical functional forms and parameters derived either from limited field data or laboratory experiments, the latter often with species and conditions of limited relevance to the actual ocean (Fasham, 1993; Evans and Fasham, 1993; Evans and Garcon, 1997). This type of compartment ecosystem model has been used extensively in oceanography (Steele, 1974) and theoretical ecology (May, 1973; Case, 2000) since the early 1970’s but has roots much further back in the literature (e.g. Riley, 1946; Steele, 1958). The area was revitalized about the time of the inception of JGOFS by the seminal work of Evans and Parslow (1985), Frost (1987), Fasham, Ducklow, and McKelvie (1990), and Moloney and Field (1991).

Despite its simplifications, the PZND model (Figure 8) does an adequate job capturing the vertical structure and broad seasonal patterns of bulk biogeochemical properties in Bermuda field data (e.g. chlorophyll—Figure 9; nitrate; Doney et al., 1996). Specific features include: a winter phytoplankton bloom following nutrient injection via deep convection; low surface nutrients and chlorophyll during the stratified summer period; and the formation of a subsurface chlorophyll maximum at the top of the nutricline. The 1-D coupled biological-physical model, based on surface forcing and physics described by Doney (1996), also reproduces aspects of the observed interannual variability driven by the depth of the winter convection.

Variants on the PZND theme have been successfully applied in vertical 1-D form in a diverse range of biogeographical regimes from oligotrophic subtropical gyres (Bissett et al., 1994) to sub-arctic high-nitrate, low chlorophyll regions (McClain et al., 1996; Pondaven et al., 2000). The construction of the 1-D physical framework (vertical mixing, temperature etc.) requires explicit consideration (Archer, 1995; Doney, 1996; Evans and Garcon, 1997), but in general 1-D coupled models have resulted in useful test-beds for exploring ecological processes and implementing biological data assimilation techniques. It has been known for a while that the relatively simple PZND

dynamics belie the ecological complexity of the real system, and recent idealized and local 1-D coupled models include increasing levels of ecological sophistication. Models are incorporating a range of factors such as: size and community structure (Armstrong, 1994; 1999a; Bisset et al., 1999), iron limitation (Armstrong, 1999b; Leonard et al., 1999; Denman and Pena, 1999; Pondaven et al., 2000), and nitrogen fixation (Hood et al., 2001; Fennel et al., 2001a). One problem, however, is that most 1-D coupled models are developed and evaluated for a single site, and the generality of these models and their derived parameter values for basin and global simulations remains an open question.

Early three-dimensional basin and global scale calculations (e.g. Sarmiento et al., 1993; Six and Maier-Reimer, 1996) were conducted with single, uniform PZND ecosystem models applied across the entire domain. These experiments demonstrated that large-scale features such as the contrast between the oligotrophic subtropical and eutrophic subpolar gyres could be simulated qualitatively. Some problems arose, however, with the details. For example, the incorporation of the Fasham, Ducklow and McKelvie (1990) model into a North Atlantic circulation model by Sarmiento et al. (1993) showed too low production and biomass in the oligotrophic subtropics and too weak a spring bloom at high latitudes. The Six and Maier-Reimer (1996) result required careful tuning of the phytoplankton growth temperature sensitivity and zooplankton grazing in order to control biomass in the Southern Ocean HNLC. A number of coupled 3-D ecosystem models now exist for regional (Chai et al., 1996; McCreary et al. 1996; Dutkiewicz et al., 2001) and global (Aumont et al., 2001) applications, and these 3-D ecosystem models are beginning to include many of the features already addressed in 1-D including multiple nutrient limitation and community structure (Gregg et al., 2001; Christian et al., 2001a; 2001b). Often, however, these models are not used to fully explore the coupling of upper ocean biology and subsurface carbon and nutrient fields because of the short integration time (a few years) or limited horizontal/vertical domain.

The next step is to combine reasonably sophisticated components for both ecosystem and biogeochemical dynamics in a global modelling framework. The exact form of such a model is yet to be determined. But based on the new insights emerging from JGOFS and other recent field studies, a minimal model can be envisioned covering those basic processes that govern surface production, export flux, subsurface remineralization, and the (de)coupling of carbon from macronutrients (multi-nutrient limitation; size structure and trophic dynamics; plankton geochemical functional groups; microbial loop and dissolved organic matter cycling; particle transport and remineralization).

As part of such a project, we have developed an intermediate complexity, ecosystem model incorporated within a global mixed layer framework (Moore et al., 2001a; 2001b). The model biology is simulated independently at each grid point and then composited to form global fields. The model has a low computational overhead, and thus can be used for extensive model evaluation and exploration. Sub-surface nutrient fields are from climatological data bases, and the mixed layer model captures the local processes of turbulent mixing, vertical advection at the base of the mixed layer, seasonal mixed layer entrainment/detrainment, but not horizontal advection. Other forcings include sea surface temperature, percent sea ice cover, surface radiation, and the atmospheric deposition of iron (Fung et al., 2000; Figure 10). The physical forcings are prescribed from climatological data bases (e.g. Levitus et al., 1994; Conkright et al., 1998) and NCOM (Large et al., 1997). A preliminary version of the ecosystem model also has been tested in a fully coupled, 3-D North Atlantic basin configuration (Lima et al., 1999; in prep.), and the full ecosystem model is currently being implemented in the new global NCAR-Los Alamos model. The mixed layer ecosystem model is discussed in some detail to suggest highlight new modeling directions and approaches

to model–data evaluation.

The ecosystem model (Figure 8) is adapted from Doney et al. (1996) and consists of eleven main compartments, small phytoplankton, diatoms, and diazotrophs; zooplankton; sinking and non-sinking detrital classes; and dissolved nitrate, ammonia, phosphorus, iron, and silicate. The small phytoplankton size class is meant to generically represent nano- and pico-sized phytoplankton and may be iron, phosphorus, nitrogen, and/or light-limited. The larger phytoplankton class is explicitly modeled as diatoms and may be limited by silica as well. Many of the biotic and detrital compartments contain multiple elemental pools to track flows through the ecosystem. The model has one zooplankton class which grazes the three phytoplankton groups and the large detritus. Phytoplankton growth rates are determined by available light and nutrients using a modified form of the Geider et al. (1998) dynamic growth model. Carbon fixation rate is governed by internal cell nutrient quotas (whichever nutrient is currently most-limiting), and the cell quotas computed relative to carbon are allowed to vary dynamically as the phytoplankton adapt to changing light levels and nutrient availability. There is good laboratory evidence for a relationship between cell quotas (measured as nutrient/C ratios) and specific growth rates (Sunda and Huntsman 1995; Geider et al., 1998). Photoadaptation is modeled according to Geider et al. (1996; 1998) with a dynamically adaptive chl/C ratio. The diazotrophs are assumed to fix all required nitrogen from N_2 gas following Fennel et al. (2001) and are limited by iron, phosphorus, light or temperature. Calcification is parameterized as a time-varying fraction of the small (pico/nano) plankton production as a function of ambient temperature and nutrient concentrations. Based on Harris (1994) and Milliman et al. (1999) we assume that grazing processes result in substantial dissolution of $CaCO_3$ in the upper water column.

The model output is in generally good agreement with the bulk ecosystems observations (e.g. total biomass; productivity; nutrients) across diverse ecosystems that include both macro-nutrient and iron-limited regimes and very different physical environments from high latitude sites to the mid-ocean gyres. The detailed, local data sets from JGOFS and historical time-series stations (Kleypas et al., in prep.) have been important for developing parameterizations, testing hypotheses, and evaluating model performance. As an example, a comparison of model simulated and observed mixed layer seasonal cycle for nitrate is shown in Figure 11 for nine locations across the globe. The time-series stations and regional JGOFS process studies (e.g. EqPAC, Arabian Sea) often provide invaluable constraints on biological fluxes (primary productivity, export flux, zooplankton grazing, not shown) as well, parameters that are typically sampled too sparsely to construct global data sets. The variables that are available from observations on a global scale are more limited, including seasonal (now monthly) nutrient fields (Conkright et al., 1998), satellite remotely sensed surface chlorophyll (McClain et al., 1998) (Figure 12) and diagnostic model derived products such as satellite based primary production (Behrenfeld and Falkowski, 1997) and f-ratio (Laws et al., 2001) estimates.

The incorporation of iron limitation plays a critical part in the model skill of reproducing the observed high nitrate and low phytoplankton biomass conditions in the Southern Ocean and the subarctic and equatorial Pacific regions. A small number of desert regions (e.g. China, Sahel) provide the main sources of atmospheric dust (and thus iron), mostly in the Northern Hemisphere, and the estimated iron deposition rate to these oceanic HNLC environments can be orders of magnitude lower than other locations (Figure 10). At such low deposition rates, upwelling of subsurface iron likely contributes a significant fraction of the total bioavailable iron. In the model, these regions are characterized by strong iron limitation of diatom growth and modest iron limitation and strong grazing pressure on the small phytoplankton. The observed low chlorophyll and low nitrate levels in

oligotrophic gyres are also simulated well, but the model does not fully capture the strong blooms in some of the coastal upwelling regions, most likely a result of the weak vertical velocities input from the coarse resolution physics model.

Models should allow us to do more than simply replicate what is already known, posing new (and testable) hypotheses of how the ocean functions at the system level. As an example, the global mixed layer model predicts the degree and time/space patterns of nutrient limitation. Not too surprisingly, the model suggest that both small phytoplankton and diatoms are iron limited in the classic HNLC regions (40% and 52% of the global surface area, respectively for the two phytoplankton groups), while the mid-ocean subtropical gyres are typically nitrogen or, to much smaller degree, phosphorus limited (Figure 13). Diatom silica limitation is exhibited in the subantarctic and North Atlantic waters with bands of silica-iron colimitation along the edges of the tropics. The variable cell quota approach allows for easy diagnosis of varying degrees of nutrient stress, which can be compared in the near future with global nutrient stress fields to be derived from the MODIS natural fluorescence measurements (Letelier and Abbott, 1996).

The other new aspect of global model is the inclusion of community structure through planktonic geochemical functional groups, namely diatoms (export flux and silica ballast), diazotrophs (nitrogen fixation), and calcifiers (alkalinity and ballast). The model spatial patterns of annual nitrogen fixation (Figure 14) agree well with the limited information known from in situ work (Capone et al., 1997), high trichodesmium biomass and/or nitrogen fixation rates reported in the Caribbean Sea and eastern tropical North Atlantic (Lipschultz and Owens, 1996) as wells as the subtropical North Pacific (Letelier and Karl, 1996; 1998). The total model nitrogen fixation of 58 Tg N, which accounts only for the mixed layer production, is somewhat less than, though of comparable magnitude to, the 80 Tg N estimate of Capone et al. (1997) and the Gruber and Sarmiento (1997) geochemical estimates of >100 Tg N.

The parameterization of phytoplankton calcification is an active research topic, but the spatial patterns shown in Figure 14 are generally similar to those estimated by Milliman (1993) and Milliman et al. (1999). CaCO_3 production/export is lower in the mid-ocean gyres and higher in the North Atlantic, coastal upwelling zones and mid-latitude Southern Ocean waters. The high latitude North Atlantic in particular is known to be a region with frequent coccolithophore blooms (e.g. Holligan et al., 1993). The model production/export is lower in the equatorial Pacific and Indian ocean compared with Milliman et al. (1999), but the global sinking export of 0.46 Gt C is in good agreement with their integrated estimate.

Two main factors limiting progress on ecosystem modelling are the conceptualization of key processes at a mechanistic level and the ability to verify model behavior through robust and thorough model-data comparisons (Abbott, 1995). The phytoplankton iron limitation story is an illuminating example. Atmospheric dust/iron deposition flux estimates vary considerably (perhaps as large as a factor of ten or more in some areas) and the bioavailable fraction of the dust iron is not well known. Surface and subsurface ocean iron measurements are limited (particularly from a global modeller's perspective), and there remain serious analytical and standardization issues. Organic ligands may play a role in governing both bioavailability and subsurface iron concentrations. Not enough is known about the effect of iron limitation and variability on species competition at ambient low iron levels as well as a host of other relevant processes, iron release by photochemistry and zooplankton grazing, advection of iron by ocean margin sediments, and iron remineralization from sinking particles.

5 Other Topics

In a recent review paper, Doney (1999) described a set of key marine ecological and biogeochemical modeling issues to be addressed in the next generation of numerical models: multi-element limitation and community structure; large-scale physical circulation; mesoscale space and time variability; land, coastal, and sediment exchange with the ocean; and model–data evaluation and data assimilation. In the preceding three sections we have presented in some detail the nature of several of these challenges and specific initial progress made by our group. Below we more briefly outline some of the remaining items.

5.1 Mesoscale Physics

The ocean is a turbulent medium, and mesoscale variability (scales of 10 to 200 km in space and a few days to weeks in time) is a ubiquitous feature of ocean biological fields such as remotely sensed ocean color (e.g. Doney et al., 2001). Based on new in-situ measurement technologies (Dickey et al., 1998) and mesoscale biogeochemical models (McGillicuddy and Robinson, 1997; Oschlies and Garcon, 1998; Spall and Richards, 2000; 2001) it has become clear that mesoscale variability is not simply noise to be averaged over, but rather a crucial factor governing the nature of pelagic ecosystems. The ecological impacts of disturbance are diverse, and the initial research emphasis on the eddy enhancement of new nutrient fluxes to the euphotic zone (McGillicuddy et al., 1998; Figure 15) is broadening to include light limitation, community structure, organic matter export, and subsurface horizontal transport effects as well (Garcon et al., 2001).

Quantifying the large-scale effect of such variability will require concerted observational, remote sensing and numerical modeling programs with likely heavy reliance on data assimilation. The computational demands of truly eddy resolving basin to global calculations are significant, however. Recent, high resolution physical simulations of the North Atlantic show that dramatic improvement in eddy statistics and western boundary current dynamics is reached only at 1/10 of a degree resolution (Smith et al., 2000), and even higher resolution may be needed for biology if submesoscale processes are as important as suggested by preliminary results (Levy et al., 2000). Over the near term, long time-scale equilibrium and climate simulations will be limited primarily to non-eddy resolving models in which mesoscale eddy effects will have to be incorporated via subgrid-scale parameterizations.

5.2 Climate Variability and Secular Change

A key measure for the skill of numerical models is their ability to accurately hind-cast oceanic responses to natural climate variability on timescales from the seasonal cycle to multiple decades. Large-scale modeling studies, with some exceptions, have tended to focus primarily on the mean state of the ocean. But biological oceanographic time series exhibit significant variability on inter-annual to interdecadal scales associated with physical climate phenomenon such as the El Nino-Southern Oscillation (ENSO) and the Pacific Decadal Oscillation (PDO) (Venrick et al., 1987; Karl et al., 1995; McGowan et al., 1998; Karl, 1999). The ecosystem response to physical forcing may be quite nonlinear, manifesting in the North Pacific, for example, as a major biological regime shift in the mid-1970s due to the PDO (e.g. Francis and Hare, 1994). Retrospective models can help explain the underlying mechanisms of such phenomena (e.g. Polovina et al., 1996). Because of an interest in separating terrestrial and oceanic signals in the atmospheric CO₂ network, there is also

a growing effort to model the oceanic contribution to atmospheric variability, which appears to be small except for the tropical ENSO signal (Rayner et al., 1999; Le Quéré et al., 2001).

Numerical models are also being used to project the potential marine biogeochemical responses to anthropogenic climate change (e.g. Sarmiento et al., 1998; Matear and Hirst, 1999). Coupled ocean-atmosphere model simulations differ considerably in their details, but most models suggest general warming of the upper ocean and thermocline, increased vertical stratification in both the low latitude (warming) and high latitude (freshening) surface waters, and weakening of the thermohaline circulation. Combined, the physical effects lead to a 30-40% drop in the cumulative anthropogenic CO₂ uptake over the next century partly compensated by changes in the strength of the natural biological carbon pump. Given the low level of biological sophistication used in these early simulations, such projections must be considered preliminary, demonstrating the potential sensitivity of the system and posing important questions to be addressed through future research.

Preliminary ecosystem simulations (Bopp et al., 2000) show different regional climate change responses to enhanced stratification with decreased subtropical productivity (nutrient limited) and increased subpolar productivity (light limited) reminiscent of the PDO signal (Polovina et al., 1996). Other environmental factors to consider include alterations of aeolian trace metal deposition due to changing land-use and hydrological cycle, variations in cloud cover and solar and UV irradiance, coastal eutrophication, and lower surface water pH and carbonate ion concentrations due to anthropogenic CO₂ uptake (Kleypas et al., 1999). The decadal time-scale biogeochemical and ecological responses to such physical and chemical forcings are not well understood in detail, and prognostic numerical models will be relied on heavily along with historical and paleoceanographic climate variability reconstructions (Doney and Sarmiento, 1999; Boyd and Doney, this volume).

5.3 Land, coastal ocean, and sediment interactions

The coastal/margins zone interacts strongly and complexly with the land, adjacent atmosphere, continental shelves and slopes, and open-ocean. The specific rates of productivity, biogeochemical cycling, and organic/inorganic matter sequestration are higher than those in the open ocean, with about the half of the global integrated new production occurring over the continental shelves and slopes (Walsh, 1991; Smith and Hollibaugh, 1993). The high organic matter deposition to and close proximity of the water column to the sediments raises the importance of sedimentary chemical redox reactions (e.g. denitrification, trace metal reduction and mobilization), with implications for the global carbon, nitrogen, phosphorus and iron cycles. Finally, the direct and indirect human perturbations to the coastal environment (e.g. pollution, nutrient eutrophication, fisheries) are large, with important impacts on marine ecosystems (harmful algal blooms, coral reefs, spawning grounds) and society (e.g. commercial fisheries, tourism, and human health and aesthetics).

Because of the topographic complexity, smaller time/space scales, and specific regional character of coastal environments, basin to global scale models typically do not fully account for biogeochemical fluxes and dynamics on continental margins and in the coastal ocean. Thus coastal/open-ocean exchange and the large-scale influence on the ocean are not well quantified except in a few locations (Falkowski et al., 1994; Liu et al., 2000). Regional coastal ecosystem models have been moderately successful (e.g. Robinson, 2001; Figure 16), and an obvious next step is to meld open ocean and coastal domains through more adaptable grid geometries such as unstructured (spectral) finite element grids (Haidvogel et al., 1997) or by embedding regional domain, higher-resolution models (Spall and Holland, 1991). Dynamic marine sediment geochemistry models (Heinze et al., 1999) are needed both for the coastal problem and for large-scale paleoceanographic applications, an example

being the compensation of the sediment CaCO_3 to changes in ocean carbon chemistry on millennial time-scales (Archer and Maier-Reimer, 1994; Archer et al., 2000).

5.4 Inverse Modeling and Data Assimilation

The emerging techniques of inverse modeling and data assimilation, which more formally compare and meld model results and data, are becoming essential in model development and evaluation (U.S. JGOFS, 1992; Kasibhatla et al., 2000). In theory data assimilation provides a solution, if it exists, that is dynamically consistent with both the observations and model equations within the estimated uncertainties. Much of the art of data assimilation lies in assigning relative error weights to different data types and to the model equations themselves, the so-called cost function problem (U.S. JGOFS, 1992). A number of recent studies have used this approach to better constrain or optimize parameters for marine biogeochemical box and one-dimensional models, particularly with time series data (e.g., Matear, 1995; Fasham and Evans, 1995; Hurtt and Armstrong, 1996; Spitz et al., 1998; Fennel et al. 2001). Applications to three-dimensional models are more limited but include efforts to assimilate satellite ocean color data into ecosystem models (e.g., Ishizaka, 1990) or to estimate poorly measured fluxes such as dissolved organic phosphorus transport/remineralization (Matear and Holloway, 1995), surface export production (Schlitzer, 1999), and air-sea oxygen fluxes (Gruber et al., 2001) from the large-scale nutrient distributions and physical circulation flow fields. The utility of data assimilation will continue to grow with the import and refinement of numerical methods from meteorology and physical oceanography to interdisciplinary problems (Robinson, 1996) and with the availability of automated software systems for generating the required model adjoints (Giering and Kaminski, 1998).

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Estimated Basin Inventories of Anthropogenic DIC (Pg C)			
Ocean	NCAR CSM Ocean Model	Data-based C* Estimates	Data Reference
Indian	22.1	20±3	Sabine et al. (1999)
Atlantic	39.5	40±6	Gruber (1998)
Pacific	46.7	46±5?	Feely and Sabine (per. comm.)
Total	108.4	106±8?	

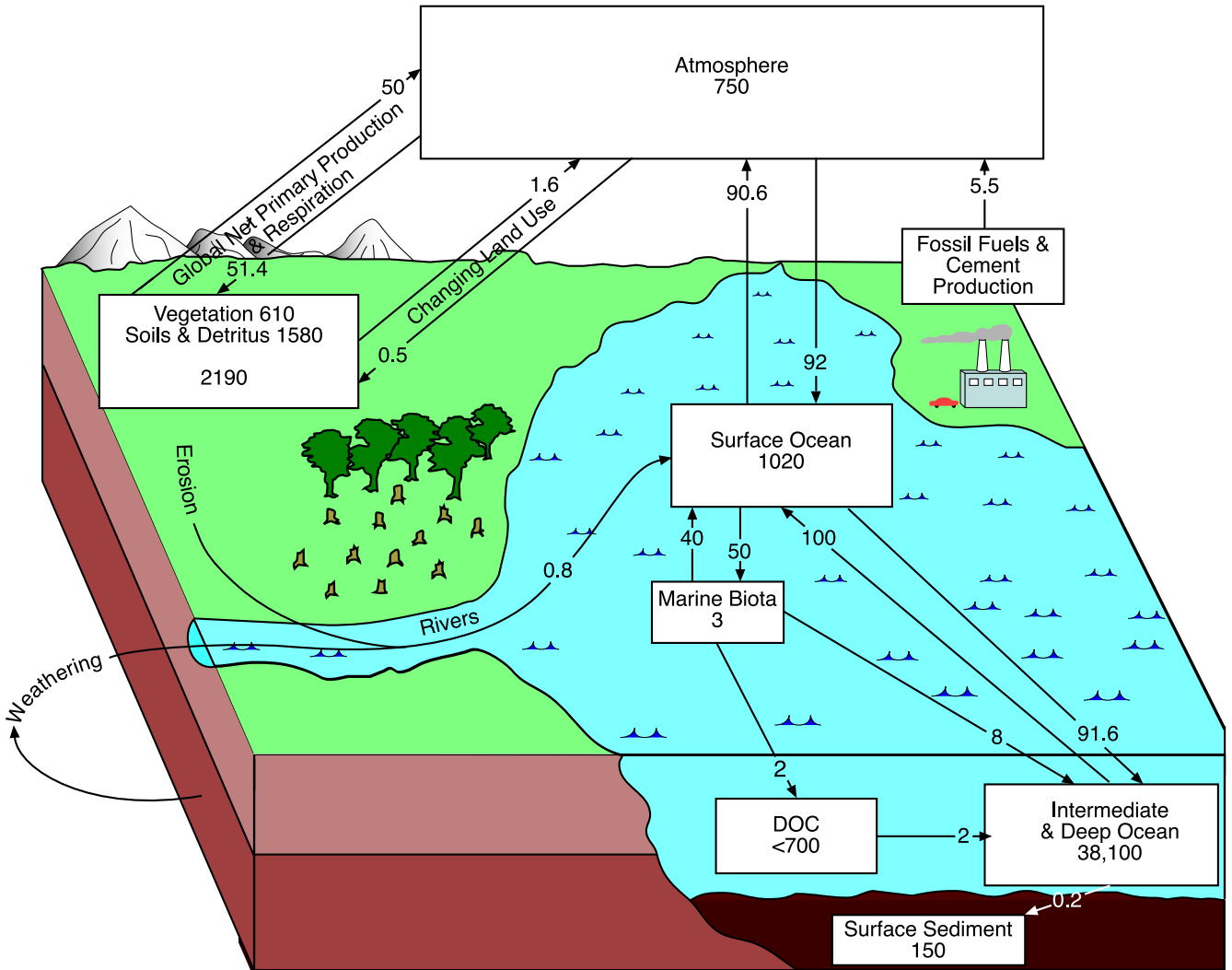


Figure 1: Schematic of present global carbon cycle budget. The budget includes the natural background cycle as well as anthropogenic perturbations. Reservoir sizes are given in units of Pg C (1 Pg equals 10^{15} g), while fluxes are given in Pg C yr⁻¹. Adapted from Schimel et al. (1995) and U.S. CCSP (1999)

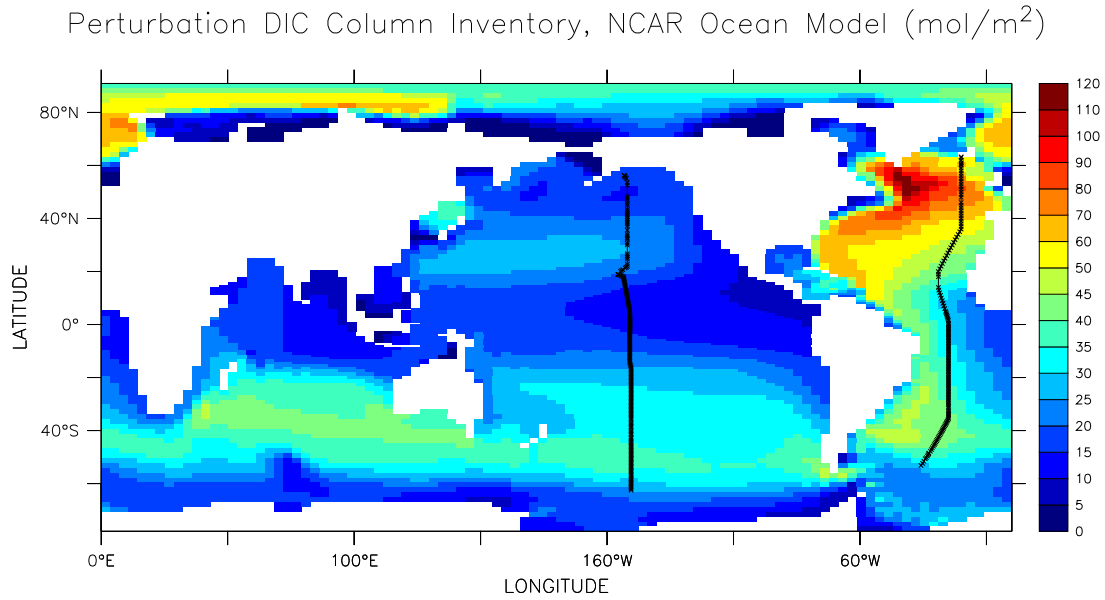
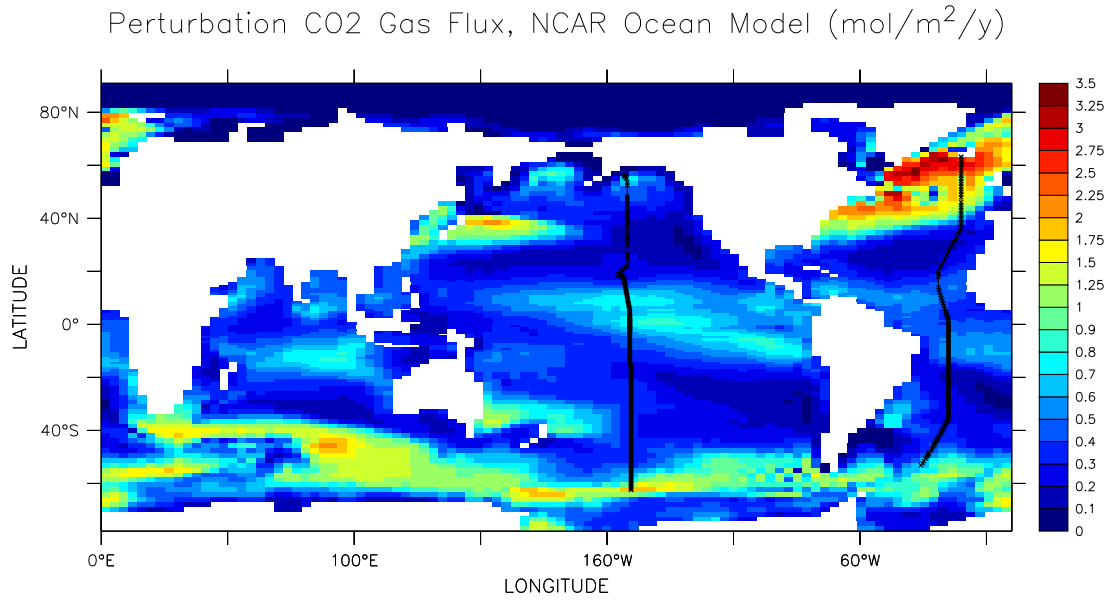


Figure 2: Spatial distributions of model simulated ocean anthropogenic (perturbation) carbon. Simulated fields are shown for a) air-sea flux (mol C m⁻² y⁻¹) and b) water column inventory (mol C m⁻²) for 1990 from the NCAR CSM Ocean Model. The two lines indicate the Atlantic and Pacific transects used for the horizontal sections in Figures 3 and 7.

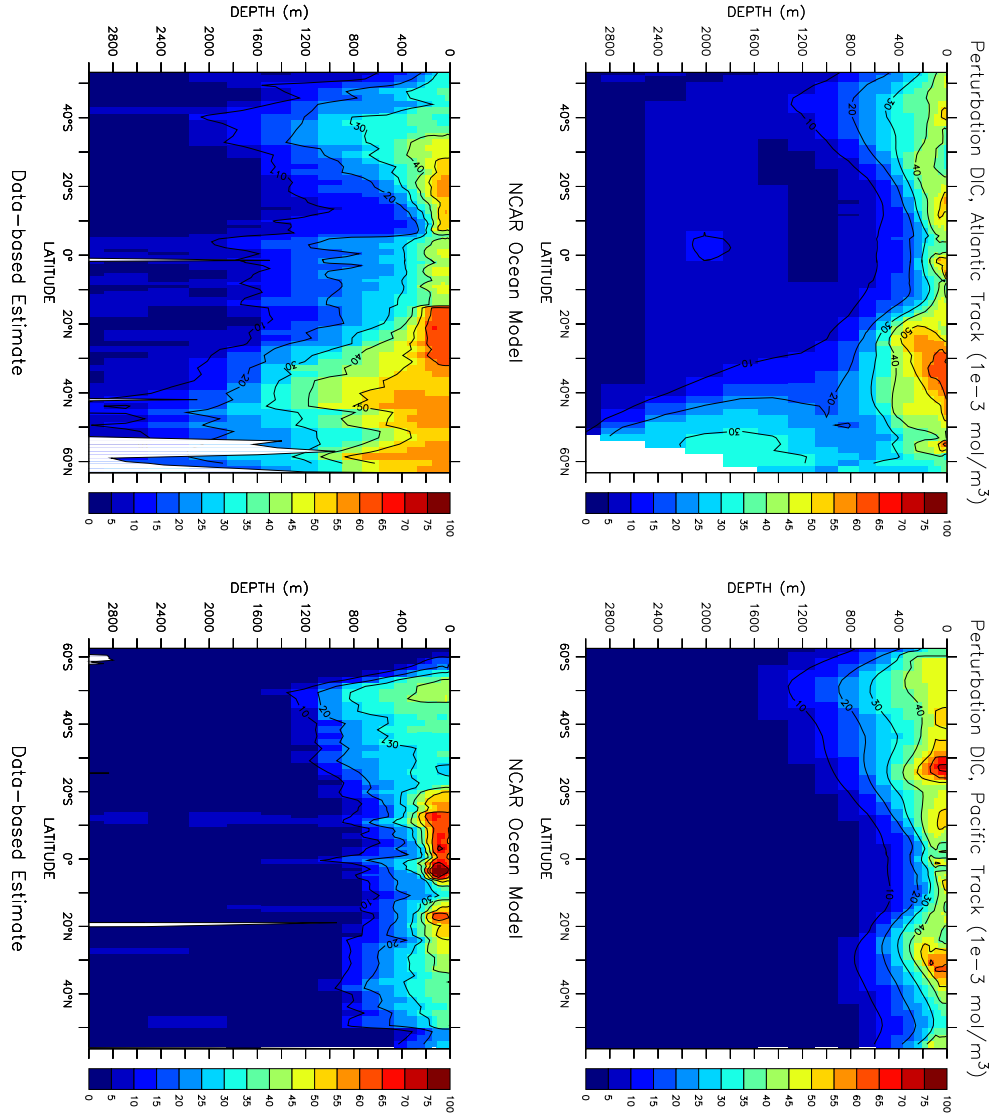
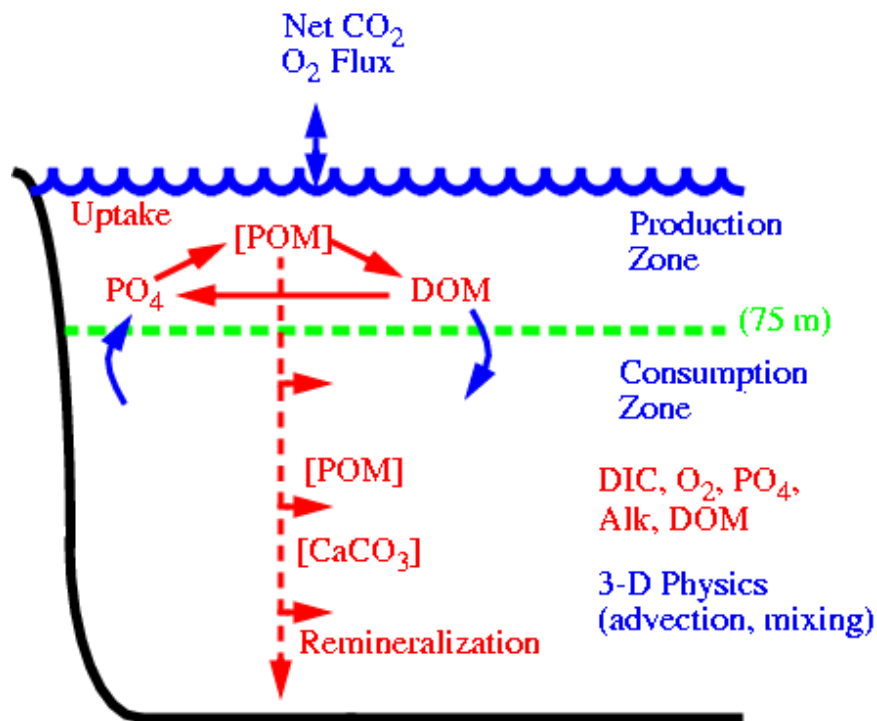


Figure 3: Depth versus latitude contour plots of anthropogenic CO_2 (mmol C m^{-3}). The panels show the simulated results from the NCAR CSM ocean model and the empirical, observation based estimates (N. Gruber, 2000, per. comm.) each for an Atlantic and Pacific section along the main path of the thermohaline circulation (see Figure 2). Note that depth is limited to 3000m.

OCMIP Biogeochemistry Model



- Phosphate Based Model
- Surface Nutrient Restoring (Monthly PO_4 Climatology)
- Fixed Redfield Ratios linking C,P, O₂
- Martin et al. Particle Remineralization Curve
- Semi-labile DOM only

Figure 4: Schematic of OCMIP global ocean carbon biogeochemical model. For more details see text and (<http://www.ipsl.jussieu.fr/OCMIP>).

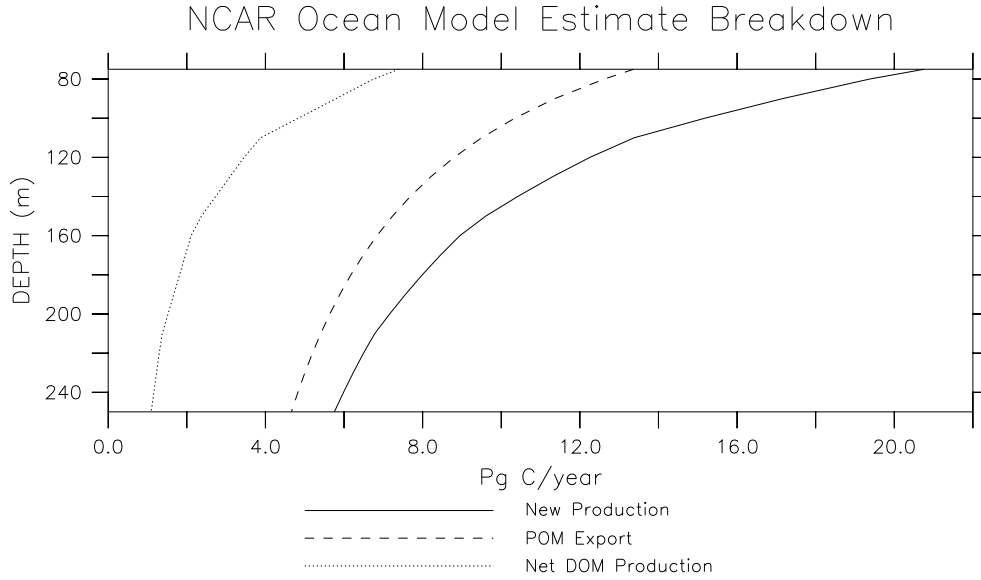
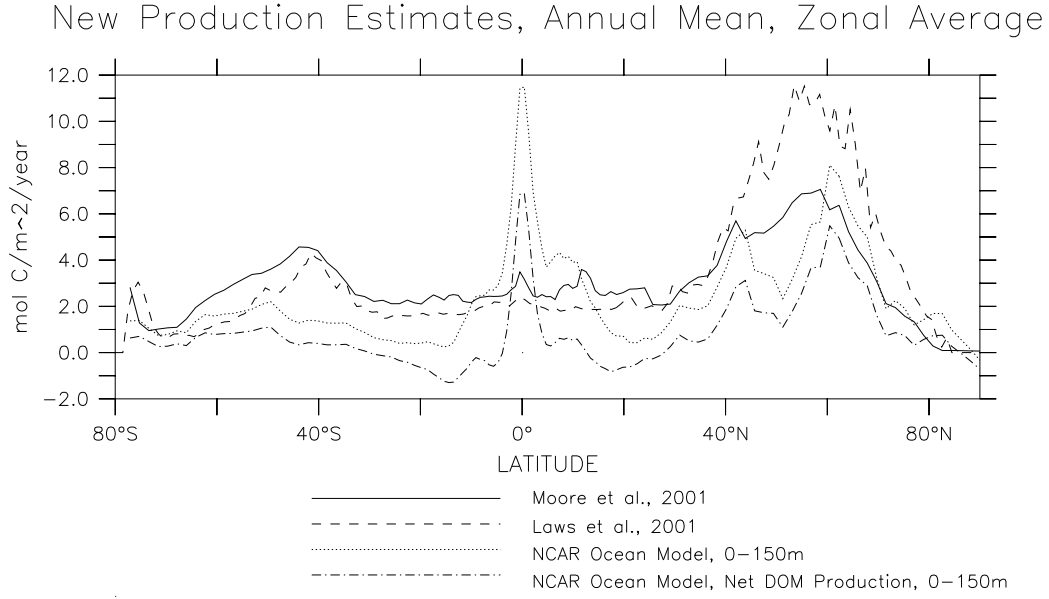


Figure 5: Annual averaged new production estimates. In panel a) the NCAR model total production (particle plus net semi-labile DOM creation) and net DOM creation computed to 150m are compared against recent new/export production estimates from Laws et al. (2001) (satellite primary production and ecosystem model based f-ratios) and Moore et al. (2001) (global ecosystem model including DOM loss from downwelling and seasonal mixed layer shoaling). In the lower panel, the NCAR model global integral total, particle and DOM new production rates are shown as a function of the bottom limit of the depth integration.

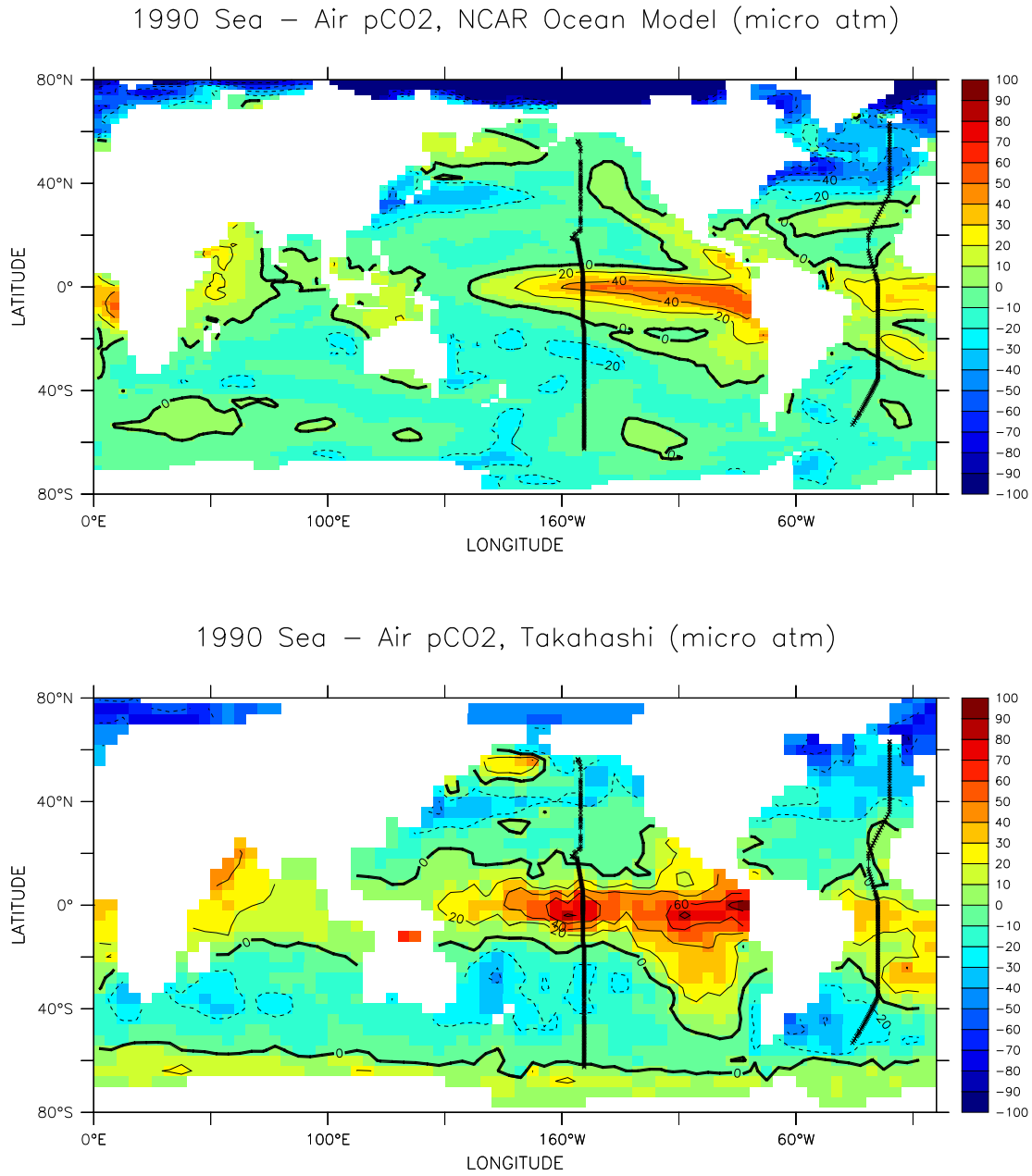


Figure 6: Spatial distributions of present (1990), annual mean surface sea–air pCO₂ difference (μatm) from a) the NCAR Climate Ocean Model and b) the Takahashi et al. (1997) climatology. The two lines indicate the Atlantic and Pacific transects used for the horizontal sections in Figures 3 and 7.

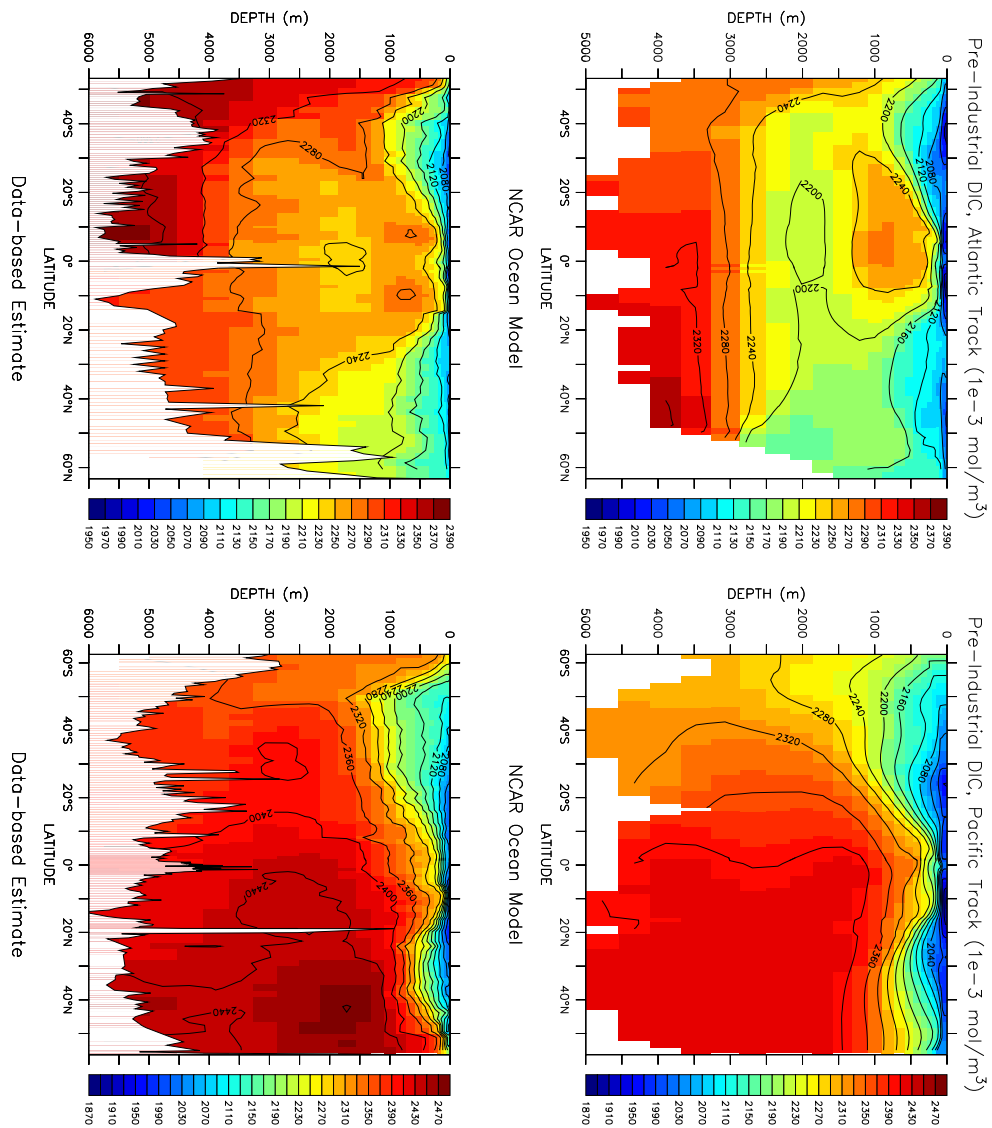


Figure 7: Depth versus latitude contour plots of pre-industrial DIC (**units**). The panels show the simulated results from the NCAR CSM ocean model and observed DIC fields with the anthropogenic DIC component removed using the C^* technique (N. Gruber, 2000, per. comm.) for an Atlantic and Pacific section along the main path of the thermohaline circulation (see Figure 6).

Ecosystem Model

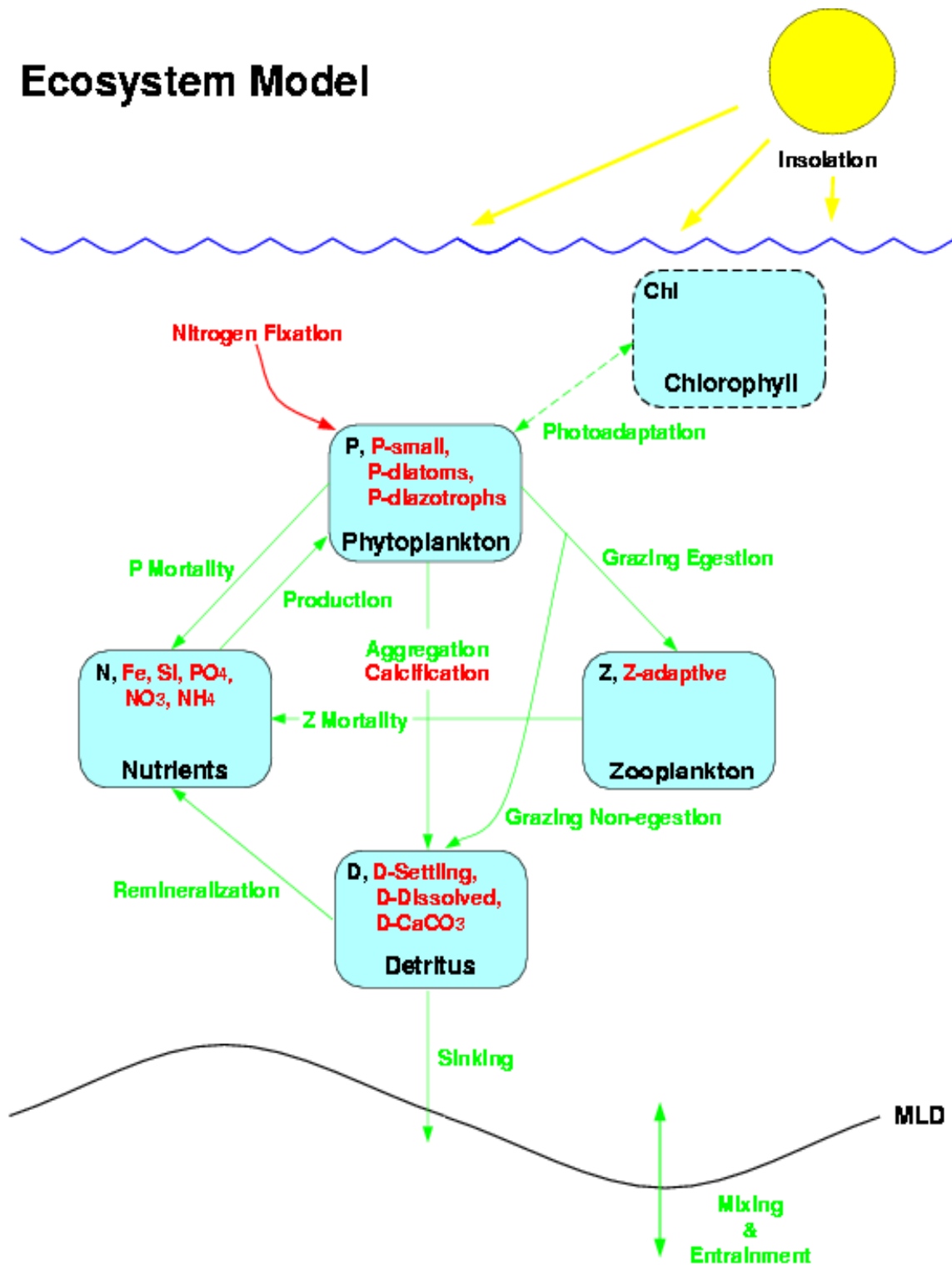


Figure 8: Schematic of a simple marine ecosystem model originally developed for the Bermuda Atlantic Time-Series Site (Doney et al., 1996) and (in red) the recent extension by Moore et al. (2001a).

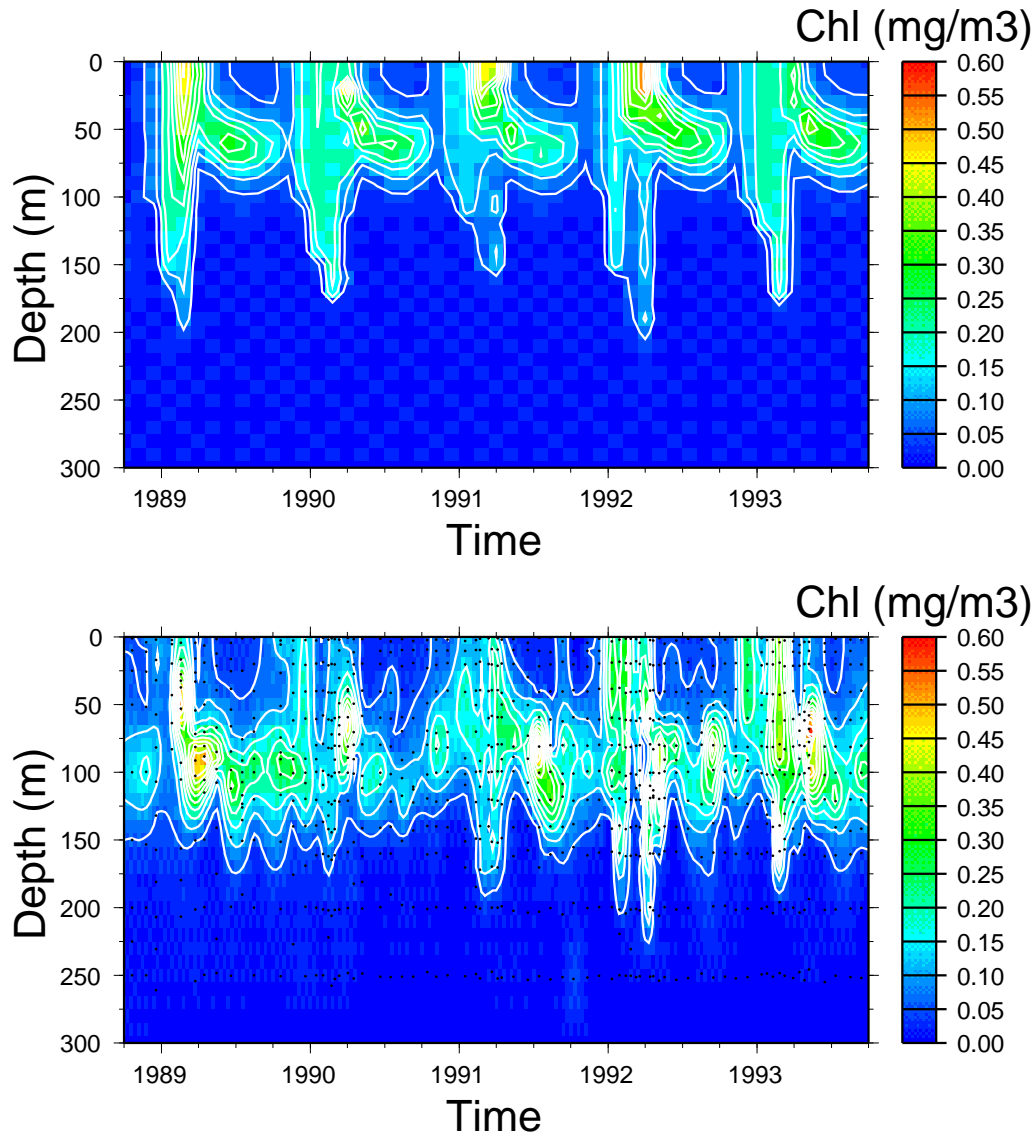


Figure 9: A comparison of the modeled and observed time-depth chlorophyll distribution for the Bermuda Atlantic Time-Series Study site in the western subtropical North Atlantic. The 1-D coupled biological-physical model is based on Doney et al. (1996) and Doney (1996).

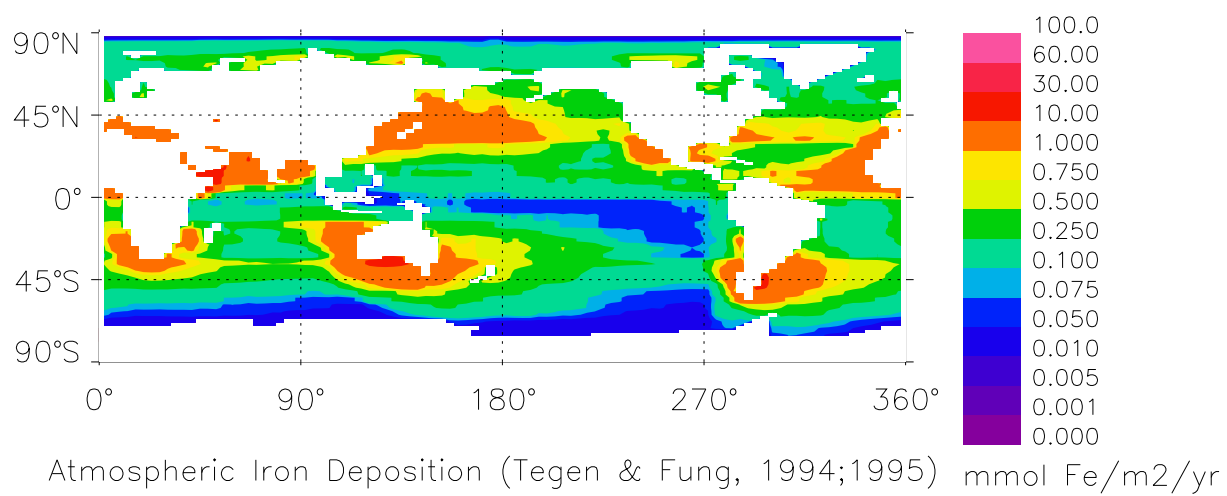


Figure 10: Annual mean map of atmospheric iron deposition to the ocean adapted from Tegen and Fung (1995) model estimates.

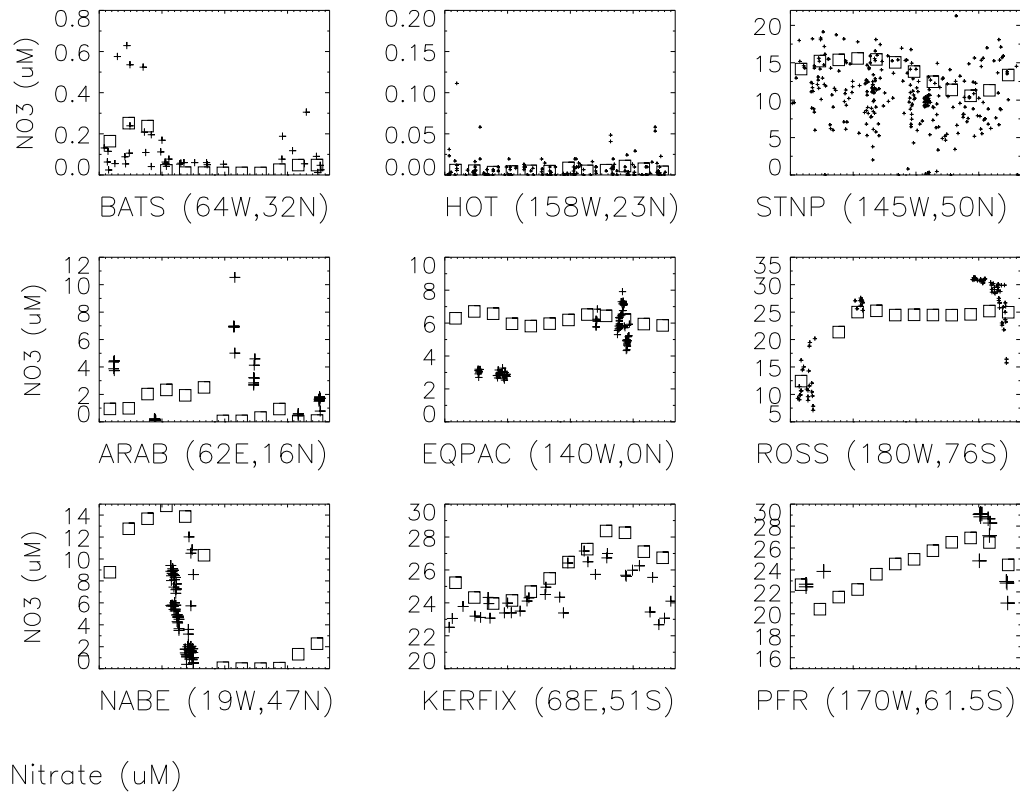


Figure 11: Comparison of simulated and observed seasonal nitrate cycle at nine JGOFS time-series stations across a range of biogeographical regimes. The model results are from a global mixed layer ecosystem model with uniform biological coefficients (Moore et al., 2001a; 2001b).

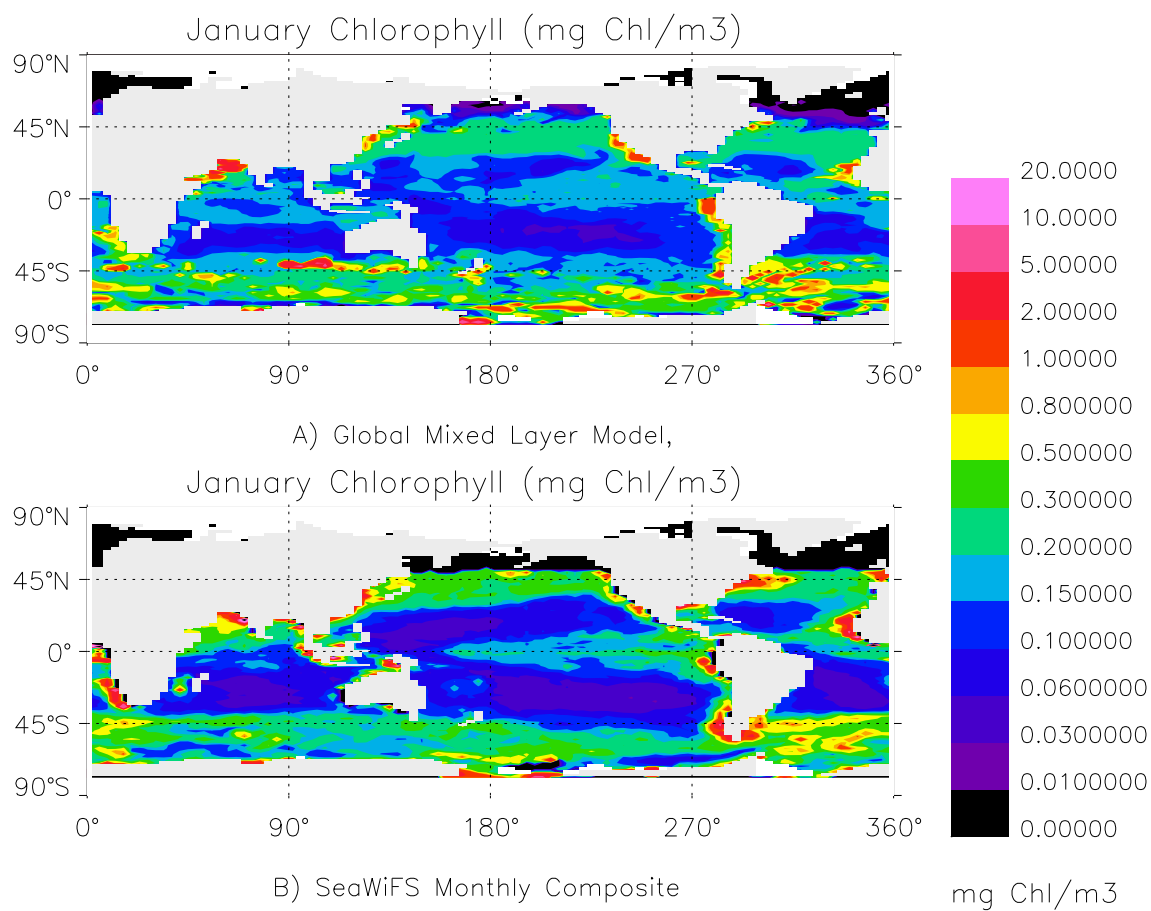


Figure 12: Global field of monthly mean surface chlorophyll concentration for January from SeaWiFS and a global mixed layer ecosystem model (Moore et al., 2001a; 2001b).

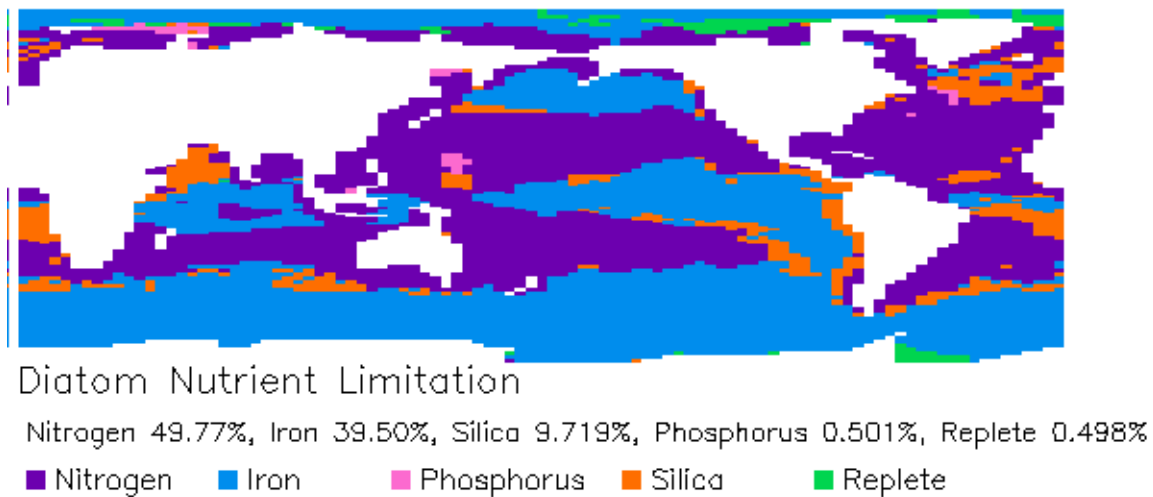


Figure 13: Ecosystem model simulated nutrient limitation patterns during summer months in each hemisphere (June-Aug. in the N. Hemisphere, Dec.-Feb. in the S. Hemisphere) for diatoms from Moore et al. (2000a; 2000b). Nutrient replete areas (here arbitrarily defined as areas where all nutrient cell quotas are $> 90\%$ of their maximum values) are largely restricted to areas of extreme light-limitation under permanently ice covered regions.

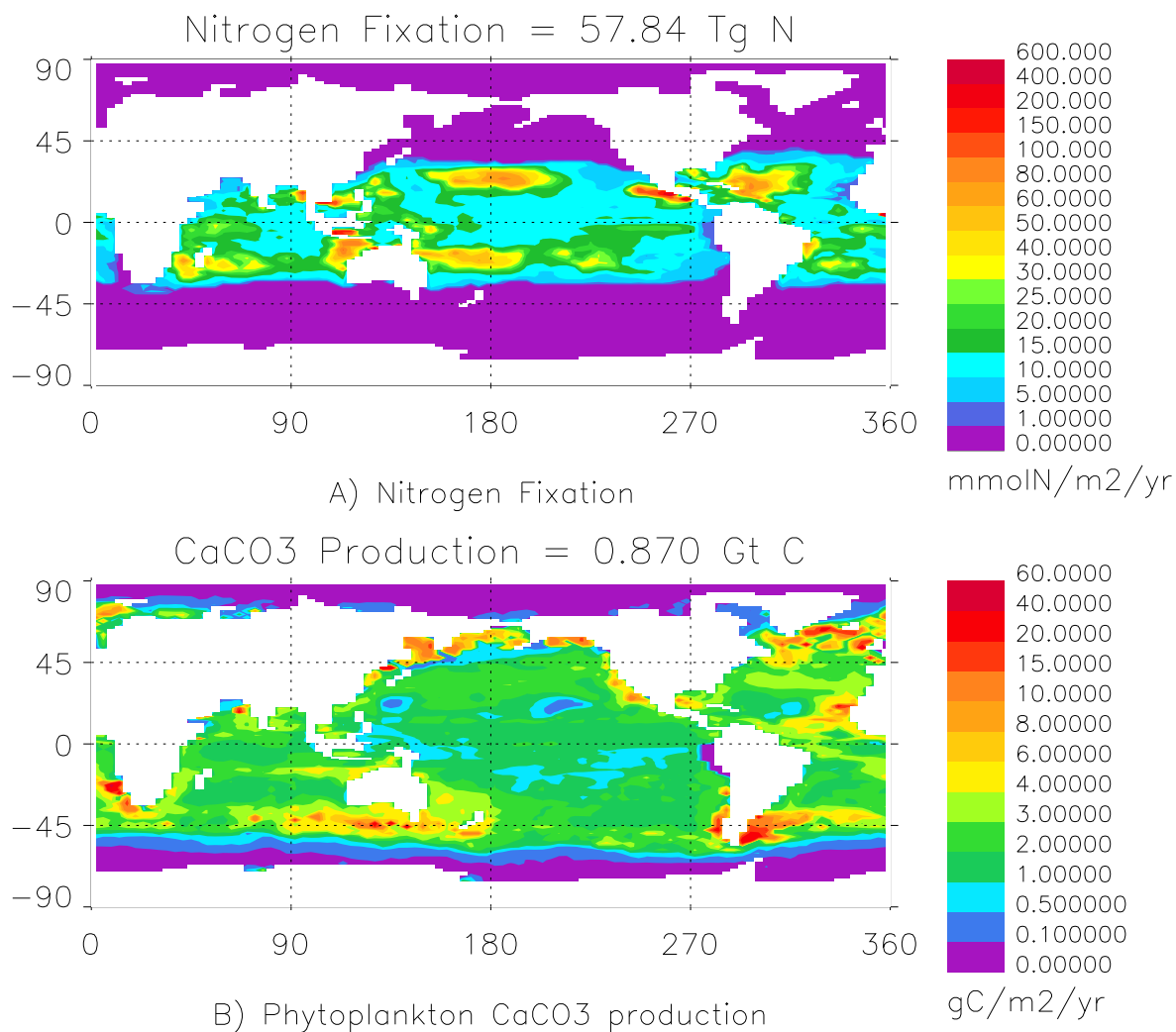


Figure 14: Model simulated annual mean nitrogen fixation and calcification fields.

Figure 15: Daily snapshot of new production from a Los Alamos-POP 0.1 deg. mesoscale simulation of the North Atlantic (Dennis McGillicuddy, per. comm.).

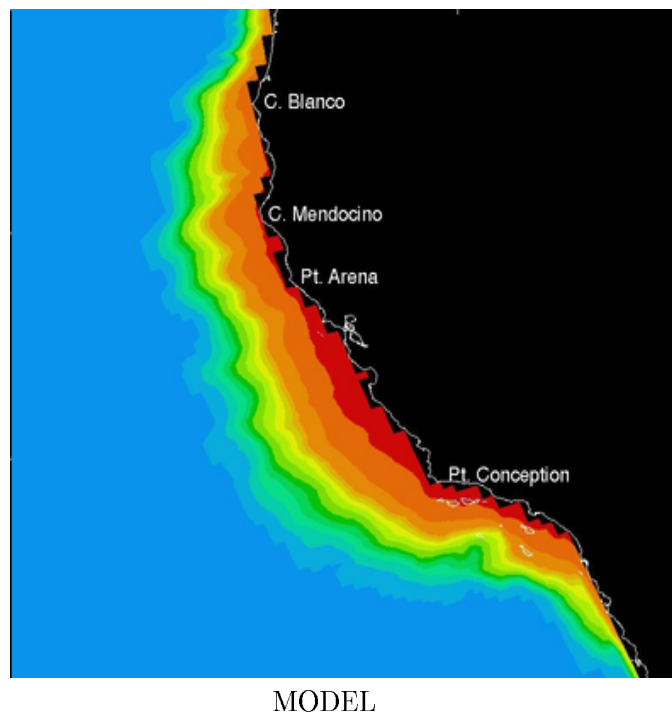
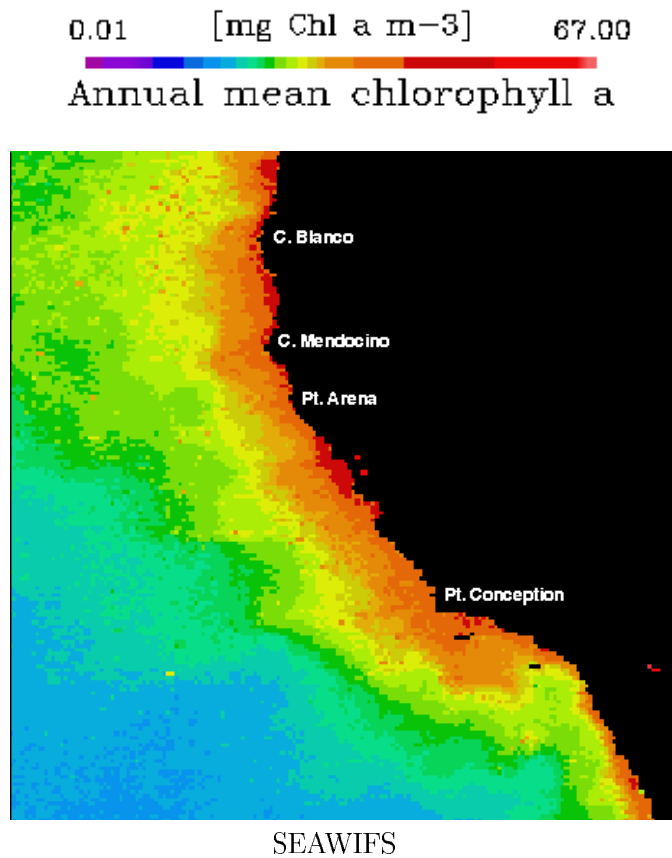


Figure 16: Annual mean chlorophyll for the California current coastal region from SeaWiFs and the UCLA regional coastal ecosystem model ROMS (Jim McWilliams, per. comm.).