Major challenges confronting marine biogeochemical modeling

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Short title: MARINE BIOGEOCHEMICAL MODELING CHALLENGES

Abstract.

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. At present, major impediments to marine biogeochemical modeling include the inadequate representation of: multi-element cycling and community structure; large-scale physical circulation; mesoscale space and time variability; and mass exchange between the open ocean and the atmosphere, land and coastal ocean. Marine biogeochemical modeling is inherently data driven, and significant progress on any of these topics will require close collaboration between the observational and modeling communities. Two main thrusts should be to develop improved, mechanistically based parameterizations of specific biogeochemical processes and to test the overall skill of integrated system models through detailed model-data comparison of both the mean state and seasonal to inter-decadal variability.

Marine biogeochemical cycles are at the heart of a series of pressing environmental issues—oceanic response to climate change [*Denman et al.,* 1996] and coastal eutrophication [*Nixon*, 1995] among the most crucial—and the scientific community will increasingly be asked to produce predictive models of demonstrated skill. The current suite of numerical models is not adequate to the task. Key processes are either excluded from present models or are crudely parameterized without clear, mechanistic basis; realistic regional and global simulations are hampered by our limited understanding of the coupled interaction of ocean biology, physics, and chemistry across all relevant time and space scales. Biogeochemical modeling is inherently data driven, and the major challenge (and opportunity) for the next decade is to integrate modeling efforts with the growing body of observations and emerging conceptual paradigms from large-scale field and satellite programs such as JGOFS, GLOBEC, CoOP, WOCE, IronEx, SeaWiFS and EOS.

Although oceanic biogeochemical modeling covers a diverse range of topics and scales, a number of common themes are evident, presented below with examples drawn from the marine carbon and nitrogen cycles.

***Models must better represent complex, often subtle biological–chemical interactions.**

The current generation of biogeochemical models, typified by the *Fasham et al.* [1990] food-web model, consist of a small number (4–12) of highly aggregated compartments, where the diversity of individual organisms and species are replaced with generic variables such as “phytoplankton” or “micro-zooplankton”. The biomass and biological flows are formulated in terms of the concentration of an elemental currency (e.g. mol m^{-3} of nitrogen or carbon), and the relationship among different biogeochemical cycles are calculated using generally constant Redfield elemental ratios. This class of models has been used with some success to capture the seasonal cycles of bulk properties (chlorophyll, primary productivity, and nutrient fields) at a single or handful of stations (Figure 1) [*Fasham*, 1995; *Doney et al.*, 1996], but the generality of these models and their derived parameter values for basin and global simulations remains a serious question. Marine biota both respond to and alter their chemical environment in intricate, sometimes poorly understood ways, and the ecological simplicity of current models belie the complexity of the real system. At a minimum, numerical models must incorporate the major shifts in biogeochemical paradigms resulting from recent field studies.

Many key biogeochemical processes are carried out by only a limited number of planktonic species—nitrogen fixation [*Capone et al.*, 1997], calcification [*Holligan et al.*, 1993], and active vertical nutrient transport [*Villareal et al.*, 1996]—which are poorly represented by bulk measures such as surface chlorophyll or total primary production. Resulting changes in the autotrophic source material and/or differential remineralization can lead to dramatic variations from the canonical Redfield ratios in the elemental composition of the dissolved, suspended and sinking organic pools in the upper ocean [*Sambrotto et al.*, 1993]. In the subtropical Pacific, for example, elevated abundances of nitrogen fixing algae were observed in the 1990's, marking a corresponding shift from a nitrogen to a phosphorus limited ecosystem [*Karl et al.*, 1997]. Net export production may be closely linked to community structure as well, largely manifest by the seasonal or episodic disturbance often leadin to the formation of diatom blooms [*Buesseler*, 1998], which because of their size are not as efficiently grazed by the ambient micro-zooplankton standing stock [*Landry et al.*, 1997]. Micro-nutrient iron limitation also may modulate community composition and has been demonstrated experimentally from the IronEx deliberate iron release studies for a portion of the high nitrate, low chlorophyll equatorial Pacific [*Coale et al.*, 1996], though a more complex interplay with silicate can not be excluded in general [*Dugdale and Wilkerson*, 1998]. Dissolved organic matter (DOM) has been shown to be an important pool for seasonal carbon storage and export [*Carlson et al.*, 1994; *Hansell and Carlson*, 1998], and the partitioning of organic matter export between dissolved and sinking particle forms is critical for large-scale model dynamics [*Najjar et al.*, 1992]. However, the dynamic controls on the production and consumption of DOM, the so-called "microbial" loop, are poorly known from a mechanistic perspective [*Azam*, 1998].

The next steps forward for numerical modeling will require explicit treatment of multiple elemental cycles (C, N, P, Si, Fe) and functional diversity within the plankton community. At the system level, the simultaneous comparison of multiple elemental budgets provides a much more stringent test of model skill, and the modeling field would greatly benefit from the construction of a standardized set of validation exercises across a range of marine environments based on existing time-series and regional data sets [e.g. *Evans and Garcon*, 1997]. Rudimentary, often incomplete community structure models also have been proposed, but as yet, no general model form has gained wide acceptance. Considerable debate has centered on whether it is better to predict species composition, or at a minimum functional characteristics, prognostically, parameterize structural responses through more simplified allometric relationships [e.g., *Armstrong*, 1994], or specify fixed biogeographical regimes in space and time [*Longhurst*, 1995]. Improved basin and global scale compilations of in-situ plankton size spectra [*Chisholm*, 1992] pigment floristics, and phyto- and zooplankton community composition are needed for model testing and satellite algorithm development. The resulting increases in model complexity must be grounded in a mechanistic understanding of the underlying processes, and traditional process studies will be fundamental in this regard but may not be sufficient. Greater reliance on deliberate ecosystem manipulation experiments and sustained time-series over multiple climatic events (e.g. ENSO, NAO, volcanic eruptions) are clearly indicated.

***Biogeochemical models are only as good as the physical circulation**

framework in which they are set.

Preliminary three-dimensional basin and global scale biogeochemical calculations [e.g. *Sarmiento et al.*, 1993; *Six and Maier-Reimer*, 1996] demonstrate that large-scale features such as the contrast between the oligotrophic subtropical and eutrophic subpolar gyres can be simulated qualitatively (Figure 2) but that more quantitative comparisons are hampered by known deficiencies in the physical ocean general circulation models. Recent comparison of four global ocean carbon models highlights dramatic differences in the effective vertical tracer transports in the southern ocean with implications for predictions of the future oceanic uptake of anthropogenic carbon [*Jim Orr, per comm.*; http://www.ipsl.jussieu.fr/OCMIP/]. 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 semi-labile dissolved organic matter—and thus obscure the validation of biogeochemical model components.

The refinement of global ocean general circulation models 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]. Biogeochemistry can contribute in this regard by providing additional, often orthogonal constraints on model performance to traditional physical measures [*Gruber et al.*, 1996]. The use of transient tracer observations (tritium, radiocarbon, chlorofluorocarbons) to assess the large-scale wind-driven and thermohaline circulation is utilized widely now [*England*, 1995], and observation based, integrated carbon, oxygen and nutrient transport calculations [*Wallace*, 1995; *Holfort et al.*, 1998] are becoming feasible, complementing the more standard heat and freshwater transport criteria [*Keeling and Peng*, 1995]. The incorporation of active biology tests new facets of the physical solutions, especially the surface boundary layer dynamics [*Large et al.*, 1994] and their interaction with the interior mesoscale field [*Gent and McWilliams*, 1990].

***Mesoscale space and time variability are fundamental aspects of the marine biogeochemical system.**

The availability of remote sensing ocean color data (Figure 3), new in-situ measurement technologies, and mesoscale biogeochemical models has spurred a growing realization that mesoscale variability is not simply noise to be averaged over, but rather a crucial trigger, governing the nature of pelagic ecosystems. Model calculations [*McGillicuddy and Robinson*, 1997], supported by moored biogeochemical time-series [*Dickey et al.*, 1998] and ship survey data suggest that mesoscale eddies can greatly enhance the net upward flux of nitrate in oligotrophic regions by lifting nutrient rich isopycnal surfaces into the euphotic zone, contributing a significant fraction of the total new production in subtropical regions [*McGillicuddy et al.*, 1998]. Tropical instability waves [*Yoder et al.*, 1994] may play a similar function by supplying dissolved iron to the surface equatorial Pacific. In both cases, disturbance, rather than background nutrient levels *per se*, is the major factor controlling community structure and integrated biogeochemical fluxes.

Quantifying the large-scale effect of such variability will require much better information on the variation and cross-correlations of biogeochemical stocks and rates on the meso- and submeso-scales. Sampling limitations for sub-surface distributions, in particular, emphasize the need for combined observational, remote sensing and regional modeling programs with heavy reliance on data assimilation. From a modeling perspective, the simulation of open-ocean mesoscale biogeochemical processes is in its infancy [e.g. *Oschlies and Garcon*, 1998], and the computational demands of truly eddy resolving basin to global calculations are significant and beyond the current capabilities of all but a small number of research groups. 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 [*F. Bryan and R. Smith, per. comm.*; http://www.cgd.ucar.edu/oce/bryan/woce-poster.html], and even higher resolution may be needed for some biological processes such as upwelling from eddy-eddy interactions [*McGillicuddy and Robinson*, 1997]. Over the near term, long time-scale equilibrium and climate simulations will be limited primarily to non-eddy resolving, coarse resolution models, and a primary objective of field studies and high resolution process models should be the development and testing of sub-grid scale biogeochemical parameterizations that can be scaled for basin and global applications.

***Improved constraints are required for interfacial mass fluxes across the air–sea, land–ocean, and coastal–open ocean boundaries.**

The interaction of marine biogeochemistry with the broader climate system is felt most directly through poorly quantified surface chemical mass fluxes with the atmosphere. For example, although significant advances have been made in mapping globally the surface seawater pCO_2 climatology [*Takahashi et al.*, 1997], significant uncertainties remain for the air-sea CO_2 flux because of difficulties in sampling the highly variable pCO_2 field particularly in remote, high latitude sites, the potential for significant regional, inter-annual variability [*Lee et al.*, 1998], and a near factor of two uncertainity in estimates of gas exchange kinetics [*Wanninkhof*, 1992]. Most estimates of the net oceanic uptake of anthropogenic carbon, therefore, have been based on numerical simulations alone (Figure 4). The situation is compounded for other climatically relevant species (e.g. organo-halides, organo-sulfides) because of limited surface concentration data and predictive modeling capability [*Lee-Taylor et al.*, 1998]. Conversely, the oceanic biogeochemical response can be forced, at least in part, by external inputs of material, a topical example being the trace metal inputs from rivers and estuaries, aeolian deposition, and margin sediments [*Duce and Tindale*, 1991; *Johnson et al.*, 1997]. The air-sea flux sampling problem will become more tractable with the advent of more satellite based approaches and autonomous chemical measurement systems [*Friederich et al.*, 1995] deployable on non-traditional platforms (e.g. moorings, drifters and floats), and developing work on direct eddy covariance measurements may resolve many of the linger unknowns regarding gas exchange kinetics [per. comm. W. McGillis, 1998, http://www.whoi.edu/air-sea/airsea.htm]. Considerable effort, however, will be required to develop the coupled ocean-atmosphere biogeochemical models required for climate studies.

Because of its limited size and proximity, the coastal ocean is particularly susceptible to perturbations in terrestrial runoff and atmospheric deposition, as demonstrated by local nutrient eutrophication and the apparent rise in harmful algal blooms [*Anderson*, 1995; *Paerl*, 1997], and ecosystem shifts due to over-fishing [*Fogarty and Murawski*, 1998]. Relative to their area, the coastal oceans also play a disproportionate role in many biogeochemical processes including nitrogen denitrification, organic carbon burial, and fisheries [*Walsh*, 1991; *Smith and Hollibaugh*, 1993; *National Research Council*, 1998]. Yet the regional character of most coastal studies and the historical disconnect between "blue-water" and coastal oceanography has limited the quantification of coastal/open-ocean exchange and its large-scale influence on the ocean [*Falkowski et al.*, 1994]. Because of their complexity and smaller scales, many global models simply neglect the continental shelves all together, an issue than can be overcome in part 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].

***Model–data comparisons must be extended to better utilize the diversity of oceanic measurements.**

The validation of present basin to global-scale numerical ecosystem models generally focuses on only a small sub-set of the wealth of available oceanic biogeochemical data, typically relying on climatologies of bulk biogeochemical concentrations, such as nutrients [*Conkright et al.*, 1994] and dissolved inorganic carbon [*Goyet et al.*, 1997], and a few rates, such as primary production [*Behrenfeld and Falkowski*, 1997]. The underlying processes within such models are often crudely represented at best, in part because the model predictions are not explicitly tested against observations. A clear example is the dynamics of particle sinking, remineralization, production and repackaging in the aphotic zone. Most large-scale models apply some form of empirical depth-particle flux relationship often derived from the work of *Martin et al.* [1987]. Considerable amounts of relevant but often under-utilized data exist on deep-sediment trap particle fluxes [*Lampitt and Anita*, 1997], particulate organic carbon standing stocks [*Bishop*, 1998], bacterial respiration from electron transport activity [*Packard et al.*, 1988], chemical transformations of organic bio-markers in particulate and dissolved organic matter [*Wakeham et al.*, 1997], partitioning of radiocarbon [*Druffel et al.*, 1992] and natural trace metal radionuclides [*Murnane et al.*, 1994] among organic pools, and radiocarbon levels of specific organic compounds in surface sediments [*Eglinton et al.*, 1997]. In part, this reflects the need for better compilation and synthesis of field data onto scales appropriate for model-data comparison. Present simulations, however, only crudely represent reality, and straightforward matching of observed and modeled variables and parameters is often difficult. The situation should improve as models capture more of the complexity of the real system, but explicit diagnostics need to be developed for more direct comparisons.

Equally important are the emerging techniques of inverse modeling and data assimilation, which more formally compare and meld model results and data [*U.S. JGOFS*, 1992]. Data assimilation in theory provides a solution, if it exisits, that is dynamically consistent with both the observations and model equations within the estimated uncertainities. 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]. 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] and surface export production [*Schlitzer*, 1999] 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 availabity of automated software systems for generating the required model adjoints [*Giering and Kaminski*, 1998].

Another 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 as given by global climatologies such as the NODC nutrient data [*Conkright et al.*, 1994] and similar inorganic carbon products forthcoming from the JGOFS/WOCE global survey [*Goyet et al.*, 1997]. But biological oceanographic time-series exhibit significant variability on inter-annual to inter-decadal scales associated with physical climate phenomenon such as the El Nino-Southern Oscillation (ENSO) [*McGowan et al.*, 1998]. The ecosystem response to physical forcing, however, may be quite non-linear, manifesting in the North Pacific, for example, as an apparent major biological regime shift in the mid-1970's [*Francis and Hare*, 1994], with a two fold increase in subtropical chlorophyll and primary production [*Venrick et al.*, 1987; *Karl et al.*, 1998]. On slightly shorter time-scales, the extended ENSO signal of the mid-1990's appears to have caused an enhancement in nitrogen fixation in the North Pacific subtropics related to increased water column stability [*Karl et al.*, 1995]. The number of historical, multi-decadal ocean biological time-series is limited [e.g. Reid et al., 1998], but their utility is almost invaluable. Despite the promise of near continuous satellite ocean color coverage for the indefinite future, subsurface, in-situ measurements are key to answering questions about why observed changes occur, and such long-term oceanographic time-series are not feasible without vigorous, on-going support from both the observational and modeling communities.

Although the availability of computational resources is and will certainly remain an issue in marine biogeochemical modeling, the main factors limiting progress are more fundamentally related to our conceptualization of the key processes and our ability to verify model behavior through robust and thorough model–data comparisons [*Abbott*, 1995]. The latter helps drive development by highlighting model deficiencies and is crucial if we are to have any confidence in the skill of our predictions on seasonal, inter-annual and decadal time-scales. The scientific challenges of the next decade increasingly will be accessible only through coordinated efforts joining numerical modeling, in-situ and remote observations and data assimilation, both because of the complexity, spatial and temporal scales, and interdisciplinary nature of the problems and because of the limitations placed on field work by finite resources. Modelers and observationalist can no longer work in relative isolation, nor can the biological and chemical communities be viewed simply as consumers of the end-product of physical models. Both groups have to be involved from the beginning in the formulation and analysis of large model simulations while modeling studies must be a standard, integral component of field programs from their conception.

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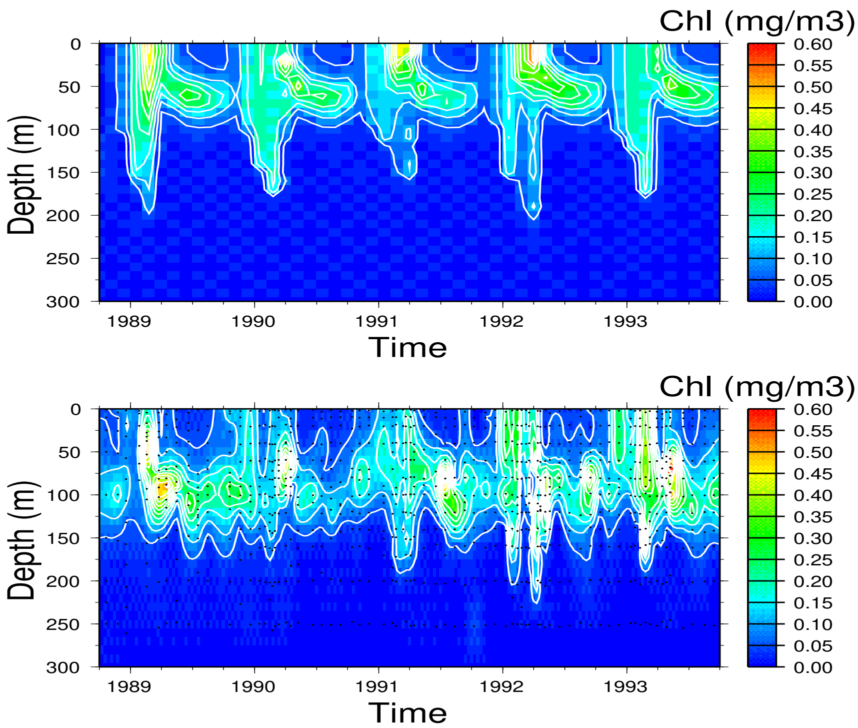

Figure 1. Comparison of multi-year, time-depth contour plots of modeled and observed chlorophyll from the JGOFS Bermuda Atlantic Time-series Site. The model results are generated by combining 1-D biogeochemical [*Doney et al.*, 1996] and synoptically forced physical mixing [*Doney*, 1996] models. Note the siginificant interannual variability in both the model and observations.

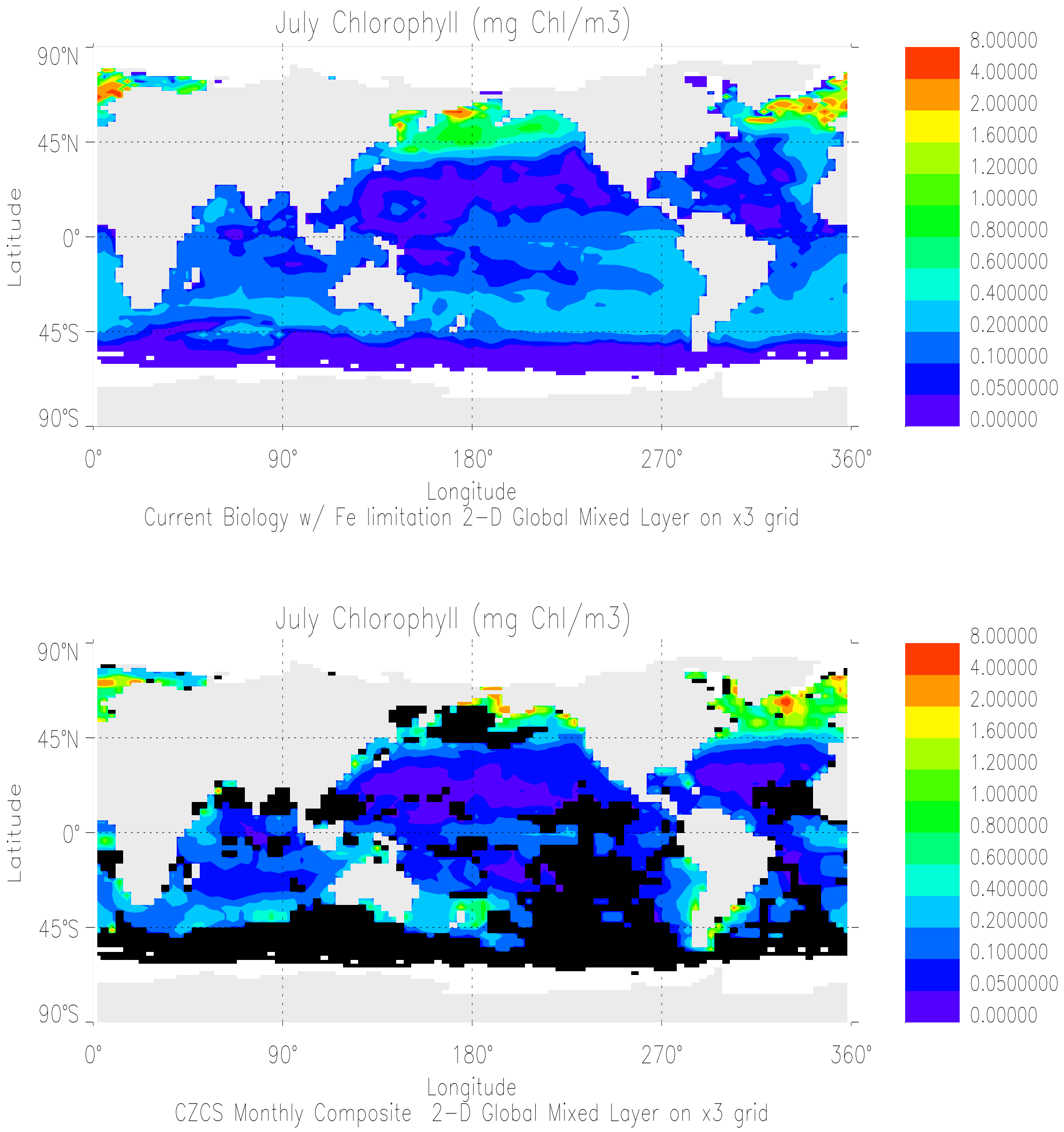

Figure 2. Comparison of observed and modeled surface ocean chlorophyll for the month of July from a global, biogeochemical mixed layer model [*Glover and Doney*, 1996] and the CZCS climatology.

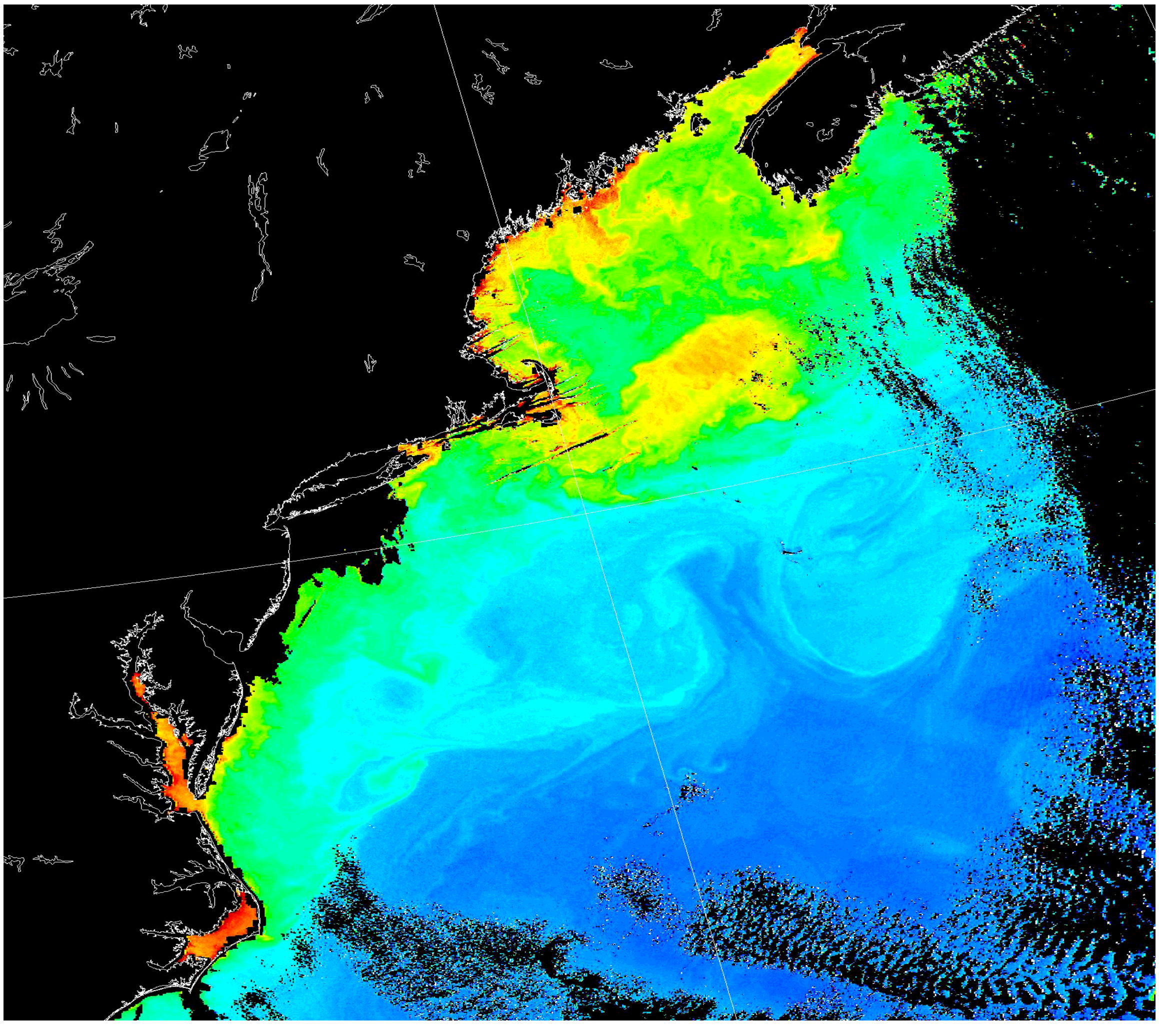

Figure 3. Satellite surface chlorophyll image of the Gulf of Maine and Mid-Atlantic Bight from the SeaWiFS instrument for October 8th, 1997 [*SeaWiFS Project*, http://seawifs.gsfc.nasa.gov/SEAWIFS.html].

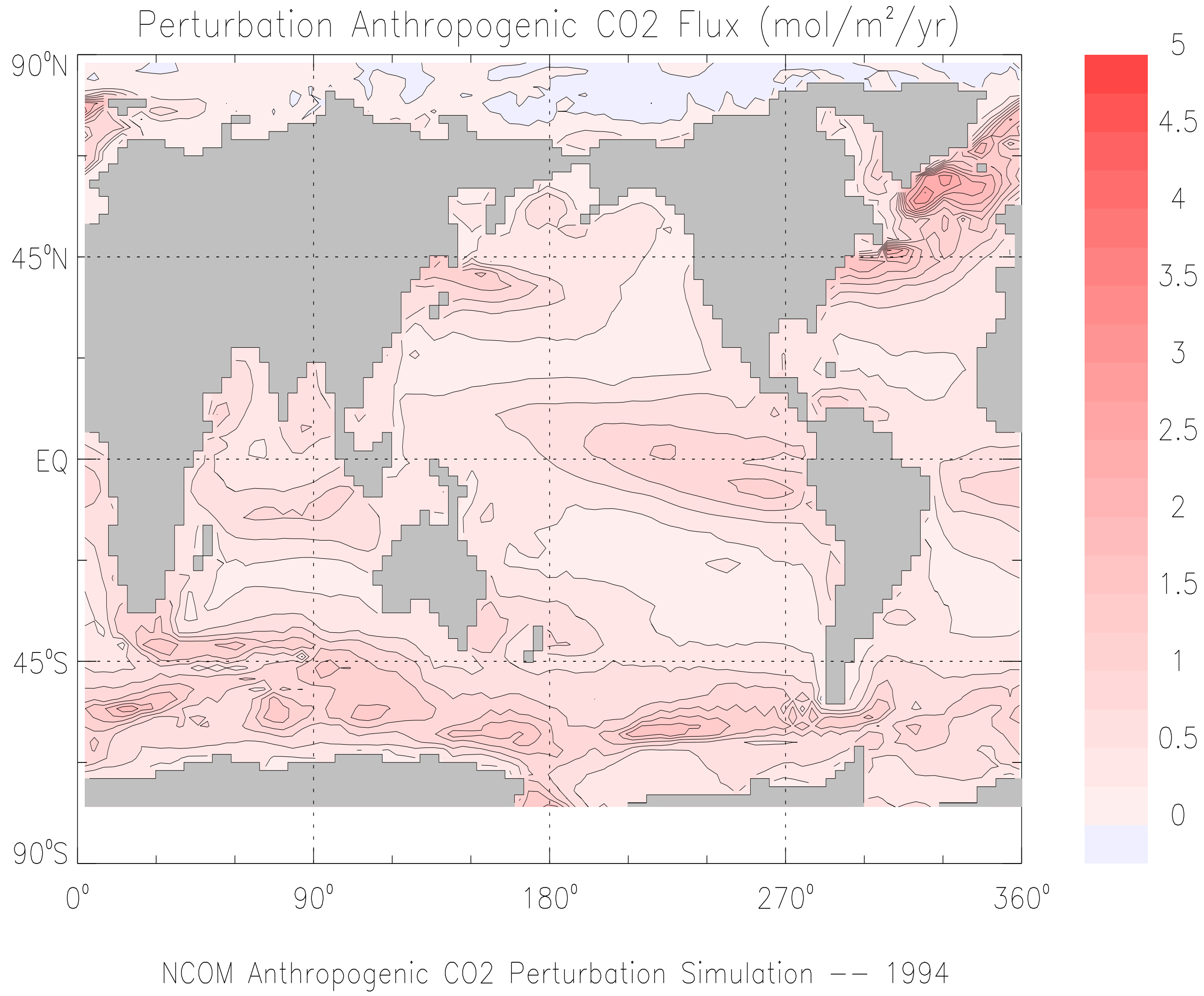

Figure 4. Annual average air-sea flux of anthropogenic CO_2 (mol C m^{-2} y^{-1}) for 1994 from a perturbation simulation of the NCAR CSM Ocean Model (NCOM); the global integrated model uptake is 2.11 PgC y^{-1} for 1994. Note that the perturbation flux of anthropogenic CO_2 differs considerably from the natural background and is largest in regions where older waters not recently in contact with the atmosphere are brought to the surface such as the equatorial upwelling bands and high latitude oceans.