

PARADIGM: The Partnership for Advancing Interdisciplinary Global Modeling

Annual Report – Year 2

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I. SUMMARY – YEAR 2

The program has seen good progress in this, its second year. The highlights include:

- Significant scientific progress towards our overall objectives, much too numerous to list here (but highlighted below in this report).
- 18 publications to appear in, or submitted to, peer-reviewed journals.
- A special session at the 2004 ASLO/TOS devoted to PARADIGM research.
- An invitation from Elsevier to produce a special issue of Progress in Oceanography devoted to PARADIGM and PARADIGM-related research.
- Establishing a PARADIGM web site: <http://www.gso.uri.edu/paradigm/>
- Invited PARADIGM presentations at the 2003 GODAE Workshop and an NSF/ONR sponsored workshop on data assimilation, as well as numerous other presentations at ocean conferences and university seminars.

The scientific accomplishments are detailed below in Section V: Work Completed and Results - Second Year.

II. LONG-TERM GOALS

To develop an efficient, community-based coupled biogeochemical-physical modeling framework that will enable the addition of new oceanographic processes in a straightforward and transparent manner, allowing new model structures to be developed and explored as our understanding of ocean ecology and biogeochemistry improves.

To develop such a modeling framework within the context of our initial, specific overarching scientific focus: an inter-comparison study between the subtropical-subpolar gyre systems of the North Pacific and North Atlantic basins, including an explicit coastal component, with particular emphasis on understanding:

- new paradigms for physical and chemical control of plankton community structure and function,
- the consequences for biogeochemical cycling,
- the effects of sub-mesoscale and mesoscale forcing, and
- the dynamics of long-term, climate driven ecosystem regime shifts.

To meet the challenge of merging observations and models through:

- advanced data assimilation techniques,
- the development of interdisciplinary data products for incorporation into models, and
- the application of new statistical and complex dynamical systems analysis techniques.

The merging of observations and models supports a rigorous model validation program that is central to PARADIGM.

III. OBJECTIVES

Our primary scientific objective is to improve our understanding of the mean state, seasonal cycle, and natural interannual to decadal variability of global and basin-scale biogeographical patterns. Why do different ecosystems reside where they do? What combination of forcing and biological responses drives the observed long-term variability and apparent ecosystem regime shifts? The intrinsic scales of ocean ecology are set by the growth and removal of phytoplankton, with time-constants of one to a few days. Our project scope, therefore, encompasses the range of coupled dynamics of ocean ecology, biogeochemistry, and physics on scales from sub-diurnal to multi-decadal and submesoscale to global.

The project is divided into four major scientific themes, with associated fundamental questions:

- 1) Biogeochemical cycles.** *What factors govern phytoplankton biomass, productivity and export, the net remineralization of organic matter below the euphotic zone, and the spatial (e.g., biogeographical regimes) and temporal (e.g., climate regime shifts) variations in these global processes?*
- 2) Community structure.** *What processes govern plankton community structure and function and how do physical-chemical-biological interactions influence biogeochemical processes in the ocean system?*
- 3) Scales of physical forcing.** *How do mesoscale and sub-mesoscale physical variability impact ecosystem fluxes and community structure?*
- 4) Advanced interdisciplinary models.** *How do we best merge observations and models?*

IV. APPROACH

PARADIGM is a group of 16 scientists committed to building and deploying new, advanced models of ecology and biogeochemistry for understanding and predicting the future states of the ocean. The group combines expertise of observers and modelers, ecologists and physicists, biogeochemists and numerical specialists. Our overall scientific goal is a rigorous, model- and observation-based intercomparison of ecosystem/biogeochemical dynamics of the North Pacific and Atlantic subtropical - subpolar gyres. Our central objective is creation of new global ocean biogeochemistry community models, comprising complex ecosystem dynamics based on functional groups (e.g., *Archaea*, diatoms, copepods, gelatinous predators), individual keystone species (e.g., *Trichodesmium*, *Euphausia superba*) and multielement limitation and cycling (e.g., C, N, P, Si, Fe). The physical model platform is composed of a hierarchy of mature, general circulation models each the focus of extensive community model development

programs. PARADIGM models will be capable of emergent behavior testing the hypothesis that fundamental regime shifts occur in response to climate change. Community models will be developed by interdisciplinary teams devoted to five program elements: (1) data fusion, synthesis and validation; (2) ecosystem model development; (3) high-resolution basin scale and regional process studies; (4) focus sites (i.e., regional testbeds) and (5) numerical method development (including data assimilation).

V. WORK COMPLETED AND RESULTS – SECOND YEAR

There has been a good deal of scientific progress in the second year of the program, which can be measured against our proposed Work Plan for Years 1 and 2:

Year 1. Initiate community model activities (Tasks 1.1, 1.2), data mining (2.1), ecosystem model development (3.1), work on regional models at focus sites (5.1, 5.3.2) and assimilation (6.1) and multi-scale grid coupling (6.2) algorithm tasks, including the following specific activities: a) finalize initial coupled model configuration for the community model, establish base state through multi-year and long equilibrium spin-up experiments and emphasize physical model outputs and physical-biogeochemical model couplings; b) obtain validation data (e.g., satellite, underway, moored, discrete), construct and analyze statistical property fields and networks of rate processes (ecosystems); and c) initiate model R&D activities, i.e. new model foodweb configurations, formulations, parameterizations, assimilation approaches, and test in 1-D or other appropriate modes with various physical testbeds (ongoing).

Year 2. Conduct first multi-decadal experiments with the community model (Tasks 1.2). Begin the high-resolution basin scale experiments (4.1.1, 4.1.2) and one of our process studies (4.2.1). Assimilation *research* (2.2) and model validation (2.3) programs start, as do new ecosystem model development (3.2) and two additional focus site (5.2, 5.3.1) programs. Finally, the open source code development program and the development and utilization of new approaches for data visualization (6.3) begins.

The following reports progress, in turn, on the activities “Global, High Resolution Basin-Scale, and Regional (Focal Site) Modeling”, “Ecosystem Model Development”, “Data Assimilation”, “Data Mining”, and “Numerical Methods” while referencing the task numbers above.

- **Global, High Resolution Basin-Scale, and Regional (Focal Site) Modeling**

One of the primary foci of PARADIGM funded research is the construction and validation of a new, coupled 3-D eco-biogeochemistry code for the global Parallel Ocean Program (POP) physical model. The new model includes multi-nutrient limitation, trace metal (Fe) cycling, multifunctional phytoplankton groups, and full carbonate chemistry. An extensive series of multi-decadal, coarse resolution (~3 deg.), global sensitivity experiments starting with “observed” subsurface nutrient fields have been conducted to fine tune parameter values. A manuscript has been submitted (Moore, Doney and Lindsay) documenting the model skill at representing large-scale biogeochemical/ecological patterns and exploring the behavior of the simulated, upper ocean iron cycle. This code has been transferred to the Los Alamos group and forms the basis for the first version of the Generalized Community Ecological-Biogeochemical Module (Task 1.1). An adjoint has been written for an off-line, global 2-D version of the eco-biogeochemistry model, and preliminary parameter optimization/data assimilation

experiments are being undertaken (Task 2.2; see Data Assimilation below). In preparation for regional modeling work, a reanalysis of the historical helium isotope data was conducted for the subtropical BATS/Bermuda site (Task 5.1). This led to a revised (and larger) estimate of the physical supply of nitrate and a new proposed mechanism involving a 3-D circulation pathway and extensive diapycnal transformations in the Gulf Stream/mode water formation regions (Jenkins and Doney, 2003).

On a related track for Task 1.1, we have developed an explicit mechanistic model of the oceanic iron cycle, and examined its interactions with a coupled ecosystem model in the global context of the MIT GCM. In addition we have developed an algorithm for solving the carbonate chemistry system in numerical models which is compact to code, more efficient in CPU cost and, significantly, easily differentiable for adjoint modeling and data assimilation. Three manuscripts are in preparation and soon to be submitted on these topics: Parekh et al. (2004), Follows et al. (2004), and Dutkiewicz et al. (2004).

The preferred version of the Moore, Doney and Lindsay ecosystem module (above) has been ported to POP2 and adapted to the LANL computing environment (Task 1.2). This was necessary since POP1 will not be supported in the not too distant future. Short validation runs in both the 3 degree and 0.4 degree configurations, with full biogeochemistry, have begun. Much effort has been put into validating the general circulation of the model setups (including the use of passive dye tracers and chemical tracers such as CFC's) so that decadal-long production runs can commence immediately once the ecosystem model parameters have been chosen and validated. We have also continued our interpretation of the important regions and mechanisms for the interannual variability of the global air-sea carbon flux in the MIT GCM and biogeochemistry model (also part of Task 1.2). The model suggests little role for the extra-tropical oceans, in contrast to the inferences from some atmospheric inverse models. A manuscript has been submitted and is accepted conditionally (McKinley et al., 2004).

We continue to analyze our high-resolution basin-scale simulations of the North Atlantic (Task 4.1.1), focusing on eddy-driven sources and sinks of nutrients in the upper ocean. A nitrate-based model of new production has been incorporated into eddy-resolving (0.1 degree) simulations. The biological model consists of light and nutrient limited production within the euphotic zone and relaxation of the nitrate field to climatology below. Sensitivity of the solutions to the parameters of the biological model is assessed in a series of simulations. Model skill is quantitatively evaluated with observations using an objective error metric; simulated new production falls within the range of observed values at several sites throughout the basin. Results from the "best fit" model are diagnosed in detail. Mean and eddy components of the nutrient fluxes are separated via Reynolds decomposition. In the subtropical gyre, eddy-driven vertical advection of nutrients is sufficient to overcome the mean wind-driven downwelling in the region and fuels a significant fraction of the annual new production in that area. In contrast, eddies constitute a net sink of nutrients in the subpolar gyre. Geostrophic adjustment to deep winter convection through mesoscale processes causes a net flux of nutrients out of the euphotic zone; the magnitude of this sink is sufficient to counterbalance the mean wind-driven upwelling of nutrients over much of the region. On the basis of these simulations it

appears that the oceanic mesoscale has major impacts on nutrient supply to, and removal from, the euphotic zone.

PARADIGM work during 2003 also supported high-resolution basin scale modeling work in the North Pacific (Task 4.1.2) by leveraging Pacific basin and regional HYCOM modeling efforts and supporting a postdoctoral scientist to incorporate a project ecosystem model into HYCOM. A 1/12th degree resolution, 20 layer HYCOM model for the Pacific Ocean north of 20°S was forced by ECMWF Reanalysis 6 hourly surface fluxes for the period 1979-1993; the simulation will be extended to 2001 during FY04. Evaluation of this high resolution Pacific HYCOM experiment reveals good agreement with observations in many areas throughout the Pacific basin. Additionally, in preparation for the incorporation of a project ecosystem model into HYCOM, a regional HYCOM model for the Northeast Pacific was developed. This regional model, which nests into the Pacific basin HYCOM (Task 6.2; see Numerical Methods below), will be used to test the coupled bio-physical model prior to implementing it into the full Pacific HYCOM. Results from the regional HYCOM may be evaluated in comparison to the coupled bio-physical model at NRL using the Navy Coastal Ocean Model (NCOM) that extends over the same domain and uses the same ecosystem model. Dr. Orlascoaga, a postdoctoral researcher at RSMAS who is also working directly with NRL, has initiated the incorporation of the ecosystem model into HYCOM.

Regional modeling of the subtropical gyres (Task 5.1) was also active in Year 2. Two processes were modeled: a) the role of remineralization and b) light limitation effects.

a) The role of remineralization from a modeling perspective The ecosystem models that are presently coupled to one- and three-dimensional circulation models either resolve the microbial loop or parameterize it via a constant remineralization rate. In addition, if the microbial loop is not resolved, phytoplankton exudation is either treated as a source of detritus that is in turn remineralized (Hurtt and Armstrong, 1996; Loukos et al, 1997; Friedrichs and Hofmann, 2000; Christian et al., 2001, Spitz et al., 2003) or as a source of dissolved inorganic nitrogen (Doney et al., 1996, Lawson et al., 1996; Fennel et al., 2001, 2003). The modeler has then to define a remineralization rate as well as a sinking rate and often chooses them such that the remineralization length scale matches the observed one. We have assessed the implications of resolving the microbial loop versus choosing a traditional parameterization of remineralization. We considered two sites, the Hawaii Ocean Time-series (HOT) and the Bermuda Atlantic Time Series (BATS) stations, since they reside in an oligotrophic environment with different biological and physical dynamics. The constant remineralization rates were computed such that they correspond to the 10-year average of the remineralization rate of the full microbial loop model. We found that not resolving the microbial loop and treating exudation as source of detritus leads to an increase of mesozooplankton and PON but a decrease of chlorophyll-a (Figure 1). In addition, we observed a shift in the timing of maximum concentrations. Treating exudation as an instantaneous source of ammonium led to a deep chlorophyll maximum (DCM) that was much smaller and deeper.

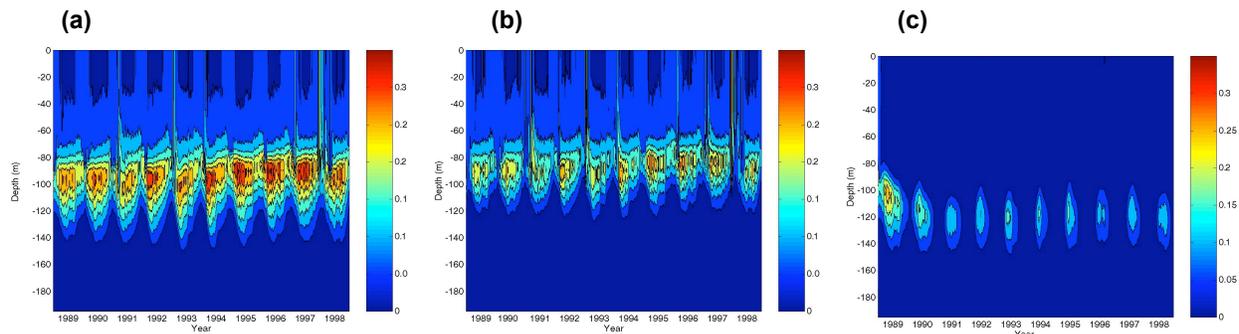


Figure 1. Vertical sections of Chlorophyll-a (mg Chl m^{-3}) for the HOT case. a) corresponds to the model with microbial loop, b) to the model with exudation to detritus and c) to the model with exudation to ammonium.

The largest export of nitrogen at 140 m (Figure 2) happens in case (a) when bacteria are able to regenerate ammonium based upon the composition of the dissolved organic pool. The export is also slightly larger when exudation is directed toward the dissolved inorganic pool without any delay (case (c)) than when exudation is directed towards the detritus pool (case (b)). In addition, the interaction between detritus and nano/microzooplankton seems to be the most sensitive to the choice of sinking and remineralization rates (not shown) while keeping the remineralization length scale constant. The same behavior as at the HOT station is observed at BATS when changing the parameterization of the remineralization process. However, the effect is stronger, especially after the spring deep mixing. In addition, increasing the remineralization and sinking rates such that the remineralization length scale is the same as in case (b) lead to a larger decrease of the DCM.

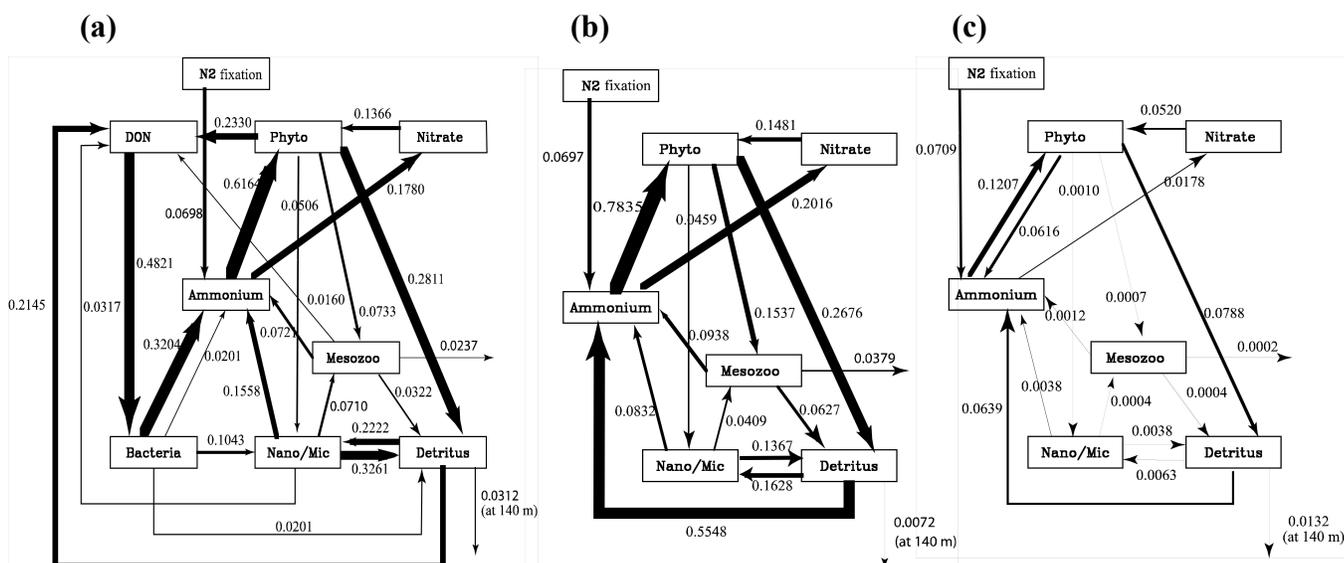


Figure 2. Mean annual fluxes at HOT calculated from 10-year runs (1989-1999).

From this sensitivity analysis, we can conclude that remineralization is an important component of the ecosystem. The parameterization of this component has a large impact not only the biomass but also on the export of nitrogen (carbon). This will have direct impact on the estimate of carbon fluxes from model simulations.

b) P versus I curve and effect on model results In ecosystem model, the light limitation formulation usually considers constant α in the vertical. New sets of observations (G. Corno and R. Letelier, personal communication) at HOT showed that α varies by a factor 5 between the surface to about 180 m. To test the importance of a variable α , we ran the 1D ecosystem model (Spitz et al., 2001) with a constant α and a varying α similar to the observations. We found that the increase of α with depth is necessary to model accurately the deep chlorophyll-a maximum (DCM) and the chlorophyll-a below the DCM (Figure 3).

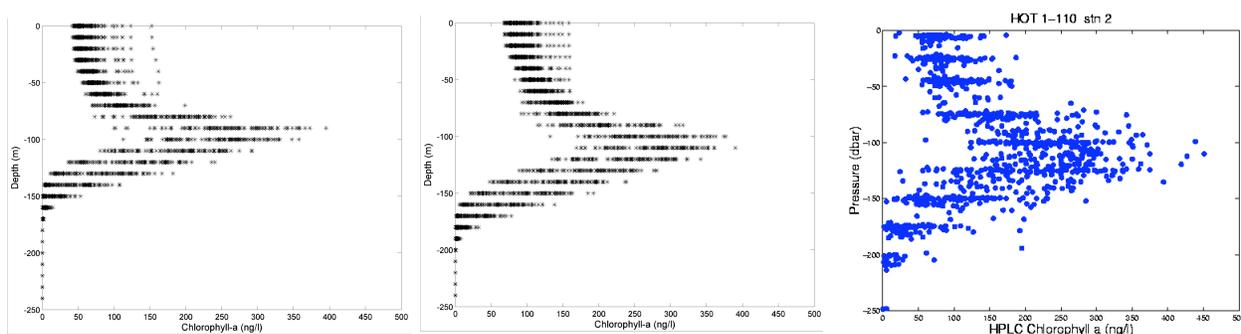


Figure 3. Chlorophyll-a profile from 1989 to 2000 using a constant (left panel) and a vertically varying α (middle panel) compared to the observations at HOT (right panel).

Continuing with our reporting of PARADIGM regional modeling efforts in the subtropical North Atlantic (in this case leveraged against the NASA Biogeochemistry Program), a coupled, one-dimensional mixed-layer/ecosystem model was developed and applied to the BATS (Bermuda Atlantic Time Series) site. The mixed-layer model uses the level 2-1/2 version of the Mellor-Yamada turbulent closure scheme (TCMLM). This scheme replaced the bulk model of the mixed layer [Garwood, 1977] used in a previous model. The biogeochemical model is an upgraded version of the Signorini et al. [2001] model, which includes additional conservation equations for diazotrophs and detritus. The addition of diazotrophs and detritus in the model follow the method of Fennel et al. [2002]. Time series of model (red lines) and observed (green lines for in situ data and blue lines for satellite data) chlorophyll concentration and primary production are shown in Figure 4. The model series is daily, while the in situ data were obtained on a nearly monthly basis. The satellite data are from monthly composites. The timing of the spring bloom is well represented by the model. It is quiet clear that the model under-predicts the summer-fall primary production. The predicted chlorophyll concentration tracks the observed values well, except for the 1995 spring transition where the fluorometric

Blue=SeaWiFS and OCTS Chlorophyll at BATS Site
 Green with Black Crosses=Observed at BATS (32.25°N, 65.75°W)
 Red=Model

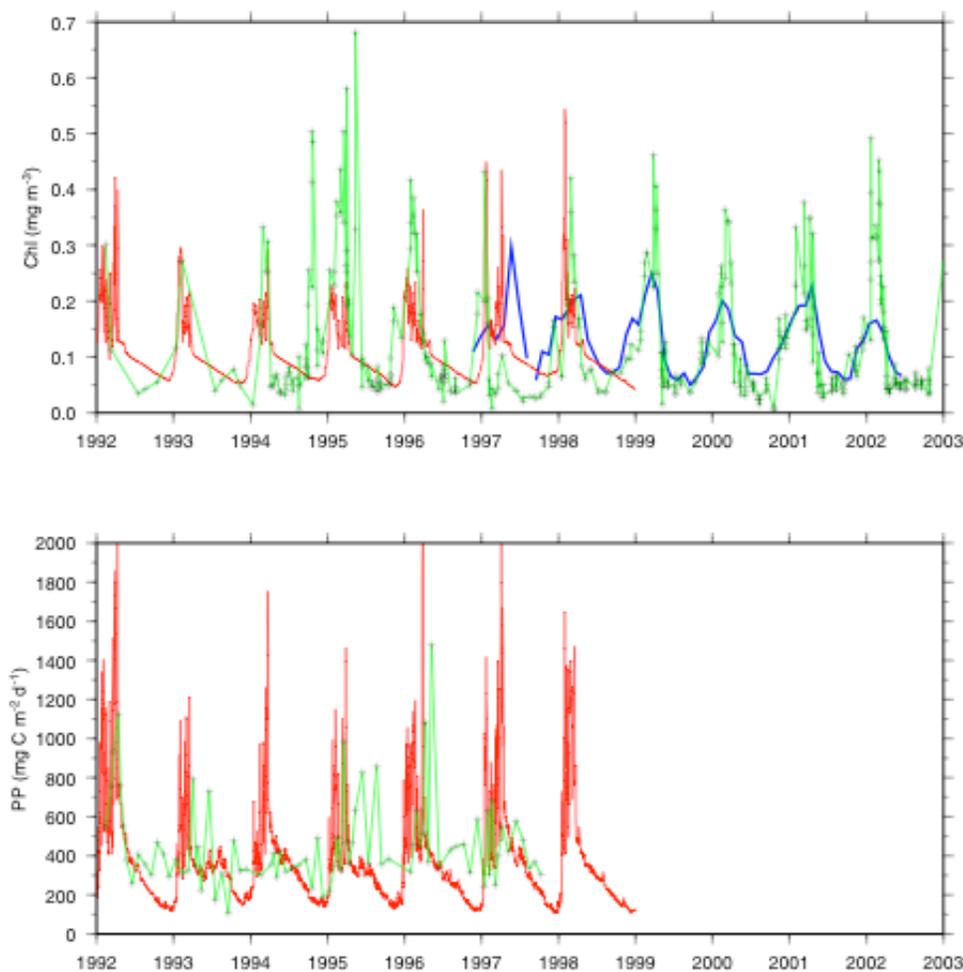


Figure 4. Time series of OCTS and SeaWiFS (blue), observed (green), and model surface chlorophyll at the BATS site.

chlorophyll measurements have a few high values (as high as nearly 0.7 mg m^{-3}). The satellite-derived (OCTS and SeaWiFS) chlorophyll concentrations are from monthly composites and therefore are much smoother but still in good agreement with the in situ data. Note that the OCTS and model records in early 1997 show anomalous high values compared to in situ data. Otherwise, monthly mean satellite values during peaks are low.

The use of the TCMLM contributed to some improvements in the model simulation of chlorophyll, PAR, nitrate, phosphate, and oxygen, but most importantly, the current model achieved good agreement with the data with much more realistic background eddy

diffusivity. However, sensitivity tests showed that the TCMLM does not provide adequate vertical mixing (convective mixing is ~50m shallower than indicated by the data) in winter-spring. In addition, off-line calculations of horizontal divergence of nutrients, heat, salt, and dissolved inorganic carbon, using seasonal climatologies, revealed that the BATS site lies in a region where horizontal transport of physical and biogeochemical properties by the ambient flow is an important process that cannot be neglected in studies of nutrient, biomass, and carbon balances. Also, mesoscale eddies play a role in the vertical transport of nutrients (eddy pumping) to the euphotic zone, as shown by several previous studies in the region [McGillicuddy et al., 1998; Siegel et al., 1999]. However, Oschlies [2002], using a three-dimensional eddy-resolving ($1/9^\circ$ resolution) model, concluded that eddy pumping has a much more limited role in nitrate supply at BATS than reported by previous studies. Also, Martin and Pondaven [2003] argues that mesoscale eddy pumping may not be able to close the Sargasso Sea nitrate budget. Therefore, future studies in the BATS region will require comprehensive three-dimensional field studies, combined with three-dimensional eddy resolving numerical experiments, to adequately quantify the impact of the local and remote forcing on ecosystem dynamics and carbon cycling.

A biogeochemical regional model of the **subarctic** North Pacific (Task 5.2) was also developed. A nitrogen-only version of the 1D model used to simulate iron fertilization was stochastically forced for thousands of years with stochastic functions derived from long term weather observations and NCEP reanalysis for Ocean Station P. Occasional years of complete nitrogen limitation occur from years with weak wind forcing and stronger than normal radiation. The transition in ecosystem structure along line P from an iron-limited regime (OSP) to a nitrogen-limited regime (P04 off Vancouver Island) was explored (Monahan, and Denman (in revision, February 2004). Discussions within the group have started concerning N. Pacific / N. Atlantic and subarctic / subtropical N. Pacific comparisons.

The coastal ocean is an important regional ‘focal’ site for PARADIGM, especially for the development and evaluation of data products from ocean observation systems that can be used in the guidance and evaluation of biological-physical models which include ecosystem variability (Task 5.3.2). Recognizing the need for observations corresponding to the predictions of advanced ecosystem models (e.g., size structure and possible species composition of phytoplankton assemblages; penetration of photosynthetically utilizable sunlight) we have analyzed observations of ocean color and near-surface attenuation of solar radiation to develop optical data products that go well beyond the conventional assessments of chlorophyll concentration and the attenuation of photosynthetically available radiation in surface waters. Using a novel inversion method, we (C.A. Brown, Y. Huot, C. Normandeau and J. Cullen) used measurements of both ocean color and attenuation to retrieve estimates of the dominant cell size of phytoplankton assemblages from the Bering Sea; the method effectively distinguished between representatives of two major functional groups, diatoms and *Phaeocystis*. A related analysis of hyperspectral ocean color as measured from a mooring in Nova Scotia coastal waters resolved variability of both phytoplankton absorption (a index of phytoplankton arguably more relevant than chlorophyll concentration) and the quantum yield of sun-induced

chlorophyll fluorescence (a promising, but incompletely understood measure of physiological status). Fluorescence yield in coastal waters was much less variable than for records from drifters in the Bering Sea (C. Schallenberg et al., in prep); we have developed a new mechanistic interpretation of this variability and plan to explore it with PARADIGM partner Mark Abbott. Measurements of attenuation have also been incorporated into a new, biologically relevant description of the penetration of solar radiation into the water column. We showed that a derived variable, weighted transparency, accounts very well for the variability of optical properties of water in models of depth integrated primary productivity (Lehmann et al. in press).

A coupled physical-biogeochemical model has been implemented for the continental shelf and adjacent deep-ocean of the U.S. east coast (Task 5.3.1) using the Regional Ocean Modeling System (ROMS v2.0). The shelf region model is embedded within a basinwide North Atlantic ROMS and has a horizontal resolution of 10 km. The model adequately captures spatial and temporal patterns of surface chlorophyll in comparison with SeaWiFS satellite chlorophyll, spring and autumn phytoplankton blooms, and the phytoplankton maximum near the pycnocline in summer. Simulations have been performed to investigate the fate of riverine inputs of nutrients and organic matter, and the effect of denitrification on the nitrogen and carbon balances. A nitrogen budget has been established for the Mid Atlantic Bight (MAB). Results suggest that the riverine inflow of DIN and PON combined is significantly smaller than nitrogen exchange with the adjacent deep ocean. Denitrification removes 60% of all the nitrogen entering the MAB, with the remainder being exported as PON. Hence, the shelves represent a net sink of nitrogen. This implies that the ocean margins play a role in the basin-wide nitrogen and carbon cycles through the material exchange between the continental shelves and the adjacent deep ocean.

- **Ecosystem Model Development**

A primary PARADIGM objective is ecosystem model development (Activity 3). One component of our program's research this year has developed along three main lines:

- extending ecosystem models coupled to 1D mixed layer models and applying them to specific ecosystem studies (the 2002 SERIES iron fertilization experiment near Ocean Station P; studies in the Arctic of under ice algal blooms and subsequent carbon-related fluxes);
- developing and testing a coupled atmospheric single column model (SCM) coupled with a community turbulent mixed layer model (GOTM) for gas flux and sulphur cycle studies; and
- implementing and testing a simple 4-component ecosystem model in the global CCCMA ocean GCM, in preparation for simulations in the Canadian Climate Model with carbon as a prognostic variable.

Task 3.1 is formulated to explore the background state hypothesis. Moritz, Lehmann and colleagues have developed a multi-component ecosystem model to explore the influence of stochastic environmental forcing with different dominant frequencies on the size

structure of phytoplankton communities (Lehmann et al. ASLO meeting presentation). This effort is designed to complement studies by other PARADIGM members, particularly the efforts for modeling structures of reduced complexity with a 'background-bloom' formulation and a preference algorithm for nitrogen uptake rather than an ammonium inhibition algorithm (Denman, 2003). Meantime, Lehmann has been assembling and analyzing data on phytoplankton size fractions in relation to environmental forcing. The research is designed to relate the relative importance of larger phytoplankton to temperature and derived environmental variables related to irradiance regime and nutrient flux to the photic zone.

Another of our fundamental ecosystem model tasks is Task 3.2, "Nutrient Ratios – Multiple Limitations – Functional Groups. A 1D coupled model was extended to include two functional groups of phytoplankton, inorganic carbon and alkalinity, nitrate, ammonium and silica and a simple algorithm for iron limitation in order to address the planktonic community responses to the 2002 SERIES iron fertilization experiment near Ocean Station P. The observed community responses can be simulated with the same iron dependence for both groups of phytoplankton. The proportion of small phytoplankton assumed to be calcifiers must be less than a few percent for sensible alkalinity values to emerge. Sensitivities of carbon export to formulations of diatom sinking and aggregation were explored and will be reported at the TOS/ASLO PARADIGM Session. A 1D snow-ice-ocean mixed layer model has also been developed for modeling the seasonal cycle of under ice algae showing the importance of careful light formulation, silica dependence and a variable-thickness under ice viscous boundary layer in simulating observations. This work will also be presented at the TOS/ASLO Session.

PARADIGM funds were leveraged with funds from the JGOFS Synthesis and Modeling Project, and the Palmer, Antarctica, LTER for an inverse model analysis of plankton foodwebs in the North Atlantic and Western Antarctic Peninsula. The relationship between food web structure and function across two ocean biomes was investigated using an inverse method to recover solutions of food web carbon and nitrogen flows. The majority of flows in food webs are unknown quantities that leave open many questions about food web function. The inverse method, first used on plankton food webs by Vezina and Platt (1989) is a least squares approach of recovering flows from plankton food webs that have not been observed or measured in the field. The inverse method provides a solution that is consistent with the observations of the system and biological constraints set forth in the model. The study focused on phytoplankton blooms in the North Atlantic Ocean and the western Antarctic Peninsula.

Plankton food web data were synthesized for input into the inverse solution method, including measured flows and biomasses from the North Atlantic Ocean (JGOFS NABE study) and the western Antarctic Peninsula (WAP: Palmer Station LTER study). Inverse food web solutions were recovered for NABE and the WAP. The inverse model solutions were analyzed with network analysis, sensitivity analysis and other techniques.

North Atlantic carbon and nitrogen inverse solutions were found representing 2 weeks in

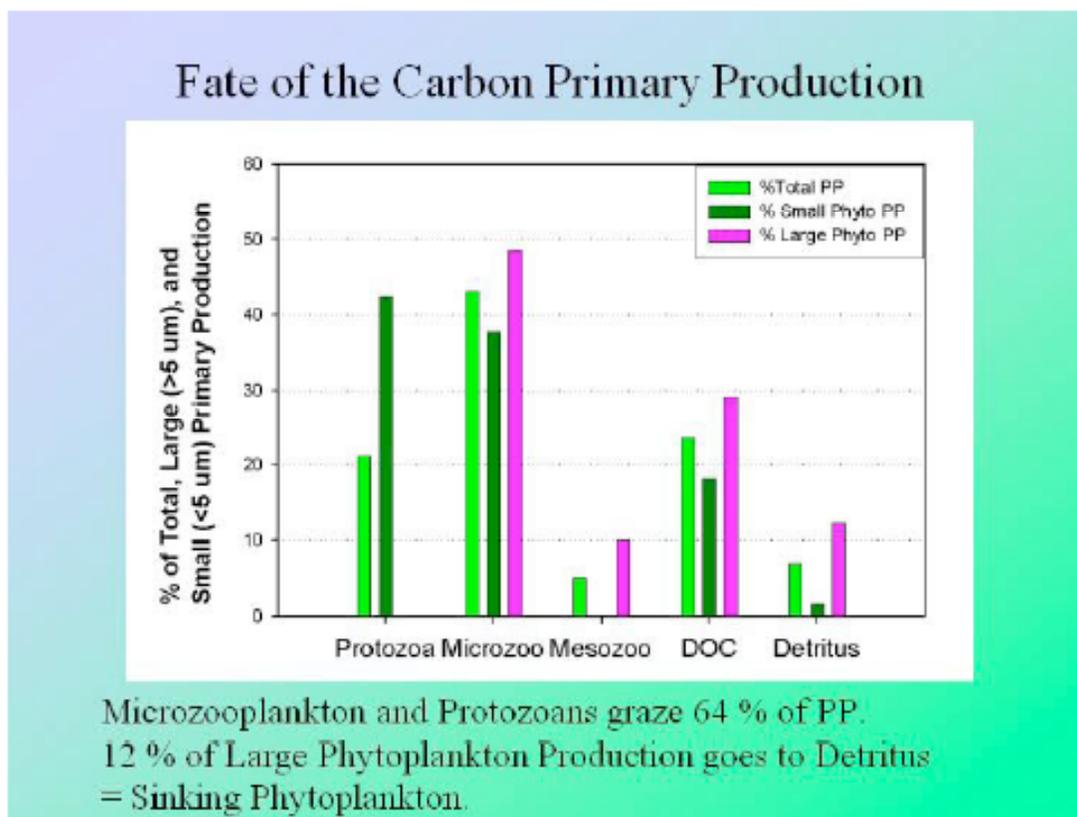


Figure 6. Fates of primary production as represented by the inverse solutions. Small grazers and DOC release are the major sinks for primary production in this solution.

Table 1. Dissolved Organic Matter and Detritus Flows in the North Atlantic Bloom Experiment (NABE) and West Antarctic Peninsula Phytoplankton (WAP) Blooms. Flows normalized to Primary Production (PP).

Flow component	NABE	WAP
Particulate detritus throughput (% of PP)	25	25
Dissolved organic matter throughput (% of PP)	74	14

Finally, contributions to Task 3.3 (studies of complex emergent behavior) were accomplished through experiments with full-scale, multi-species copepod populations, which provide insights into copepod-copepod interactions and the degree to which these interactions impact the success of the copepod population as a whole. The results from single and multi-species interaction simulations are now being used to develop parameterizations for inclusion of species-specific zooplankton behavior in large-scale three-dimensional coupled physical-biological models. If successful, this will allow inclusion in larger scale of a degree of biological complexity and realism that has previously not been possible.

- **Data Assimilation**

One of the more important PARADIGM activities is data assimilation, both for research into new techniques for multi-component data assimilation (Task 6.1) and for validation studies (Task 2.2). Data assimilation into coupled physical-biological models requires quantitative estimates of errors in the model and in the data. The data errors must include the error of representativeness, i.e., that part of the signal that cannot be represented in terms of the model state, as well as sampling variability and instrument error. The error of representativeness is particularly important for coupled models, since computer resource limitations may preclude the use of coupled eddy resolving physical/biological models. While the coarse resolution (0.7°) circulation model that we are using simulates the upper ocean remarkably well, we know that the lack of mesoscale eddies prevents the model from correctly simulating the long-term behavior of the circulation and its heat, salt and nutrient transports. We have used a reduced state space Kalman filter and an ensemble Kalman filter with AVHRR observations of SST to explore these errors and determine the relative importance of model errors versus surface forcing errors. In the first method, the forecast error covariance is estimated by fitting multivariate EOF's from the model to the EOF's of the AVHRR/model SST misfit. The observation error, including representativeness error, is folded into the misfit, so our forecast error covariance also contains observation errors. In the second method, the forecast error covariance is based on an ensemble, and the observation error covariance is assumed to be diagonal, an assumption that is almost certainly incorrect. The difference in error models is the major difference between the two methods, since both rely on the same ensemble to calculate the basis of the space of corrections. The combination of the two techniques will allow us to analyze model versus forcing errors. The results of the two assimilations methods have been presented at the 2004 AGU Ocean Sciences meeting and are the subject of an upcoming manuscript.

The eleven component ecosystem model of Spitz et al. (2001) has been coupled to the North Pacific Ocean circulation model. The coupled system has been run for 15 years (1988 to 2002). The coupled simulation reproduces the general features of the spring bloom over the entire North Pacific, even though the model was developed to describe the subtropical ecosystem and calibrated at the Hawaii Ocean Time-series (HOT). While the qualitative agreement between SeaWiFS observations and the model is reasonable, the differences pose substantial challenges for data assimilation compared to assimilation for the circulation model. The time and space scales of the spring bloom are much shorter and smaller than the SST signals used in the Kalman filter. Developing an error model for the ecosystem is far more challenging. As a first approach, we have tested the concept of estimation of model errors from assimilation by considering two stations, HOT and OSP. The first two leading EOFs in the vertical for chlorophyll-a at HOT and OSP (Figures 7 and 8) explain 77% and 71% of the variance, respectively. The first leading EOF at both stations shows strong correlation between the surface and subsurface. At both stations, the second EOF shows anti-correlation between surface and subsurface chlorophyll-a. For data assimilation using a reduced state space Kalman filter, this indicates that surface chlorophyll-a information can be used to update the subsurface chlorophyll-a. However, additional information is needed to partition between the first and the second modes. At

HOT, a simple model based upon projecting the satellite remote sensed data onto a single mode will produce qualitative agreement between surface and subsurface structure but will underestimate the strength of the subsurface chlorophyll-a. Multivariate analysis might be necessary to correct the subsurface deficiencies. In agreement with the HOT observations, the amplitude of the model EOFs shows that the surface chlorophyll-a bloom is out of phase with the deep-chlorophyll-maximum. At OSP, contribution to the subsurface chlorophyll-a comes only from the second mode and therefore a multivariate analysis will be needed. These results will be presented at the 2004 TOS/ASLO Ocean Research Conference.

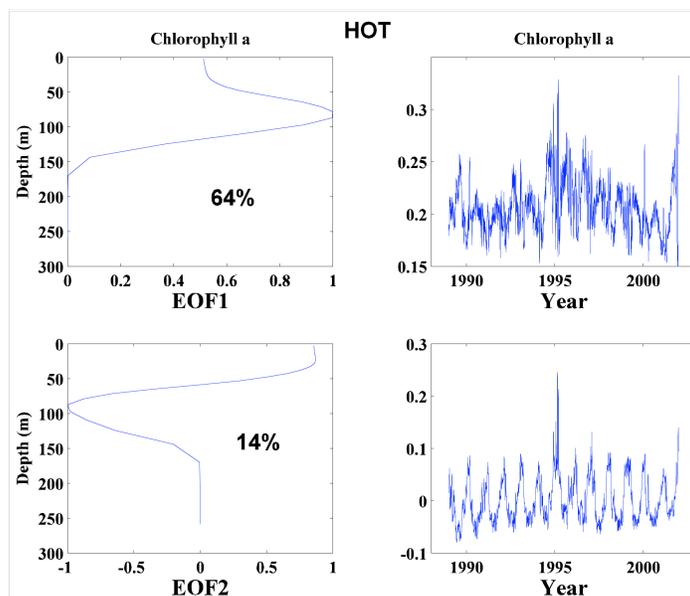


Figure 7. First two leading EOFs at HOT and time series of corresponding amplitudes.

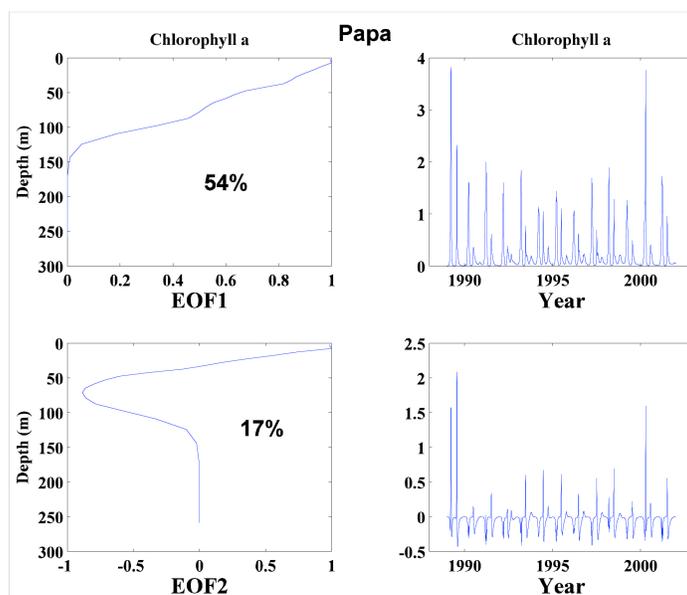


Figure 8. First two leading EOFs at OSP and time series of corresponding amplitudes.

In addition to the Kalman filter approach, we have written the adjoint code of the Spitz et al. (2001) ecosystem model for 1D and 3D assimilations. This code has been fully tested using twin experiments in 1D mode. Experiments in 1D mode with observations at the HOT station are being undertaken.

- **Data Mining**

An important sub-component of our Activity 2 is data mining in support of the PARADIGM modeling activities (Task 2.1). These efforts have a direct impact on our ecosystem modeling activities, either through direct accounting of processes or parameterization of those within our global, basin-scale, and regional models. Field programs (not supported by PARADIGM) continue to provide important data sets for scrutiny with PARADIGM objectives in mind. During the past year we continue to evaluate the relationships between microbial community structure, in situ function and rates and controls of biogeochemical cycling in the North Pacific Subtropical Gyre. This work includes data and information synthesis, mostly from Station ALOHA, as well as new laboratory and field experimentation (again, not directly supported by PARADIGM) designed to evaluate the ecophysiology of key microbial groups, and to test hypotheses regarding key ecosystem processes. Significant progress has been made in two related areas: (1) N and P cycling, especially the role of P in structuring oligotrophic marine ecosystems, and (2) the net metabolic balance of the sea.

With regard to P, three related papers and a major review article have been published. The first was a laboratory study of the elemental composition of *Prochlorococcus* and *Synechococcus*- the two dominant photoautotrophs in low nutrient marine ecosystems worldwide- under P-sufficient and P-limited conditions (Bertilsson et al. 2003). Contrary to expectation, neither species grows in the laboratory with the expected “Redfield” C:N:P stoichiometry, even under nutrient replete conditions. Furthermore, the quotas of C, N and P in these cells appear to be flexible, with especially low P requirements. In fact based on the measured P cell quota and the known P requirement for its genome, *Prochlorococcus* appears to invest about >50% of the cell P for DNA leaving very little P remaining for other structural (phospholipids, RNA) and metabolic functions. We hypothesize that this low P cell quota may be an important strategy of this species for slow growth in a nutrient poor environment, and if so would have ecological implications ranging from grazing to viral lysis. This is an initial report of an ongoing collaboration with Sallie Chisholm (MIT). In a previous study of P concentrations in the North Atlantic, Wu et al. (2000) hypothesized that the order of magnitude lower dissolved inorganic P (DIP) content of the N. Atlantic gyre relative to the North Pacific gyre was a result of a higher dust (and therefore Fe) deposition in the N. Atlantic. The Fe-induced drawdown of DIP is a result of enhanced bacterial nitrogen fixation. Near Hawaii the near surface DIP is about 10-30 nM whereas south of Bermuda the values are <1 nM (Cavendar-Bares et al. 2001). This Fe-control of DIP hypothesis was tested by conducting an investigation of the South China Sea. We predicted that since the South China Sea was much closer to the dust (Fe) source in China, it should look more like the N. Atlantic (subnanomolar DIP) than the N. Pacific. The field results failed to support this hypothesis (Wu et al. 2003), and we presented several alternative hypotheses regarding the intersections of Fe deposition, bacterial nitrogen fixation and DIP cycling.

This work is continuing. Finally, we have investigated the simultaneous utilization of dissolved organic P (DOP) and DIP in waters near Sta. ALOHA. Our results indicate that the biologically active pool of P greatly exceeds the measured DIP pool, by about a factor of two (Bjorkman and Karl, 2003). This indicates an important role for the very large and mostly uncharacterized pool of DOP in the sea (near Hawaii DOP exceeds DIP by nearly an order of magnitude). This work is ongoing. Our next challenge is to determine if there is simultaneous usage of both pools by all (or most) organisms, or whether there is a resource partitioning in the plankton with some groups using exclusively DOP while others use DIP. A major review article on the subject of DOP has recently appeared (Karl and Bjorkman, 2002).

There has been a recent and very lively discussion over the past two years regarding the metabolic balance of the sea (summarized by del Giorgio and Duarte, 2002). This topic of discussion is central to any marine ecosystem modeling program. We decided to conduct some field experiments and have recently begun to contribute our own, new views to this ongoing controversy (Karl et al. 2003; Williams et al. 2004). This is ongoing work that is germane to the stated PARADIGM mission.

We have also “mined” the available physiological, ecological and distributional literature for tropical copepod species for developing a Lagrangian particle model that will be useful in our modeling hierarchy. A fundamental question regarding marine copepods in tropical oceans is how the many species exist, co-exist, and persist within an environment characterized by dilute phytoplankton concentrations. During the past year we have addressed this question by developing a three-dimensional Lagrangian particle model that includes explicit parameterization of feeding and behavioral dynamics of four abundant copepod species found in tropical waters: *Clausocalanus furcatus*, *Paracalanus aculeatus*, *Oithona plumifera*, and *Oncaea mediterranea*. These species employ diverse prey acquisition strategies that have been sufficiently characterized by observational studies to develop species-specific parameterizations of translational ambits and grazing attributes. In addition to the individual copepods, the model tracks individual phytoplankton and phytoplankton aggregates, where the motion of each particle consists of a combination of sinking, a random component meant to emulate isotropic turbulence, and active swimming (where applicable). Results from single copepod experiments demonstrate that the model successfully simulates observed prey acquisition and feeding rates. This single copepod framework is also used to explore sensitivities to various characteristic movement behaviors, such as somersaulting and jumping.

In the remainder of this subsection the PARADIGM funding complements the funding from the NASA Biogeochemistry Program, which supported a major portion of the work discussed next. There are two major activities here related to the goals of PARADIGM: a study of the mid-ocean gyres using time series of satellite ocean color data, a global study of the influence of wind climatologies and gas transfer algorithms on the sea-air CO₂ exchange.

(1) Seasonal and Interannual Variability of North Atlantic and North Pacific Gyres

Ecosystem indicators in the subtropical gyres, such as biomass (e. g., chlorophyll concentration) and new and export productions, respond to long-term trends in climate variability [Karl et al., 2001; Oschlies, 2001]. This physical-biological coupling between the climate cycles and ecosystem dynamics is a consequence of altered nutrient flux pathways that result from changes in the stratification and circulation of the subtropical gyres. Seasonal and interannual variability in the areal extent of the subtropical gyres were examined [McClain et al., 2004] using 8 months (November 1996 - June 1997) of Ocean Color and Temperature Sensor (OCTS) and 6 years (September 1997 - October 03) of Sea-viewing Wide Field-of-View Sensor (SeaWiFS) ocean color data. Although the available ocean color record is still very short to unequivocally correlate climate variability indices to observed trends in biomass, some consistent patterns are emerging. Figure 9 shows the time series of the size of the five mid-ocean gyres. The seasonal range is significant for all gyres and all gyres display systematic trends. The North Pacific and North Atlantic gyres have the largest upward trends, 3%/yr and 4%/yr, respectively. Curry and McCartney [2001] show evidence that variability in the intensity of the North Atlantic gyre circulation is related to the NAO. The transport index, derived from the differences in potential energy anomaly between the central Labrador Basin and Bermuda, showed significant decadal variability related to the NAO. There was also an upward trend in transport during 1970-1995 of 0.8 Sv (20 Sv/25 years), which translates into 1.6%/yr increase in the strength of the gyre. This transport trend is consistent with the upward trend in the fractional size of the oligotrophic waters inside the North Atlantic gyre found in this analysis. The upward trend in the size of the oligotrophic region (4.1%/yr) is accompanied by a 2.7%/yr reduction in chlorophyll concentration and a 0.5%/yr increase in dynamic height inside the gyre [McClain et al., 2004]. These trends imply a coupling between the gyre circulation and upper-ocean nutrient supply, although the two studies do not overlap in time. The positive state of the NAO reflects changes in wind pattern as well as strength. The NAO plays a role in modulating interannual hydrographic and biogeochemical variability. In the Sargasso Sea, there are oceanic responses to the NAO forcing characterized by changes in vertical mixing, subtropical gyre circulation, and mesoscale eddy frequency [Bates, 2001; Williams et al., 2000]. The positive state of the NAO index in the 1970s and 1990s reflect enhanced midlatitude westerlies, with related shifts in air-sea exchanges of heat, freshwater, and momentum [Curry and McCartney, 2001].

(2) Seasonal Variability of Sea-Air CO₂ Flux A global study of the seasonal variability of sea-air CO₂ flux was conducted with emphasis on its dependence on climatological wind speeds and gas transfer algorithms. In this report, the results for the North Pacific and North Atlantic are contrasted with the other global ocean regions. As shown in Figure 10, the Southern Ocean has the largest seasonal cycle with a peak in ocean uptake during January-February (-1.1 to 2.9 Gt/yr).

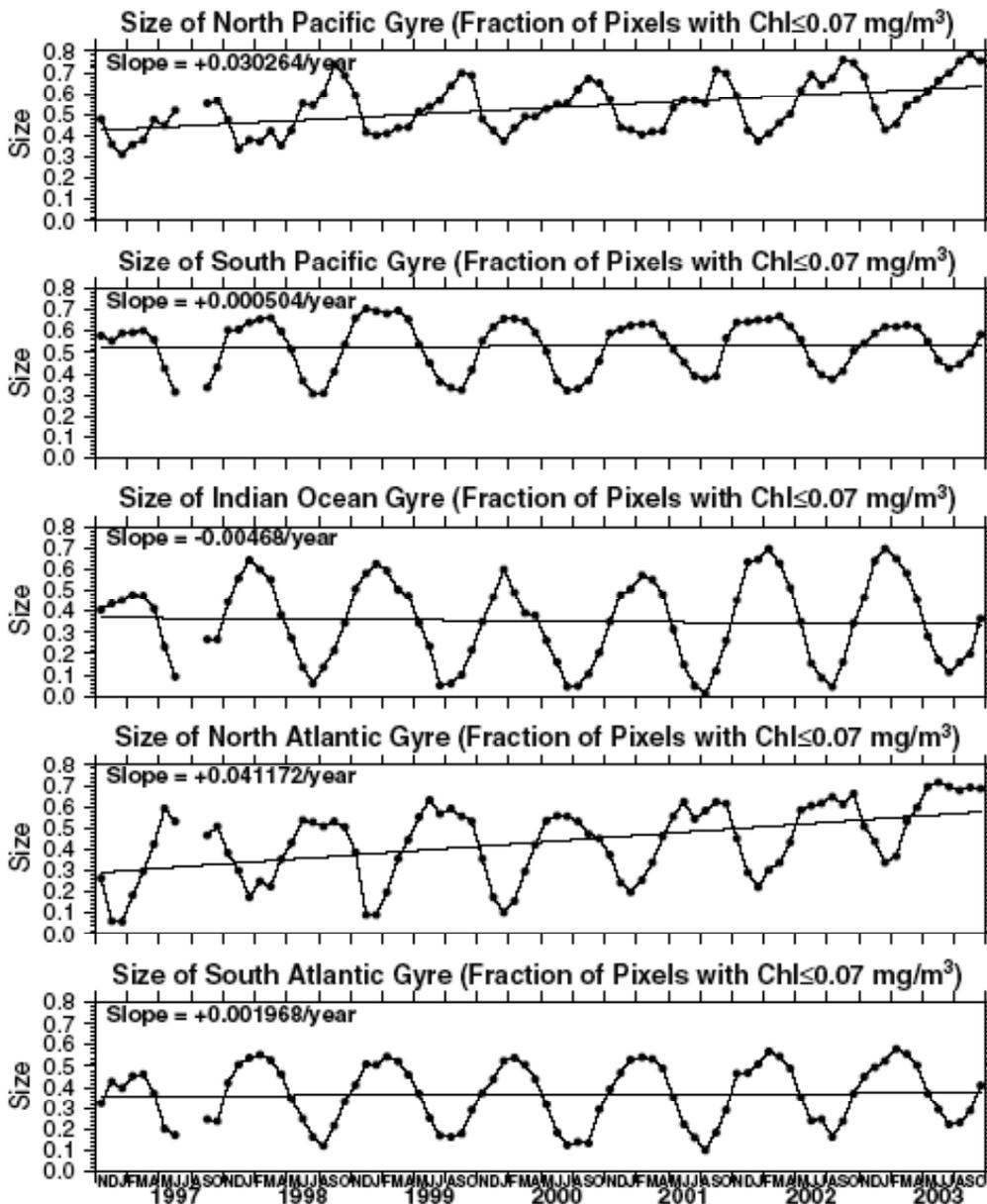


Figure 9. Time series of the fractional size of the oligotrophic areas (chl , 0.07 mg m^{-3}) inside the North Pacific, South Pacific, Indian Ocean, North Atlantic, and South Atlantic subtropical gyres. The values were derived from OCTS (November 96 – June 97) and SeaWiFS (September 97 – October 03) data. The linear trends are superimposed on each plot and represent seven complete years of data (November 96 – October 03).

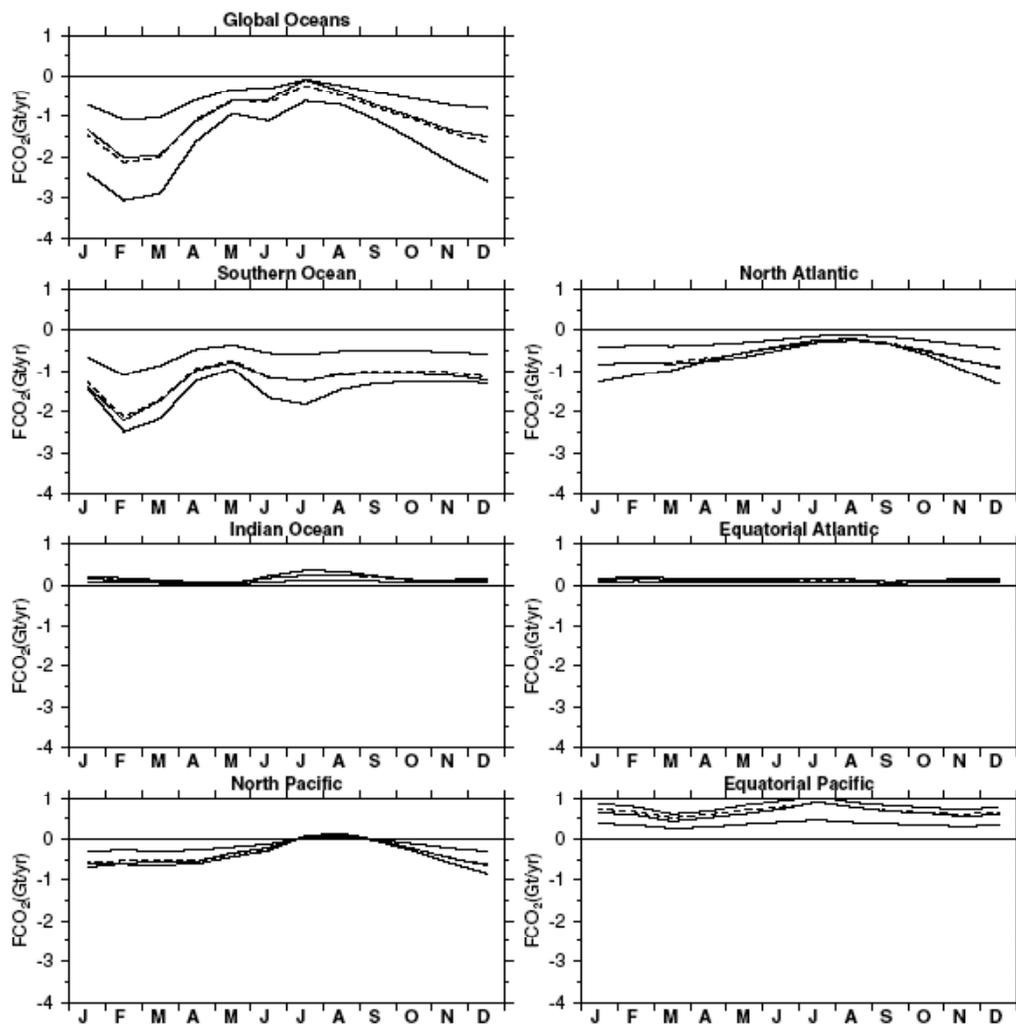


Figure 10. Seasonal variability of air-sea CO_2 flux derived with SSM/I winds for the global oceans and six different oceanic regions. The four separate lines, solid, dashed, dotted, and thick, solid, represent the Liss and Merlivat (1986), Wanninkhof (1992), Tans et al. (1990), and Wanninkhof and McGillis (1999) algorithms, respectively.

The North Atlantic and North Pacific Oceans have a reduced seasonal cycle, with strongest uptake during fall-winter and nearly neutral conditions during the summer months. These regions have small outgassing (North Pacific) or small ingassing (North Atlantic) of CO_2 during the summer months because the potentially high pCO_2 values due to elevated SST conditions are counterbalanced by an increased pCO_2 drawdown by biological activity. The Indian Ocean, equatorial Pacific, and equatorial Atlantic have no distinctive seasonal cycle. Our global CO_2 flux estimates agree reasonably well with the estimates of Takahashi et al. [1997] using Esbensen and Kushnir [1981] winds. Their estimates using the Liss and Merlivat [1986], Wanninkhof [1992], and Tans et al. [1990]

gas transfer algorithms are -0.71, -1.14, and -1.34 Gt/yr, respectively. Our equivalent estimates are -0.65, -1.28, and -1.22 Gt/yr. Lefèvre et al. [1999] compiled quarterly maps of $\Delta p\text{CO}_2$ interpolated from $p\text{CO}_2$ measurements in the North Atlantic and the North Pacific Oceans. Their estimates of the CO_2 flux for the Northern Hemisphere north of 10°N using SSM/I winds and the Liss and Merlivat [1986], Wanninkhof [1992], and Tans et al. [1990] algorithms are -0.45, -0.70, and -0.86 Gt/yr, respectively. Our equivalent estimates are -0.52, -1.02, and -1.08 Gt/yr. Lefèvre et al. [1999] estimates using Esbensen and Kushnir [1981] winds and the same three gas transfer algorithms are -0.37, -0.60, and -0.76 Gt/yr, respectively. Our equivalent estimates are -0.50, -0.98, -1.03 Gt/yr. Overall, our estimates are 15% to 35% higher than those of Lefèvre et al. [1999]. Since we used $p\text{CO}_2$ data based on Takahashi et al. [1997], and Lefèvre et al. [1999] used revised $p\text{CO}_2$ maps based on additional observations, we attribute our CO_2 flux overestimates to the different $p\text{CO}_2$ data sets used for the estimates.

- **Numerical Methods**

Task 6.4 is designed to examine the accuracy and competitiveness of performing biogeochemical model simulations “offline” at high resolution, and we are ahead of schedule on this task. We compared “online” and “offline” simulations of a point source tracer in the context of a $1/6$ degree resolution North Atlantic circulation model. We find the computational cost of the offline method (in terms of CPU clock time) to be about an order of magnitude less than online calculations even with very high temporal resolution in the stored flow fields (6 hourly). A manuscript (Jones et al., 2003) is in preparation.

Finally, in support of our program’s computer visualization component (Task 6.3), we have developed significant advances to the Vis5D+ OpenGL-based visualization program for scientific datasets in 3+ dimensions that improve utilization for viewing data intensive coupled bio-physical models. These improvements will be submitted for public use in the summer of 2004.

VI. IMPACT/APPLICATIONS

PARADIGM will develop new community models of ocean biogeochemistry and ecology on global scales, comprising complex ecosystem dynamics based on functional groups (e.g., *Archaea*, diatoms, copepods, gelatinous predators), individual keystone species (e.g., *Trichodesmium*, *Euphausia superba*) and multi-element limitation and cycling (e.g., C, N, P, Si, Fe). These models will include new parameterizations of mesoscale and submesoscale processes that are especially important in biological/physical coupling. Data assimilation and data fusion will be used to improve model formulation and to validate model performance. New approaches to software development will be used to simplify the addition of new ocean processes. The models will be capable of emergent behavior, testing the hypothesis that fundamental domain shifts occur in response to climate change.

PARADIGM will improve linkages between modelers and field oceanographers by creating an environment where model assumptions can be explored, model performance rigorously evaluated, and new ideas and hypotheses formulated and tested. Through

regular interactions, data visualization, and focused workshops, PARADIGM will serve as an intellectual hub for the study of ocean ecology and biogeochemistry with numerical models as the tool. By making such models more transparent to the non-modeler, we will enable the study of complex, global-scale processes in a rigorous open manner.

VII. TRANSITIONS

To benefit from relationships outside our consortium, a fundamental objective will be *to make all of our research widely available to the scientific community*, both through traditional mechanisms (e.g. workshops) and innovative modes of communication (web-based interactive exchanges). Two important events that will take place near the end of the second year of PARADIGM (the ASLO/TOS PARADIGM special session) and into the third year of the program (a special issue of Progress in Oceanography devoted to PARADIGM and PARADIGM-related research) demonstrate how serious we take this objective. This responsibility will also include the distribution of forward model and data assimilation products, computational algorithms, etc. through workshops, summer schools, etc. For that, we have established a PARADIGM web site (<http://www.gso.uri.edu/paradigm/>).

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