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Eastern U.S. Continental Shelf Carbon Budget: Integrating Models, Data Assimilation, and Analysis

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The U.S. East Coast Continental Shelf (USECoS) project was initiated in 2004 with the overall goal of developing carbon budgets for Mid-Atlantic and South Atlantic regions of the eastern U.S. coast. We addressed this goal through a series of specific research questions that were designed to understand carbon inputs and fates in the two regions, dominant food web pathways for carbon cycling, and similarities/differences in carbon cycling in the two continental shelf systems. The USECoS project represents a major effort to simultaneously synthesize and integrate diverse data sets, field measurements, models, and modeling approaches. We expect that the type of approach taken here will result in more insight than would be possible if each component of the program moved forward independently. The primary significance of this project is in providing a strong quantitative basis for the development of future observational and modeling studies of carbon budgets of continental shelf systems. A strong aspect of the USECoS project is the integration of modeling and extensive physical, chemical, and biological data sets, which provides an opportunity for modeling and data analyses to inform one another from the outset. This research is particularly germane to NASA's carbon cycle research focus and coastal research initiative and the U.S. Climate Change Research Program, all of which support the goals of the North American Carbon Program. We highlight primary approaches that have been used, and some of the challenges and results that have come from interactions among our team of investigators. The global scale and interdisciplinary nature of the science questions that we now face in Earth Science are such that integrated teams of investigators are needed to address them.

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The past two decades have seen the development of large multidisciplinary oceanographic programs with a focus on understanding carbon cycling processes in coastal and oceanic environments. Synthesis and modeling activities typically followed towards the end of these programs (e.g., Joint Global Ocean Flux Study), usually long after the field experiments had been planned and carried out. A lesson from these programs that has been articulated in subsequent community planning reports (e.g., the Ocean Carbon Transport, Exchanges and Transformations (OCTET) and Ocean Carbon and Climate Change (OCCC) reports) is that future ocean carbon cycle research programs should promote close collaborations among scientists with expertise in measurement, data analysis, and numerical modeling at every stage of development: formative stages of hypothesis building, planning and execution of field programs, data analysis, numerical modeling, and synthesis.

The advantages of this collaborative approach for numerical model development are clear: data are collected with algorithm development in mind, and quantitative models are based on the best current understanding. But there are distinct advantages for

observational and experimental programs as well. Collaborations with numerical modelers allow the analyst to see data in a more holistic context, and thus to understand better what other parameters should be measured and modeled as well as understand better the inherent limitations and uncertainties in the modeling approaches. That collaboration of modelers and analysts results in better model construction with justifiable assumptions and in more appropriate data selection has been recognized for some time (e.g., Walsh, 1972) and has been re-emphasized by recent discussions of approaches for development of marine biogeochemical and ecosystem models (e.g., Doney, 1999; Doney et al., 2001; Flynn, 2005; Anderson, 2005). For an analytical measurement where no standards exist, it may be only through sensitivity studies with numerical models that the analyst can predict what the values of certain parameters are likely to be. Modeling and data-intensive programs often have the same goals, but they bring different tools to bear. The box models and statistical techniques common to data analyses are part of the quantitative view of data. But using *all* the methods available (e.g., empirical and deterministic approaches) will ensure greater progress towards the common goal of understanding large ecological systems.

We combined the expertise of modelers and empiricists in a collaborative project as part of the NASA Earth Interdisciplinary Science initiative. The U.S. East Coast Continental Shelf (USECoS) project was initiated in 2004 with the overall goal of developing carbon budgets for the Mid-Atlantic Bight (MAB) and South Atlantic Bight (SAB) along the eastern U.S. coast (Figure 1). We addressed this goal through a series of specific research questions that were designed to understand carbon inputs and fates in the two regions, dominant food web pathways for carbon cycling, and

similarities/differences in carbon cycling in the two continental shelf systems. The nature of the research questions required a team approach that included expertise in areas of remote sensing, oceanographic data analysis, numerical models including data assimilation, carbon cycling, and knowledge of the physics and biogeochemistry of the MAB and SAB. As a result, the team assembled for the USECoS project consists of a diverse group of science investigators, with varying degrees of experience in crossing disciplinary boundaries. This mixture of expertise and the interactions that have resulted has proven to be as important in successfully addressing the project goal as any infrastructure (e.g., computers), data sets, and numerical model codes that we used. However, the fruitful scientific collaborations have come with a steep learning curve.

Integrating results from different disciplines and expertise included using measurements from satellites, field studies, historical data, and one-dimensional data assimilative modeling. Simplified mathematical descriptions (parameterizations) were developed that captured the essential features of each disciplinary model; these were then implemented in the circulation and biogeochemical models used in this study (Figure 2). Satellite-derived data products were evaluated with field and historical data to ensure their accuracy; results of parameterization studies were incorporated into the circulation and biogeochemical models; simulation results (models run separately and coupled) were evaluated using a suite of approaches that included escalating statistical evaluations; and results of the evaluation phase were used to revise parameterizations. This iterative process of model improvement and evaluation continued until simulations were deemed sufficiently realistic, and thus ready to provide the basis for development of nutrient and carbon budgets and serve as a baseline for climate-related simulations.

This iterative approach (Figure 2) has worked well for the USECoS research program and provides the basis for the primary objective of this paper: to give insight into how collaborations between analysts and modelers have resulted in a stronger program that is yielding results that likely would not have been achieved otherwise. These collaborations are illustrated by examples of how model simulations and processes were evaluated using comparisons with historical *in situ* and satellite-derived data sets, quantitative statistical estimates of model skill, and data assimilation. The accompanying text boxes provide details of the Northeast North America (NENA) circulation (Box 1), biogeochemical (Box 2) and dissolved organic matter (DOM, Box 3) models, and satellite dissolved organic carbon (DOC) algorithm development program (Box 4) associated with the USECoS program.

This paper also demonstrates how the ongoing US ECoS program is enhancing our understanding of carbon cycling processes on the MAB and SAB continental shelves. This research is particularly germane to NASA's carbon cycle research focus and coastal research initiative and the U.S. Climate Change Research Program, all of which support the goals of the North American Carbon Program (Wofsy and Harriss, 2002). We highlight primary approaches that have been used, and some of the challenges and results that have come from interactions among our team of investigators. The global scale and interdisciplinary nature of the science questions that we now face in Earth Science are such that integrated teams of investigators are needed to address them. Thus, lessons we have learned provide insights and a way forward for future programs.

MAB AND SAB CIRCULATION AND PRODUCTIVITY PATTERNS

The continental shelf of the eastern U.S. is a relatively well-studied region of the ocean, providing abundant historical data for a first-order physical and biogeochemical characterization. Carbon cycling in the MAB and SAB continental shelves and upper slope has been studied for 30 years in a number of programs sponsored by the Department of Energy (DOE, 1970s and 1980s). Much of the DOE-sponsored work in the SAB is summarized in Atkinson et al. (1985), and some of the earliest studies using the Coastal Zone Color Scanner (CZCS) were conducted in collaboration with the DOE SAB program (Yoder et al., 1987; McClain et al., 1988). In the MAB, the Shelf Edge Exchange Processes (SEEP) experiments I and II (1983-1989) and the Ocean Margins Program (OMP) experiment (1994-1996) provided insight into biogeochemical processes, with major findings reported in special issues of *Continental Shelf Research* (1988, 8(5-7)), and *Deep-Sea Research II* (1994, 41(2-3); 2002, 49(20)). Yoder et al. (2001) used the entire 7.5-year CZCS data set to examine phytoplankton variability of the MAB and the SAB and showed noticeable interannual variability during 1978-1986.

From these past studies we know that the circulation dynamics and the productivity and chlorophyll fields in the MAB and SAB differ significantly. In the SAB the Gulf Stream flows along the outer edge of the shelf break (e.g., Lee and Atkinson, 1983); this flow produces shelf break upwelling with subsurface bottom intrusions and frontal eddies that have a strong effect on nutrient and plankton production (Yoder, 1985). The episodic forcing of the SAB by Gulf Stream-induced upwelling results in biological production that occurs in short-lived events (McClain et al., 1984), rather than in the more traditional spring/fall blooms that are observed in the MAB. In summer,

when SAB shelf waters are stratified and the Gulf Stream tends to be nearer the shelf break, the intrusions extend across the entire shelf and produce subsurface blooms that are not discerned in ocean color imagery. In winter, when shelf waters are well-mixed, satellite-derived ocean color distributions from the SAB show the episodic nature of the chlorophyll production in this region and suggest that it occurs in multiple sites along the outer SAB shelf.

In contrast to the SAB, the MAB has an outer shelf front and a slope sea, which separates the shelf proper from the Gulf Stream. The influence of the Gulf Stream on the MAB is through warm-core eddies that move southward along the shelf break (Evans et al., 1986). The shelf circulation in both systems is influenced by estuarine and riverine inputs and wind. In the MAB, the coastal flow is to the south with offshore flow at Cape Hatteras, where much of the flow is entrained into the Gulf Stream front. Cross-shelf exchange occurs along the entire shelf edge through meandering of the shelf-break front (Lozier and Gawarkiewicz, 2001), and is at times modulated by warm-core ring interactions (Ryan et al., 2001). Ocean color distributions from the MAB show an annual April-May spring bloom (Yoder et al., 2001), as well as extensive summer phytoplankton blooms adjacent to the MAB coast in some years. The differences between these two regions provide a strong basis for comparative studies between a continental shelf region that is strongly affected by oceanic forcing (SAB) and one in which buoyancy and wind forcing are more dominant (MAB).

The USECoS study is seeking to understand how carbon is introduced into the eastern U.S. continental shelf environment, how it is transformed and transported while resident on the shelf, and its ultimate fate. Our approach to these questions is to use

remote sensing data, especially ocean color imagery from the Sea-viewing Wide Field-of-View Sensor (SeaWiFS) and the Moderate Resolution Imaging Spectroradiometer (MODIS), a synthesis of *in situ* measurements, a coupled ocean biogeochemistry-carbon-circulation model configured for the MAB and SAB, and data assimilation studies.

MODEL-DATA FUSION

Model-data fusion embraces a number of approaches for integrating discrete observations into a modeling framework, ranging from simple model-data comparisons to more formal data assimilation methodologies such as constrained parameter optimization. We have had success with a number of these approaches because of the extensive and continual collaboration between our observational (*in situ* and satellite) and modeling science investigators.

Quantitative model skill assessment (Figure 2) is a significant activity in which all components of the USECoS team are engaged. From our collective experiences, this activity is frequently not a major component of multi-disciplinary team research. Simulations from the NENA model have been evaluated by comparison with *in situ* and satellite-derived data using a suite of statistical approaches of escalating rigor, including comparisons of spatial distributions, means, variance, two-dimensional histograms and other skill assessment methods, such as Taylor/Target diagrams which reveal seasonal timing/phase relationships. Overall spatial distributions of climatological means from the model should match those from *in situ* and satellite data with little bias; the model should also capture the dynamic range over seasonal time scales, as well as regional differences in the timing of minima and maxima such as spring and fall phytoplankton blooms. This diversity of model skill assessment methods has helped us identify seasons and regions

where model improvements are required. In addition, a one-dimensional data assimilative model has provided the basis for quantitative assessment of model processes, which furthers the development of a model with improved skill. Each approach is described below, and results from these provide the basis for evaluation of model processes.

1) Model Evaluation Through Historical Data Comparisons

We focused our historical data mining efforts on temperature, salinity, and dissolved oxygen measurements in the 2005 World Ocean Database (WOD, Boyer et al., 2006), selecting only those data that have been interpolated to standard levels and that passed all WOD quality control procedures. For our study region (Figure 1, excluding the Sargasso Sea), there are about 460,000 temperature profiles, 110,000 salinity profiles, and 20,000 oxygen profiles. The median year of the temperature station distribution is 1968; 90% of the profiles were made between 1946 and 1994; similar results apply to the salinity and oxygen data.

Using these data, we developed monthly mean climatologies of mixed layer depth (MLD), salinity, and dissolved oxygen anomaly (ΔO_2, departure from saturation) which were used to evaluate equivalent distributions constructed from our circulation and biogeochemical model (Figure 3). For example, our circulation model (Box 1) captures a number of the observed patterns in MLD such as: (1) large parts of the shelf and Georges Bank are well-mixed to the bottom in March; (2) in the MAB, MLD increases away from the shelf, sometimes exceeding 250 m, but then reaches a minimum of about 50 m within the extension of the Gulf Stream northeast of Cape Hatteras; (3) in September, the mixed layer is shallower and tends to deepen away from the continent, except for Georges Bank,

which, due to tidal mixing, is mixed to the bottom. The annual mean salinity distribution is also well simulated by the circulation model (Figure 3), showing the dominant pattern of increasing surface salinity with distance from shore, the large salinity gradient located near the shelf break, the low salinity on the Scotian shelf, and the high salinity in the Sargasso Sea.

Historical data analyses are also integral to the evaluation of the marine biogeochemical model (Box 2). Dissolved oxygen, particularly its departure from saturation, has long been used as a tracer for the cycling of organic carbon. We computed the oxygen anomaly using the WOD temperature, salinity and dissolved oxygen data, with a formulation for the saturation concentration (Garcia and Gordon, 1992), and compare it with the similar quantity obtained from the biogeochemical model (Figure 3). The model captures the overall pattern of the surface ocean oxygen anomaly, reproducing the observed supersaturation in early summer and undersaturation in early winter, with particularly large seasonal ranges inshore of the shelf break north of Cape Hatteras. The annual cycle in oxygen anomaly reflects the annual cycle in surface heat flux, net community production, and vertical mixing. Because the circulation model captures the annual cycle in MLD and salinity very well, model-data differences are most likely due to biogeochemical processes not yet represented.

2) Model Evaluation Through Satellite Data Comparisons

Satellite-model comparisons. We are also using a wide range of satellite-derived distributions (Figure 4, Table 1) to quantify and understand regional, seasonal, inter-annual, and climate-related variability of phytoplankton biomass and organic carbon production within the USECoS study area and to evaluate the performance of similar

products from the simulations with the coupled circulation-biogeochemical model. We have developed several new and simple metrics that characterize the natural cycles of major annual phytoplankton biomass and carbon production events. One example is the index of 'month of maximum satellite chlorophyll concentration' (Figure 4, lower panel), which was computed from a 9-year monthly SeaWiFS climatology. This reveals that the fall phytoplankton bloom (September and October) in northern Gulf of Maine is a more significant event in the annual cycle than the spring bloom. The peak chlorophyll is during January in the inner MAB shelf but during November in the mid-shelf, and during April along the outer MAB shelf and adjacent Slope Sea. On Georges Bank the annual chlorophyll peak occurs in April, except along the northern and southern flanks of the Bank, adjacent to the tidal mixing fronts, where the peak occurs in October-November. There is also a surprising degree of spatial heterogeneity in the timing of the annual peak in the SAB. Satellite data and simple metrics such as these reveal the relevant underlying biological oceanographic scales operating on the continental shelf and reveal important differences in processes among the SAB, MAB, Georges Bank, and the Gulf of Maine regions.

Comparisons of satellite-derived fields with equivalent fields from NENA show that the model captures the north-south gradient in sea surface temperature (SST, Figure 5A), shows the general north-south gradient in chlorophyll distribution, but underestimates concentrations in the SAB except in the mid-shelf (Figure 5B), and captures the spatial pattern in DOC concentration (Figure 5C). These comparisons provide a first order evaluation of model skill and highlight areas where model improvements are needed.

A cautionary note on estimating productivity from satellite data. The ability to estimate primary production from space (e.g., the Vertically Generalized Vertical Productivity (VGPM) model, Behrenfeld et al., 2005) enables the determination of phytoplankton carbon production for the world oceans with unprecedented temporal and spatial resolutions. Accurate measurement of euphotic zone chlorophyll *a*, sea surface temperature (SST), and Photosynthetically Active Radiation (PAR) are key elements of nearly all satellite ocean color-based primary productivity algorithms (Carr et al., 2006). In shelf water north of Cape Hatteras, the broad-scale seasonal and spatial patterns from the VGPM2a satellite-productivity model (a variation of the VGPM) are consistent with results based on *in situ* measurements (^{14}C-uptake) made during earlier surveys (O'Reilly et al., 1987). However, the SAB continental shelf poses a very unique challenge for satellite measurement of chlorophyll *a* and, consequently, primary production (PP) estimates because the episodic summer subsurface intrusions of nutrient-rich Gulf Stream waters onto the shelf significantly enhance biomass and carbon production below the depths 'visible' to passive satellite ocean color sensors, such as SeaWiFS and MODIS.

Vertically-integrated chlorophyll *a* and PP within 2 weeks after a large bottom intrusion event on the middle shelf in July 1981 reached 75 mg m^{-2} and 3 to 4 g C m^{-2} d^{-1}, respectively (Yoder et al., 1985). At the peak of the bloom, 80% of the water column PP occurred below the mixed layer and new PP (NO_3-supported) exceeded 90% of the total. Most of this production occurred below the mixed layer, as well as below the penetration depth (the inverse of the diffuse attenuation coefficient) of ocean color sensors, making it impossible to use satellite ocean color algorithms to observe the effects of these sub-surface blooms on SAB phytoplankton production (Signorini et al., 2005).

As an example, cross-sections of chlorophyll *a*, nitrate, and light penetration from a transect off St. Augustine, FL (Figure 6a) show pronounced intrusion effects. Below 20 m, where Gulf Stream intrusions enhance the nitrate concentration (Figure 6b), and sufficient light (1 to 10% of surface PAR, Figure 6c) is available for photosynthesis, biomass (Figure 6a) and carbon production (not shown) increase significantly towards the bottom. The subsurface bloom intensity varies from station to station in response to the magnitude of the nutrient enrichment originating from the intrusion.

The mean chlorophyll *a* concentration estimated from the CZCS-derived chlorophyll *a* summer composite for 1981 (Figure 6d) was 0.32 mg m^{-3} versus an *in situ* estimate of 0.45 mg m^{-3} for the St. Augustine section. Near the shelf edge, where *in situ* near bottom chlorophyll *a* concentrations were largest (> 5 mg m^{-3}), the satellite coverage was good, but provided no hint of the subsurface bloom. These results illustrate the need for more than one approach for estimating rates of carbon production by phytoplankton in continental shelf waters and highlight the importance of combining satellite-derived estimates with those from mechanistic models that can extend measurements to deeper waters.

3) Model Evaluation Through Taylor/Target Diagrams

In addition to side-by-side comparisons of model-data contour plots and time series of selected simulated and observed quantities at specific depths and locations, we are applying more quantitative measures, such as Taylor and Target diagrams, to assess model skill. The Taylor diagram (Taylor, 2001) is used to quantitatively compare three statistics of the simulated and observed time series for a parameter (e.g., SST or chlorophyll in Figure 7) in a given region: the centered-pattern root-mean-square

difference of a parameter (plotted as the distance between the origin and each model symbol), the normalized standard deviation of that parameter (the radial distance from the origin), and the correlation of that parameter (the theta angle from the x-axis). Bias information can also be included through the use of colored symbols.

Taylor diagrams (Figure 7) illustrate that the simulated SST time series are well correlated with satellite SST data (with a correlation coefficient of roughly 0.9), and have nearly the same variance as the observations in each of our 58 study sub-regions (Figure 1). Not surprisingly, the model-data differences for chlorophyll are higher than for SST, with correlations rarely exceeding 0.5. In addition, the model consistently underestimates the surface chlorophyll variance in the SAB. These Taylor diagrams are proving to be extremely useful in our model development efforts, as they can quickly illustrate where and to what degree our revised model formulations are improving or degrading our model-data fit.

In Target diagrams (Joliff et al., 2007; Friedrichs et al., 2007a), bias and centered-pattern RMS are normalized by the standard deviation of the observations and plotted on the x- and y-axes, respectively (Figure 8). Because the sum of the squares of these two components of the RMS difference is equal to the square of the total RMS difference, the distance from the origin to each plot symbol represents total RMS error. Thus in this diagram, unlike the Taylor diagram, it is easy to visualize the relative magnitudes of the two components of RMS error, i.e., the bias and variability RMS errors.

Target diagrams for SST illustrate that these components of the total RMS error are typically of equal magnitude, which is not the case for chlorophyll, where total RMS error is primarily due to bias: simulated chlorophyll fields underestimate SeaWiFS-

derived chlorophyll, particularly in the SAB and in inshore MAB regions (Figure 8). In addition, the surface chlorophyll fields are biased low when compared with climatological satellite data; this bias is cut in half when the simulated fields are compared with 2004 data instead (Figure 8).

4) Model Refinement Through One-dimensional Data Assimilation

Another approach taken to incorporate discrete observations into the NENA framework and to quantitatively assess model skill is the variational adjoint method (Friedrichs et al., 2006; 2007b). Due to our incomplete knowledge, biogeochemical models are often by necessity highly empirical, have many non-mechanistic formulations, and include numerous parameters that are difficult to measure with current oceanographic instrumentation. Data assimilation techniques such as the variational adjoint method (Hofmann and Friedrichs, 2001) provide an approach for objectively estimating the best-fit set of model parameters and their associated uncertainties (Fennel et al., 2001). These methods can be used to compute sensitivities and correlations between parameters and assess predictive abilities of a given model (Friedrichs et al., 2006) and are thus a crucial component of successful marine biogeochemical modeling studies.

We are currently making use of an existing one-dimensional data assimilative ecosystem-modeling framework that has been recently developed to quantitatively compare the performance of 12 models characterized by varying levels of ecosystem complexity (Friedrichs et al., 2007a). When used in conjunction with the three-dimensional NENA model, which provides the horizontal advection terms, vertical velocity, MLD, PAR, and temperature, this framework closely reproduced the 3D fields and yielded optimal values of maximum phytoplankton growth rate, remineralization

rates, C:chl ratios, and other key parameters (Fig. 9). Since this framework includes the flexibility of assimilating remotely sensed ocean color and/or *in situ* data simultaneously from multiple sites, the best-fit set of parameter values could be obtained over multiple regions (Friedrichs et al., 2007a). Data could also be assimilated from numerous individual locations (Friedrichs et al., 2006), which reveals whether certain optimal parameter values and their associated uncertainties vary in space and/or time.

EVALUATION OF MODEL PROCESSES

In addition to using historical data sets to evaluate distributions of various concentrations predicted by our models, we also evaluated process mechanisms. For example, it is known that DOM represents the largest pool of organic carbon on the MAB shelf and may thus play a significant role in carbon cycling and transport. Furthermore, under nutrient-depleted conditions, nitrogen and carbon primary production are partially decoupled, the DOM produced is carbon-rich and thus may represent a significant source of organic carbon (Williams, 1995), which can be exported to the open ocean (Bauer and Druffel, 1998; Vlahos et al., 2002). To investigate this aspect of shelf carbon cycling, we included semi-labile dissolved organic carbon and nitrogen (semi-labile DOC and DON) in our biogeochemical model (Box 3). The inclusion of explicit DOM dynamics allows investigation of its role in biological production and carbon cycling in the MAB and SAB in conjunction with physical transport, which is difficult to do with just observations.

Analysis of our model predictions allowed us to assess the relative importance of DOM production and transport through advective and eddy-diffusive mechanisms. The simulated annual horizontal divergence of semi-labile DOC shows areas of production and export (negative values) on the continental shelf and slope and areas of import

(positive values) in the open ocean (Figure 11A). Most shelf areas can export about 1 mol C m^{-2} yr^{-1} through the seasonal production of marine semi-labile DOC to the open ocean.

It has been suggested that the U.S. northeastern continental shelf is an important site for Particulate Organic Matter (POM) burial (Thomas et al., 2002). In order to compare the magnitudes of burial of POM with the horizontal export of DOM to the open ocean, we added to the biogeochemical model a parameterization mimicking POM resuspension and burial. Resuspension rate of the POM flux reaching the sea bed was specified as a function of the bottom friction velocity. The fraction of resuspended POM is thus largely dependent of the local near bottom current velocity associated with the general circulation, tidal currents on the continental shelf, and wind-driven events in shallow waters, and further couples the physical and biogeochemical models. We used carbon and nitrogen burial to simulate the accumulation of material in the sediment, assuming that the burial efficiency of the particulate organic carbon is proportional to the vertical flux of POC reaching the seabed (Henrichs and Reeburgh, 1987). We estimated the burial efficiency for PON using a C to N ratio of buried organic matter of 9.3; values of 9-10 have been found for shelf and estuarine surface sediments and slightly lower values in deeper waters (Gelinas et al., 2001). The model gave burial rates of POC in the sediments (Figure 11B) that agreed well with estimates by Thomas et al. (2002) of 0.1-0.2 mol C m^{-2} yr^{-1} in the slope off Cape Cod, 0.5-1.0 in the Mid-Atlantic Bight, and 0.02-1.7 in the slope off Cape Hatteras. The main gradients of model organic carbon burial extended from 2 mol C m^{-2} yr^{-1} in shallow water (inner-shelf) to 0.2 mol C m^{-2} yr^{-1} on the outer-shelf.

Comparison of simulated POC burial and horizontal flux of semi-labile DOC (Figure 11) show that POC is efficiently buried in the inner- and mid-shelf while the mid- and outer-shelf export seasonally-produced DOC to the open ocean at comparable rates. This simple parameterization gives us the opportunity to assess the importance of these processes quantitatively in our coupled circulation-biogeochemical model. Our results suggest that the inclusion of a more comprehensive sediment transport and transformation model (Warner et al., submitted) should be an important future focus in model refinement.

CONCLUDING REMARKS

The USECoS project represents a major effort to simultaneously synthesize and integrate diverse data sets, field measurements, models, and modeling approaches. We expect that the type of approach taken here will result in more insight than would be possible if each component of the program moved forward independently. The primary significance of this project is in providing a strong quantitative basis for the development of future observational and modeling studies of carbon budgets of continental shelf systems. A strong aspect of the USECoS project is the integration of modeling and extensive physical, chemical, and biological data sets, which provides an opportunity for modeling and data analyses to inform one another from the outset.

The extensive collaboration between the *in situ* and satellite data analysts and modelers has improved our parameterizations and formulations for both the circulation and biogeochemical models, as well as identified areas where improvements in satellite algorithms may be needed (e.g., primary production). The example of estimating primary production in SAB shelf waters resulting from bottom intrusions highlights the need for

coupled numerical circulation-biogeochemical models capable of providing accurate estimates of primary production in continental shelf waters, especially since the SAB is not the only continental shelf system where much of the primary production is at depths greater than can be seen by ocean color satellites (e.g., Prézelin et al., 2004). However, model development should be in conjunction with *in situ* measurements of primary production made with current technology to provide rigorous evaluations of the model-derived estimates, similar to the approaches used in this study. This may not be an easy task to accomplish under the current funding limitations, but coordinated model-data efforts are needed if reducing uncertainties is a goal.

Empirical observations of process measurements such as primary production of POC and DOC, benthic primary production, remineralization rates of DOM, solubilization and remineralization of particles, burial efficiency in shallow and deep waters, and grazing-related release of DOM are critical to improving biogeochemical models as model complexity increases. Model evaluation is usually focused around measurements of concentration and biomass (cf. Figures 4,5,7,8), but model development needs measurements of rates and processes. For example, few rate measurements were available to constrain the processes included in the DOM component of NENA. The available data sets allow autotrophic processes in the NENA region to be fairly well constrained, but there are few direct measurements of heterotrophic processes, such as the processes involved in decomposition of organic matter. The coastal ocean is one place where heterotrophic processes are large enough to be measured. Without such measurements, models such as NENA will continue to include ill-constrained parameters, which results in a trial-and-error approach for developing model parameterizations and

processes, thereby limiting model skill. However, the measurements and biogeochemical model development are not independent and should progress together to ensure realization of the full benefit of each.

A primary conclusion from the approach taken in this study is that a well-coordinated interdisciplinary team with skills in field measurements, remote sensing, and modeling focused on a single coupled circulation-biogeochemical model is an effective means of addressing important and complex issues, such as carbon cycling in marine ecosystems. The focus on a single model forces the team to resolve issues and reconcile differences of opinion, i.e., a disciplined approach, rather than simply going in different directions, as can happen with a focus on more than one model.

A research team composed of members from multiple institutions, like the USECoS team, does at times hinder progress. However, a team that is dispersed may be unavoidable in achieving the desired balance of expertise. Maintaining progress requires a commitment from each team member to interactive collaborations and there is a trade off between having a critical mass and having a team that is too large to manage. A large team can lead to development of smaller groups focused on specific research problems which do not foster collaborative interactions. Many factors must come together to make a successful program (NRC, 2005) and for the USECoS program a focus on one model and common goals has allowed the overall effort to be more than the sum of the individual components.

BOX 1: Circulation model description

Realistic simulation of the circulation on the MAB and SAB continental shelves is fundamental to realizing the objectives of the USECoS program and considerable effort

has been directed at achieving acceptable simulations. The circulation model used is the Regional Ocean Modeling System (ROMS) (Shchepetkin and McWilliams, 2005; Haidvogel et al., 2007; http://myroms.org) configured for the same Northeast North America (NENA) spatial domain of Fennel et al. (2006). The model has 10 km horizontal resolution, 30 vertical levels, and is embedded within the *HY*brid *C*oordinate *O*cean *M*odel (HyCOM, http://hycom.org) North Atlantic data assimilative model (Chassignet et al., 2007). The HyCOM open boundary transports are augmented by barotropic tides from a global analysis (Egbert and Erofeeva, 2002). Coastal freshwater inputs have annual mean values from a watershed analysis (Seitzinger et al., 2005) modulated by average monthly variability observed at USGS gauged rivers. Air-sea fluxes are calculated using bulk formulae (Fairall et al., 2003) applied to daily reanalysis air temperature, pressure, humidity and winds. All tracer advection is by the positive definite MPDATA scheme which is important to accurately representing biogeochemical model constituents.

The embedding procedure imposes external remotely-forced mesoscale and seasonal variability, but to achieve realistic mean circulation in shelf waters it proved critical to correct biases in the temperature and salinity provided by the HyCOM North Atlantic model. A simple correction procedure – supplanting the HyCOM temporal mean temperature and salinity with values from the Hydrobase climatology (Lozier et al., 1995) – was devised that substantially improved the simulation of buoyancy-driven southwestward mean flow throughout the Gulf of Maine and Mid Atlantic Bight. Improvements to the properties of slope water adjacent to the South Atlantic Bight (which enters the NENA domain from the Intra-American Seas) were also noted.

The simulations exhibit well recognized features of the local and remotely-forced circulation: low salinity on the MAB inner shelf, the tidal mixing front and residual circulation around Georges Bank, Gulf Stream intrusions in the SAB, and interactions of Gulf Stream warm rings with the New England slope. Comparisons of the modeled circulation and tracer fields to observations show progress over the simulations of Fennel et al. (2006) due principally to the introduction of tides and unbiased open boundary data. Features that are the focus of on-going study are exaggerated upwelling of anomalously cold water in the South Atlantic Bight, intermittent overshoot of the Gulf Stream at Cape Hatteras, and a weak Slope Sea gyre. Model development is investigating whether higher spatial resolution is required to improve these aspects of the simulation.

BOX 2: Biogeochemical model structure

We simulate ecosystem processes in the MAB and SAB with a modified version of the Fasham et al. (1990) model that is incorporated into ROMS (Fennel et al., 2006). In our ROMS implementation we distinguish the two inorganic nitrogen species, nitrate and ammonium; include chlorophyll as a prognostic variable in addition to phytoplankton biomass; distinguish two size classes of detritus to allow for different settling rates; and include explicit DOM dynamics described in detail in Box 3.

It is important to note that none of the biological models available in ROMS explicitly represents diagenetic processes at present. However, the inclusion or at least the parameterization of diagenetic processes is important for coastal applications because a major fraction of nutrient remineralization occurs in the sediment. In our application of the Fasham-type model to the east coast continental shelves (western North Atlantic) we use a relatively simple representation of benthic remineralization processes where organic

matter settling out of the bottom-most grid box results in a corresponding influx of inorganic nutrients at the sediment/water interface (Fennel et al., 2006). This formulation conserves mass by assuming immediate equilibrium between particle deposition and influx of dissolved constituents from the sediment. Soetaert et al. (2000) showed that this intermediate complexity approach captures most of the dynamics inherent in benthic-pelagic coupling when compared to coupling with a diagenetic sub-model but is computationally much more efficient. This approach also allows for the straightforward inclusion of processes such as sediment denitrification (Fennel et al., 2006) using the relationship between sediment oxygen consumption and denitrification derived by Seitzinger and Giblin (1996).

We also included inorganic carbon and oxygen dynamics in our biogeochemical model for the MAB and SAB. Aside from physical transport (i.e., advection and mixing) the local concentration of dissolved inorganic carbon, DIC, and oxygen is affected by gas exchange with the atmosphere at the sea surface and by sources and sinks due to biological processes such as the photosynthetic synthesis of organic matter or its metabolic or microbial oxidation. We describe the sources and sinks due to biological processes based on stoichiometric ratios and parameterize gas exchange as suggested by Wanninkhof (1992). The gas exchange of oxygen depends on the temperature and salinity-dependent oxygen solubility (Garcia and Gordon, 1992) and the piston velocity. For the air-sea gas exchange of carbon dioxide the situation is more complicated because gas exchange does not directly depend on the concentration of DIC but rather on the small fraction of DIC that is present as carbon dioxide (carbon dioxide does not just dissolve in seawater, but reacts with water to form carbonic acid which subsequently

dissociates into bicarbonate and carbonate; the sum of all three makes up DIC). Only the small fraction DIC that is present in form of carbon dioxide determines the partial pressure, pCO_2, which enters the parameterization of gas exchange. Calculating this fraction (and thus pCO_2) requires knowledge of DIC, the local alkalinity, temperature and salinity, and the iterative solution of a set of non-linear equilibrium equations (Zeebe and Wolf-Gladrow, 2001).

BOX 3: Inclusion of DOM dynamics in the biogeochemical model

Since a large portion of organic carbon is stored in dissolved organic matter (DOM), the transport of DOM may be an important pathway for carbon. As a first step toward addressing this question we added two semi-labile DOM components (dissolved inorganic nitrogen, DON, and dissolved inorganic carbon, DOC) to the biogeochemical model. Note that the model does not include the biologically inert "refractory" DOM fraction which dominates DOM in deep waters and is thought to act as a conservative tracer and be relatively uniform with depth (Hansell and Carlson, 1998; Carlson, 2002) except in areas influenced by rivers (Druffel et al., 1992). The source and sink terms of DOM are phytoplankton exudation, "sloppy feeding" of zooplankton, POM solubilization and DOM remineralization. The sources and sinks of DOM are thus directly related to primary production, grazing, and detritus pool concentration.

Exudation of semi-labile DOC by phytoplankton includes two processes: nutrient-based and carbon excess-based release. The nutrient-based release reflects the exudation of semi-labile DOC and DON by healthy phytoplankton. This term is proportional to primary production. The carbon excess-based release represents the carbohydrate over-production by nutrient-stressed cells. This process is responsible for the mucilage events

that are often observed during summer in eutrophic coastal areas. The carbon excess uptake can be seen as an 'overflow' of photosynthesis under nutrient limitation. We described this process as the difference between nutrient-saturated (and light-limited) and nutrient-limited (and light-limited) primary production (Andersen and Williams, 1998; Ianson and Allen, 2002).

As a result, in nutrient-depleted conditions, the nitrogen and carbon primary production are partially decoupled and carbon-rich DOM is produced; C to N ratios for DOM range between 10 and 25 (Hopkinson and Vallino, 2005; Søndergaard et al., 2000; Biddanda and Benner, 1997; Benner et al., 1992). Values vary between 9.95 for fresh material (Hopkinson and Vallino, 2005) to 19-25 for high molecular weight DOM, i.e., mainly the semi-labile fraction (Biddanda and Benner, 1997). The accumulation and subsequent transport of carbon-rich DOM may thus present an efficient export mechanism of organic carbon from productive shelf systems to the open ocean.

BOX 4: Development of empirical algorithms for CDOM and DOC

As part of a limited USECoS field program focused on the Chesapeake Bay region, samples were collected at multiple depths for measurement of pigments, dissolved organic carbon (DOC), particulate organic carbon (POC), absorption of chromophoric dissolved organic matter (CDOM), and particles. These have provided datasets critical for development of satellite-derived DOC and POC algorithms and for evaluation of the biogeochemical model results (Figure 5).

In order to develop empirical algorithms for CDOM and DOC, we collected field measurements to correlate a_{CDOM} (CDOM absorption coefficient) to *in situ* radiometry (reflectance band ratios) and then correlated DOC to reflectance band ratios through the

a_{CDOM} to DOC relationships. Results from our current field work in the continental margin of the southern MAB and the Chesapeake Bay mouth demonstrate that we can retrieve a_{CDOM} from SeaWiFS and MODIS observations through empirical relationships similar to those described by other researchers (D'Sa and Miller, 2003; Johannessen et al.; 2003). Our a_{CDOM} algorithm takes an exponential decay form with the remote sensing reflectance band ratios (488/551nm for MODIS and 490/555nm for SeaWiFS) plotted on the ordinate and a_{CDOM} on the abscissa (Mannino et al., in preparation). Because CDOM contributes to light absorption across the visible spectrum, several band ratio solutions are possible to avoid the atmospheric correction problems associated with the 412 nm ocean color satellite band in coastal waters (e.g., negative water-leaving radiances). Furthermore, comparisons of CDOM absorption at other relevant wavelengths (e.g., 443 nm) are possible to conduct comparisons, for example, with the Garver-Siegel-Maritorena inversion model (GSM-01; Maritorena et al., 2002). Uncertainties for a_{CDOM} derived from MODIS-Aqua are on average 20-25% and <10% for DOC (Mannino et al., in preparation). Seasonal variability in CDOM absorption and DOC is quite evident along the continental margin with the estuarine plumes and near-shore regions as most dynamic (Figure 10). Our results show that at least two seasonal algorithms (fall-winter-spring and summer) are required to retrieve DOC from MODIS and SeaWiFS due to seasonal variability in the CDOM to DOC relationship caused by the accumulation of primarily non-chromophoric DOC from net ecosystem production (NEP) and the concomitant loss of CDOM through sunlight-induced photooxidation between late spring to early fall.

Satellite ocean color data and field measurements are helping us to evaluate results from our biogeochemical model. For example, the increase in DOC distributions observed from ocean color satellite data can be compared with model results on the seasonal accumulation of semi-labile DOC from net ecosystem productivity (Figure 4 and Figure 10B). The satellite ocean color data are also helping us to evaluate how well the model represents the inputs and fate of DOC to the continental shelf from estuarine and riverine systems.

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List of Figures

Figure 1. Map of the east coast of the United States showing the Middle Atlantic Bight (MAB), the South Atlantic Bight (SAB), the Gulf of Maine (G0M), the 58 sub-regions used for evaluation of model-derived distributions, and 500-m isobath (red line). Other abbreviations used are: GB-Georges Bank, GS-Gulf Stream, SSF-shelf slope front, NEC-Northeast Channel, Wbasin-Wilkinson Basin, Jbasin-Jordan Basin, Cgom-central Gulf of Maine.

Figure 2. Schematic showing the multiple approaches used by the USECoS team.

Figure 3. Climatological and model-derived distributions of mixed layer depth (upper panel), annual mean salinity (middle panel), and dissolved oxygen anomaly (lower panel). Mixed layer depth was computed using a criterion of 0.5° C with respect to the surface. Monthly MLD was binned to a 0.1° grid; monthly salinity and oxygen anomaly were binned to a 0.5° grid. Annual mean salinity was computed when a given grid box contained measurements for more than nine calendar months. White indicates no data.

Figure 4. The nine-year mean distribution of A) particulate organic carbon (POC), B) absorption by colored dissolved organic matter at 355 nm (Acdom), C) primary production (VGPM2a), and D) month of maximum concentration chlorophyll *a* constructed from SeaWiFS measurements made from 1997 to 2007.

Figure 5. Comparisons of satellite-derived and simulated distributions of annual mean A) SST, B) chlorophyll and C) DOC in the surface water (from Mannino et al. algorithm, Box 4) and simulated semi-labile DOC.

Figure 6. Cross-shelf sections of: (a) chlorophyll *a*, (b) nitrate, and (c) light penetration (PAR in percent of surface intensity) constructed from data collected during 2-3 August 1981 along a

transect offshore off St. Augustine, FL (30°N). The light penetration was calculated using a PAR attenuation coefficient developed for the ecosystem model, which is a function of chlorophyll *a* concentration and salinity. Note the high chlorophyll *a* concentration on the entire shelf below 10 m, which resulted from nutrient inputs from a subsurface Gulf Stream intrusion, and significant (>10%) light penetration to the ocean floor. A CZCS summer composite for 1981 (d) shows that ocean color retrievals miss the high chlorophyll *a* that is associated with the subsurface bottom intrusions (white thick line is transect location). Note that there are no satellite data in the transect region near the coast (black regions) due to sensor amplifier ringing off the bright coastline.

Figure 7. Taylor diagrams showing quantitative assessment of model skill as compared to satellite data (from 2004) for the SAB (left panels) and MAB (right panels). SST results are shown in top two panels and surface chlorophyll results are shown in bottom two panels. Percent bias is illustrated via model symbol colors. (See text for full description of Taylor diagram).

Figure 8. Target diagrams for showing the bias and variability components of the RMS error for model vs. satellite-derived SST (upper four panels) and chlorophyll (lower four panels) in the SAB (left panels), and MAB (right panels). Comparisons were performed with satellite climatologies as well as with 2004 satellite measurements. Circles denote lines of constant normalized total RMS error. Solid line: model-data misfit = standard deviation of data; dashed line: model-data misfit = error in data, assumed to be ± 1°; dotted line: model-data misfit = error in data, assumed to be ± 0.3°. Thus, model estimates falling within inner circle are indistinguishable in terms of skill. Model estimates with variances greater than those computed from the data are given the sign nRMS_V> 0 whereas subregions where the model underestimates

the observed variance are given the sign nRMS_V<0. Region definitions in legend refer to regions defined in Figure 1.

Figure 9. A) Comparison of time series of SeaWiFS surface chlorophyll, with pre- and post-assimilation modeling surface chlorophyll at a station on the outer continental shelf offshore of Chesapeake Bay and depth-time contour plots of B) pre- and C) post-assimilation of chlorophyll (mg Chl m^{-3}) at a station on the outer continental shelf offshore of Chesapeake Bay. Prior to assimilation of ocean color data (B), chlorophyll concentrations were overestimated but were reduced to reasonable values by adjusting the maximum growth rate and C:chl ratio (C).

Figure 10. Satellite-derived distributions of a_{CDOM} (355 nm, m^{-1}) (upper panel) and DOC (μM C) (lower panel). From spring to summer, a_{CDOM} decreases due to photooxidation and possibly from reduced inputs of terrigenous DOM as a result of reduced river discharge. From summer to fall, storm events will vertically mix the water column and introduce CDOM from depth into surface waters. Much higher DOC values are observed in summer compared to early spring due to ecosystem productivity that promotes the accumulation of semi-labile DOC. Our estimate of the DOC reservoir within the 10-100-m isobaths for the continental shelf region shown in Figure 1 is on the order of 1.2 Tg C. Source data for images shown are from NASA's MODIS-Aqua sensor.

Figure 11 A) Simulated semi-labile DOC net horizontal flux for 2005 (mol C.m^{-2}.yr^{-1}). Negative values correspond to areas of production and export, and positive values to areas of import. B) Simulated POC burial in the sediments for 2005 (mol C.m^{-2}.yr^{-1}).

Table 1. Satellite data and derived products used for analyses and model evaluation.

Measurements	Sources
Sea Surface Temperature (SST, °C)	4km nighttime composite from: AVHRR Pathfinder 1985-present, MODIS Terra 2000-, MODIS Aqua 2002-. GOES 2001-)
Chlorophyll *a* (mg m^{-3})	SeaWiFS & MODIS Aqua
Photosynthetically active radiation (PAR, $Em^{-2}d^{-1}$)	SeaWiFS
Cloud Cover/probability	SeaWiFS
Particulate Organic Carbon (POC, mgL^{-1})	D. Clark Algorithm (uses SeaWiFS / MODIS ocean color bands ~ 443nm, ~490nm, ~550nm)
Primary Production ($gCm^{-2}d^{-1}$)	SeaWiFS data and the VGPM2a model
Euphotic Depth (1% surface par)	VGPM2a model
Euphotic Chlorophyll (mg m^{-2})	VGPM2a model
Absorption coefficient of CDOM (m^{-1})	SeaWiFS and MODIS (see Box 4)
a_{CDOM}(355nm) (m^{-1})	
Dissolved Organic Carbon (μmol L^{-1})	SeaWiFS and MODIS (see Box 4)

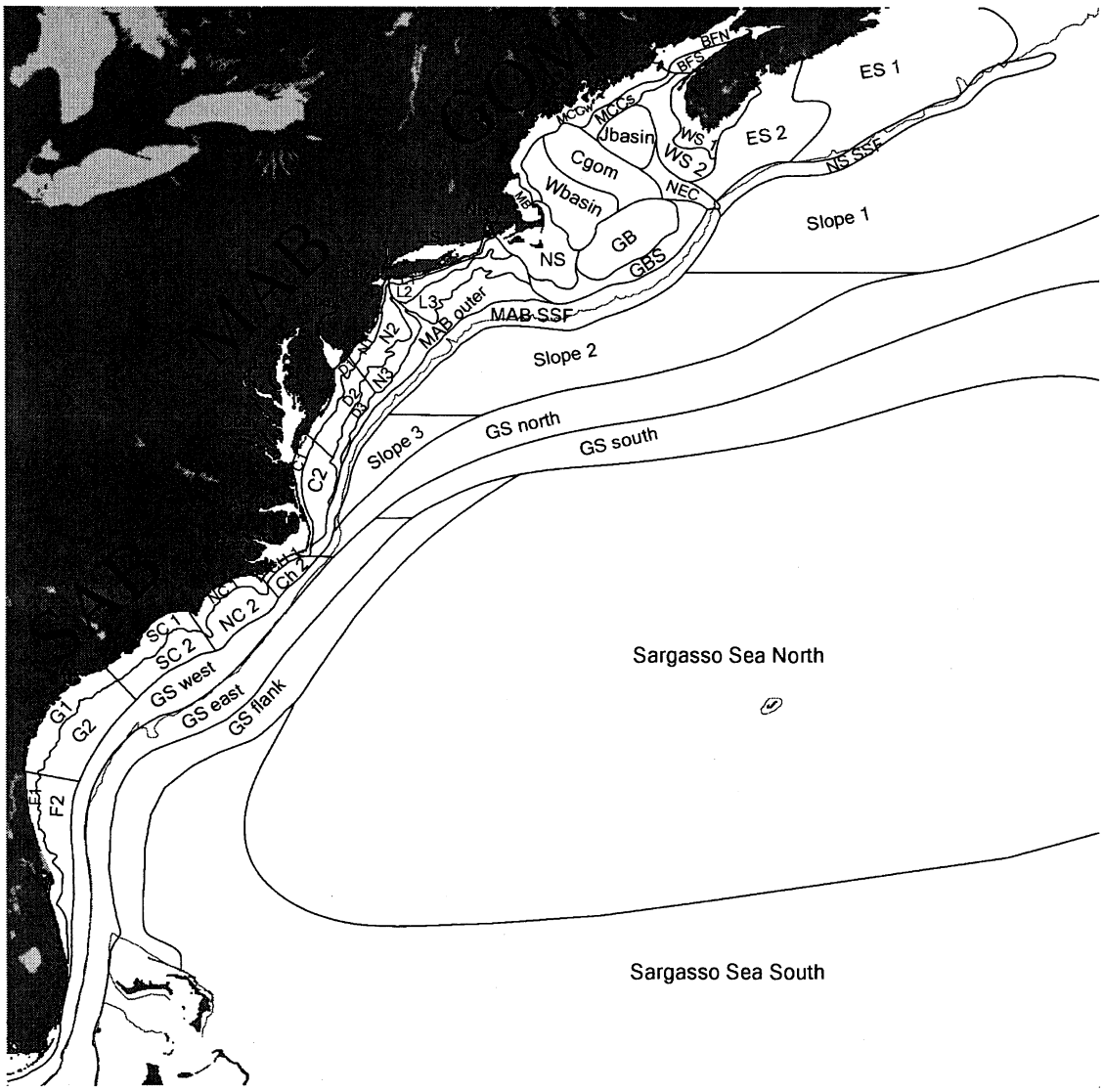
ES 1
ES 2
BFN
BFS
MCCS
MCCW
Jbasin
WS 1
WS 2
Cgom
Wbasin
NEC
NS SSF
Slope 1
NS
GB
GBS
MAB
L2
L3
MAB outer
MAB SSF
Slope 2
N2
N3
D1
D2
D3
Slope 3
GS north
GS south
C1
C2
Cb 2
NC 1
NC 2
SC 1
SC 2
GS west
GS east
GS flank
G1
G2
E1
F2
Sargasso Sea North
Sargasso Sea South

Figure 1

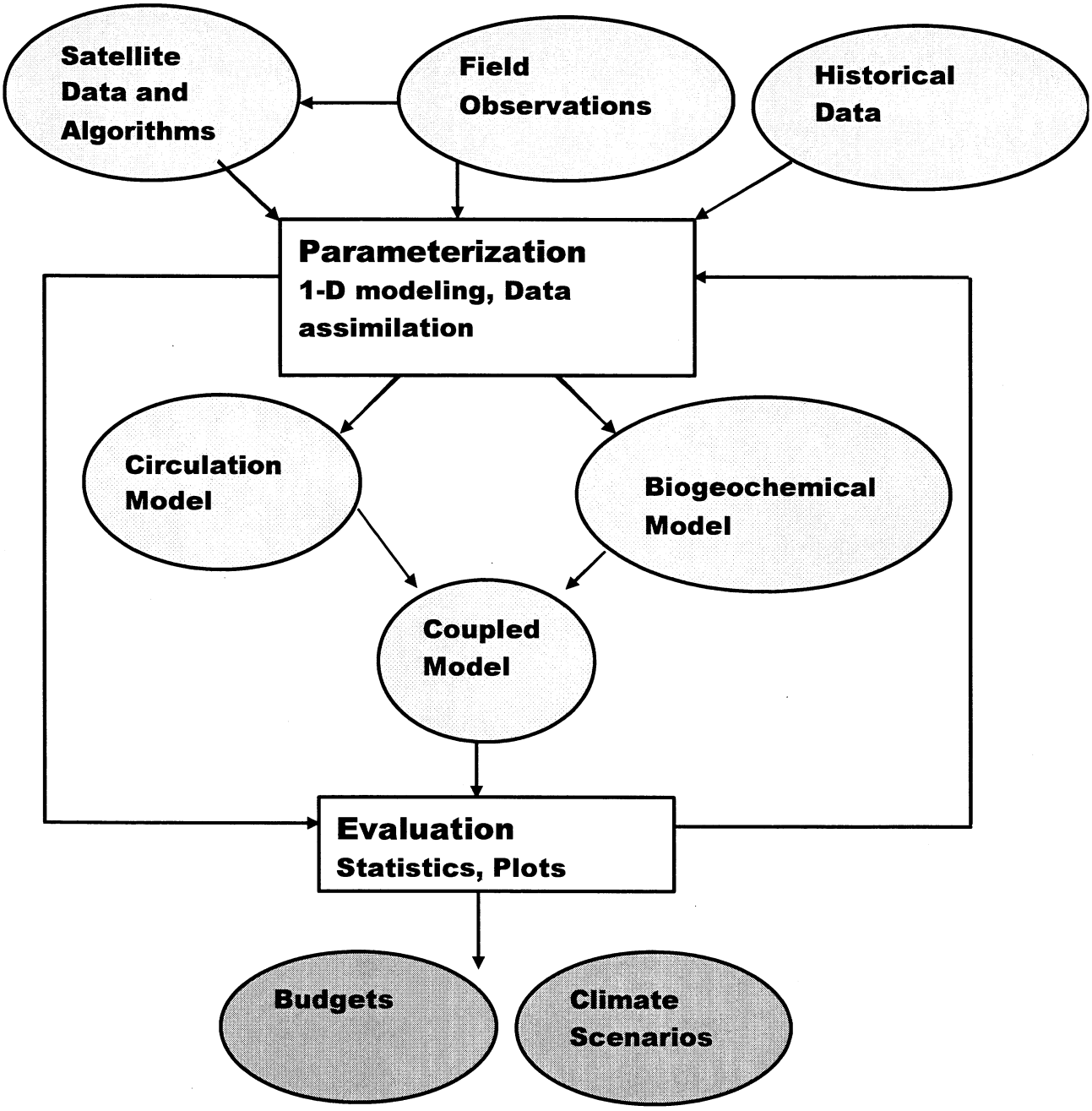
Satellite Data and Algorithms
Field Observations
Historical Data
Parameterization
1-D modeling, Data assimilation
Circulation Model
Biogeochemical Model
Coupled Model
Evaluation
Statistics, Plots
Budgets
Climate Scenarios

Figure 2

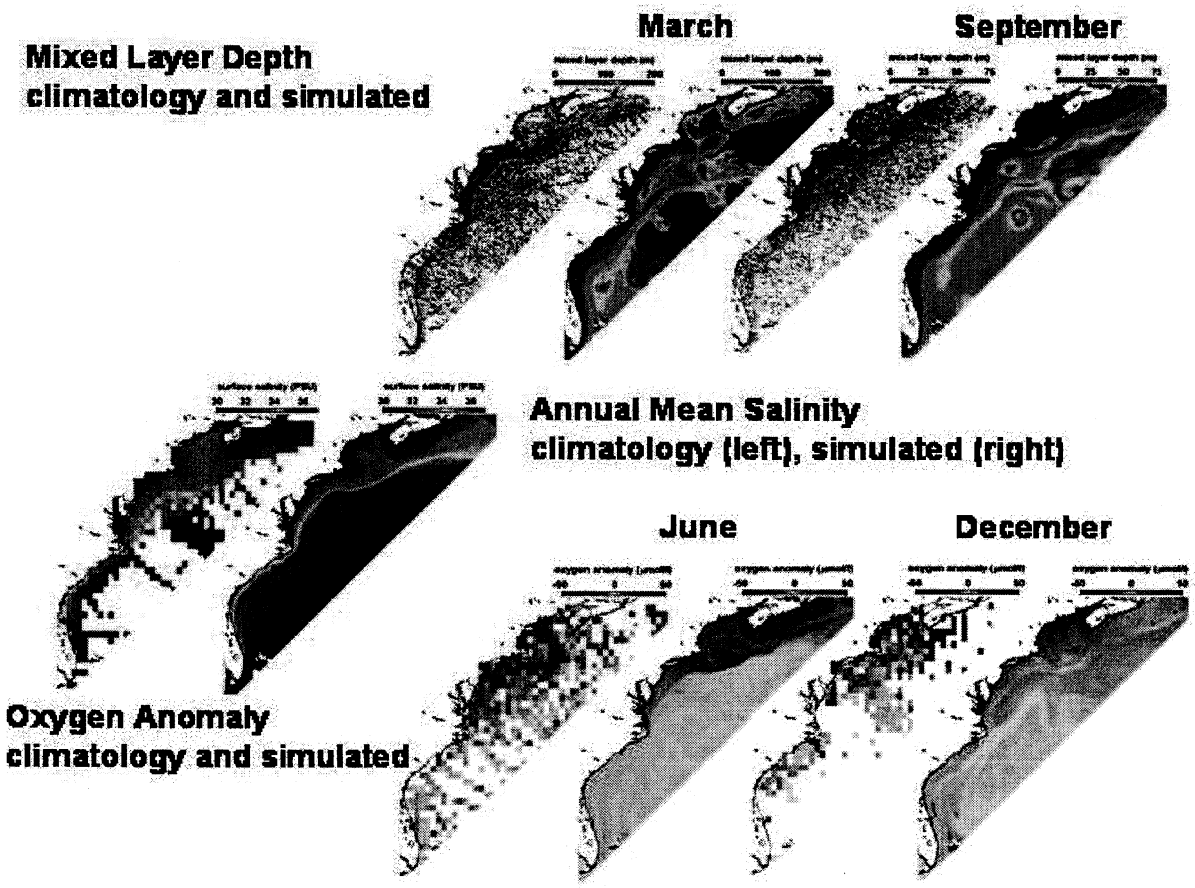
March
September
Mixed Layer Depth
climatology and simulated
Annual Mean Salinity
climatology (left), simulated (right)
June
December
Oxygen Anomaly
climatology and simulated

Figure 3

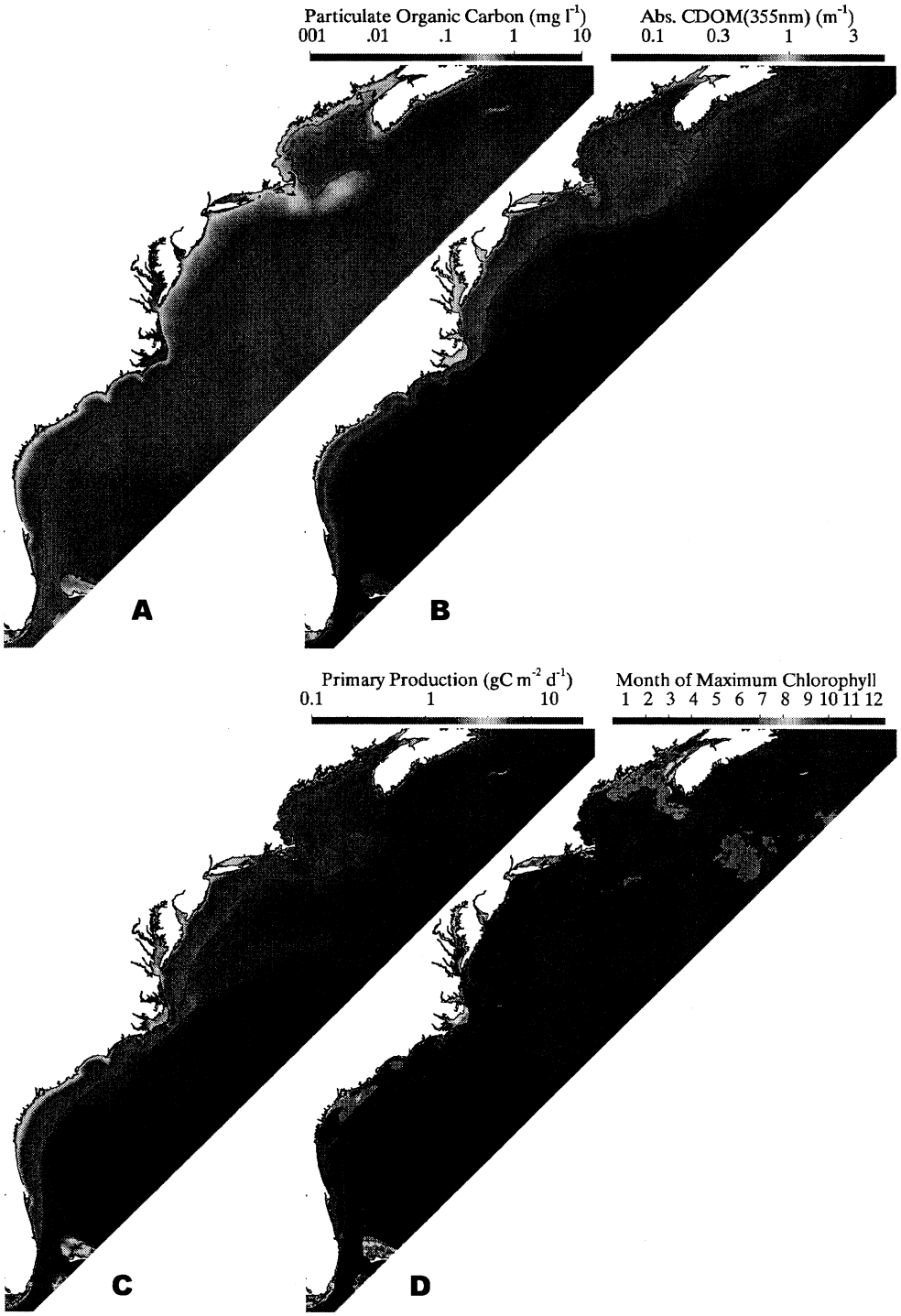
Particulate Organic Carbon (mg l-1)
001 .01 .1 1 10
Abs. CDOM(355nm) (m-1)
0.1 0.3 1 3
A
B
Primary Production (gC m-2 d-1)
0.1 1 10
Month of Maximum Chlorophyll
1 2 3 4 5 6 7 8 9 10 11 12
C
D

Figure 4

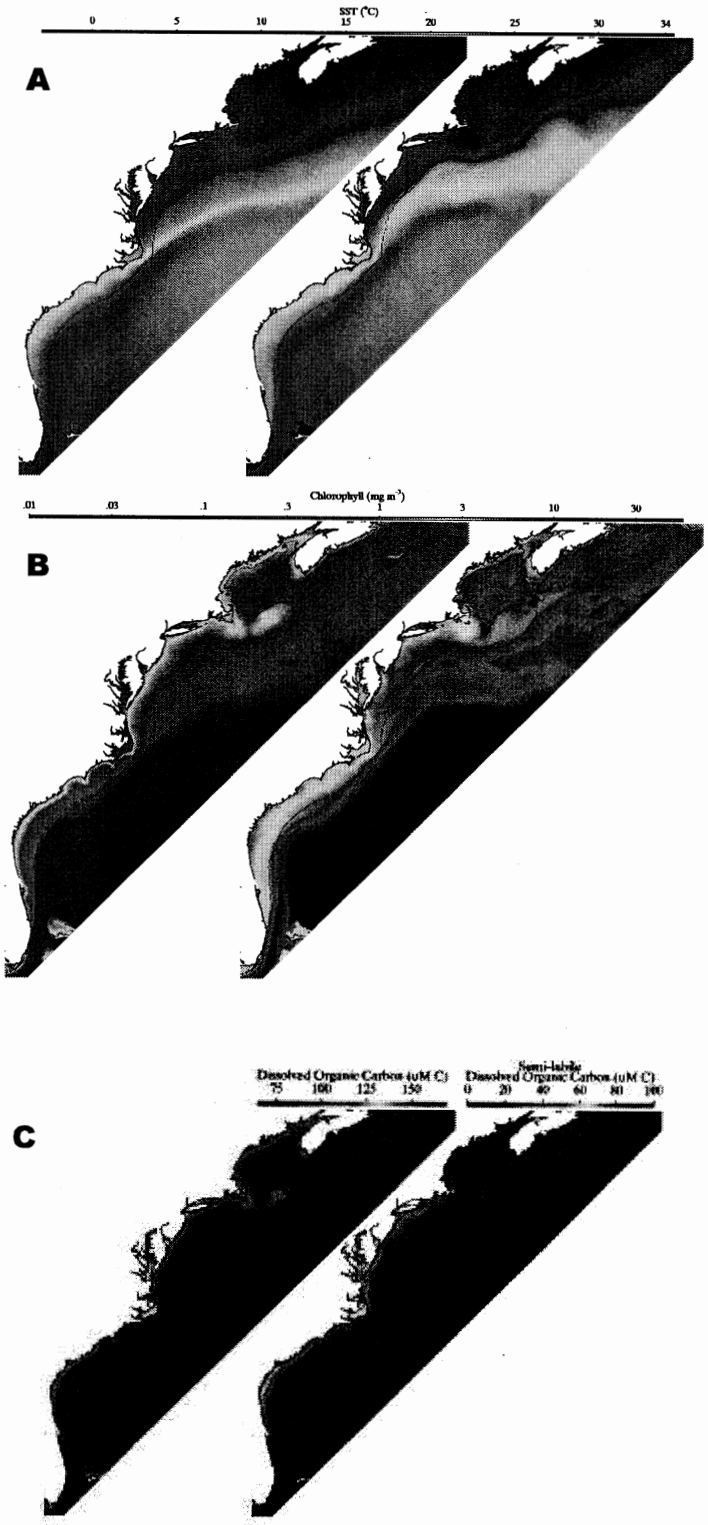
SST (°C)
0
5
10
15
20
25
30
34
A
Chlorophyll (mg m-3)
.01
.03
.1
.3
1
3
10
30
B
Dissolved Organic Carbon (uM C)
75
100
125
150
Semi-labile
Dissolved Organic Carbon (uM C)
0
20
40
60
80
100
C

Figure 5

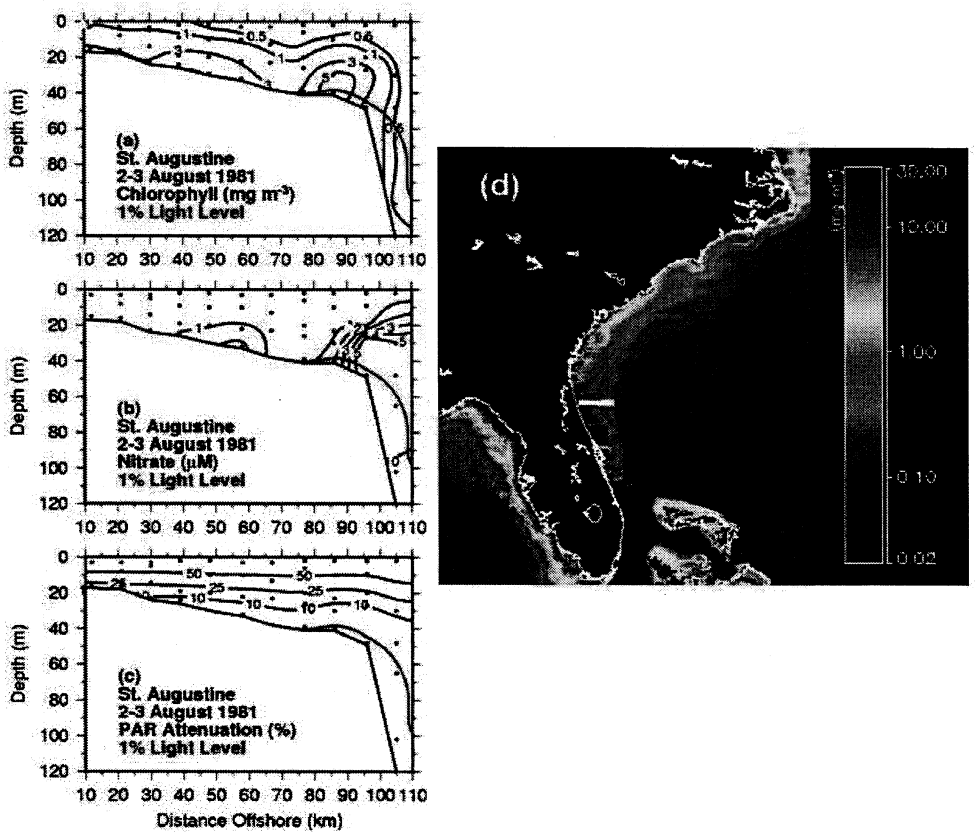
(a)
St. Augustine
2-3 August 1981
Chlorophyll (mg m⁻³)
1% Light Level
(b)
St. Augustine
2-3 August 1981
Nitrate (µM)
1% Light Level
(c)
St. Augustine
2-3 August 1981
PAR Attenuation (%)
1% Light Level
Depth (m)
Distance Offshore (km)
(d)
10.00
1.00
0.10
0.02

Figure 6

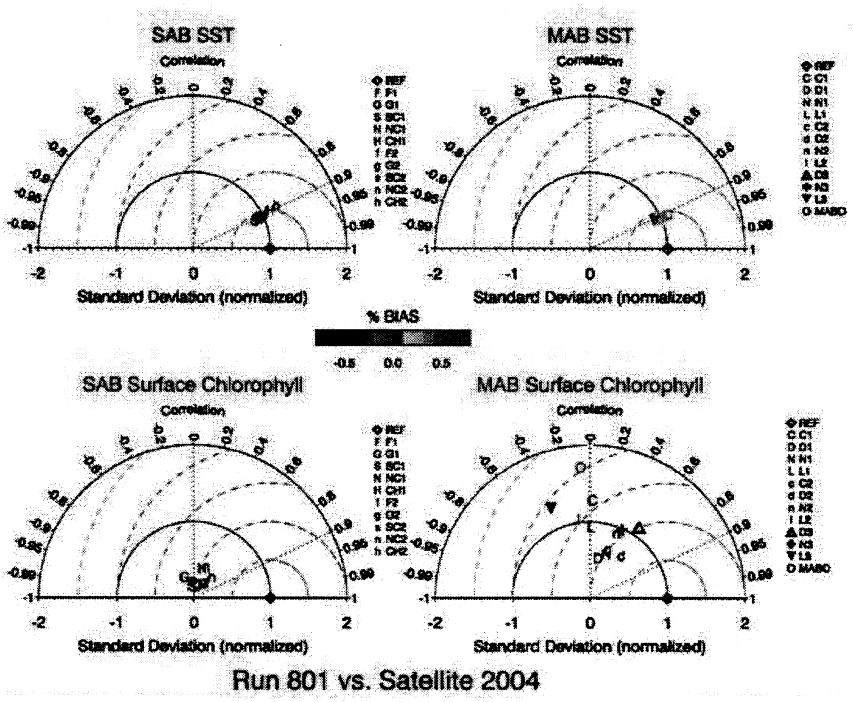
SAB SST
MAB SST
Correlation
Standard Deviation (normalized)
% BIAS
-0.5
0.0
0.5
SAB Surface Chlorophyll
MAB Surface Chlorophyll
Run 801 vs. Satellite 2004

Figure 7

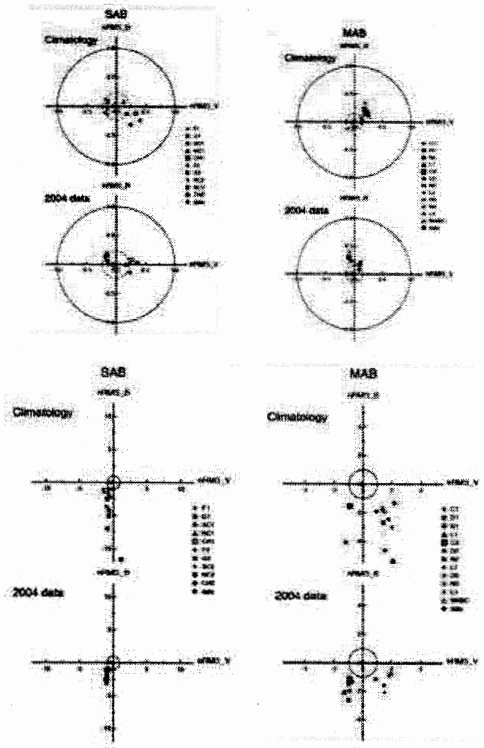
SAB
Climatology
2004 data
MAB
Climatology
2004 data
SAB
Climatology
2004 data
MAB
Climatology
2004 data

Figure 8

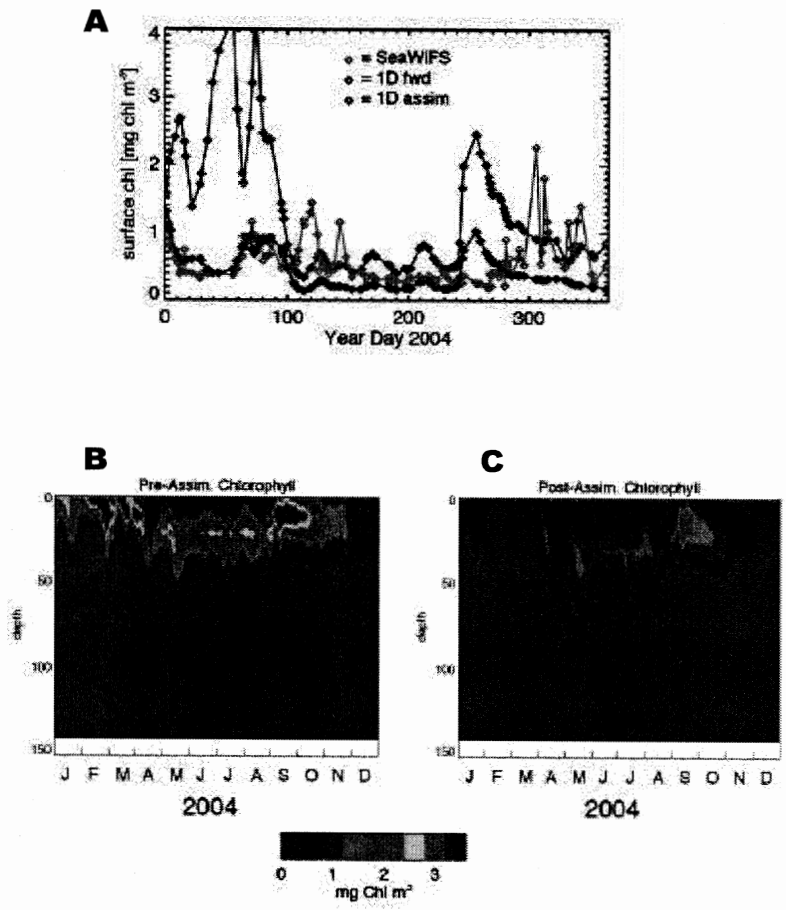
A
= SeaWiFS
= 1D fwd
= 1D assim
surface chl [mg chl m⁻³]
Year Day 2004
B
Pre-Assim. Chlorophyll
depth
J F M A M J J A S O N D
2004
C
Post-Assim. Chlorophyll
depth
J F M A M J J A S O N D
2004
mg Chl m⁻³

Figure 9

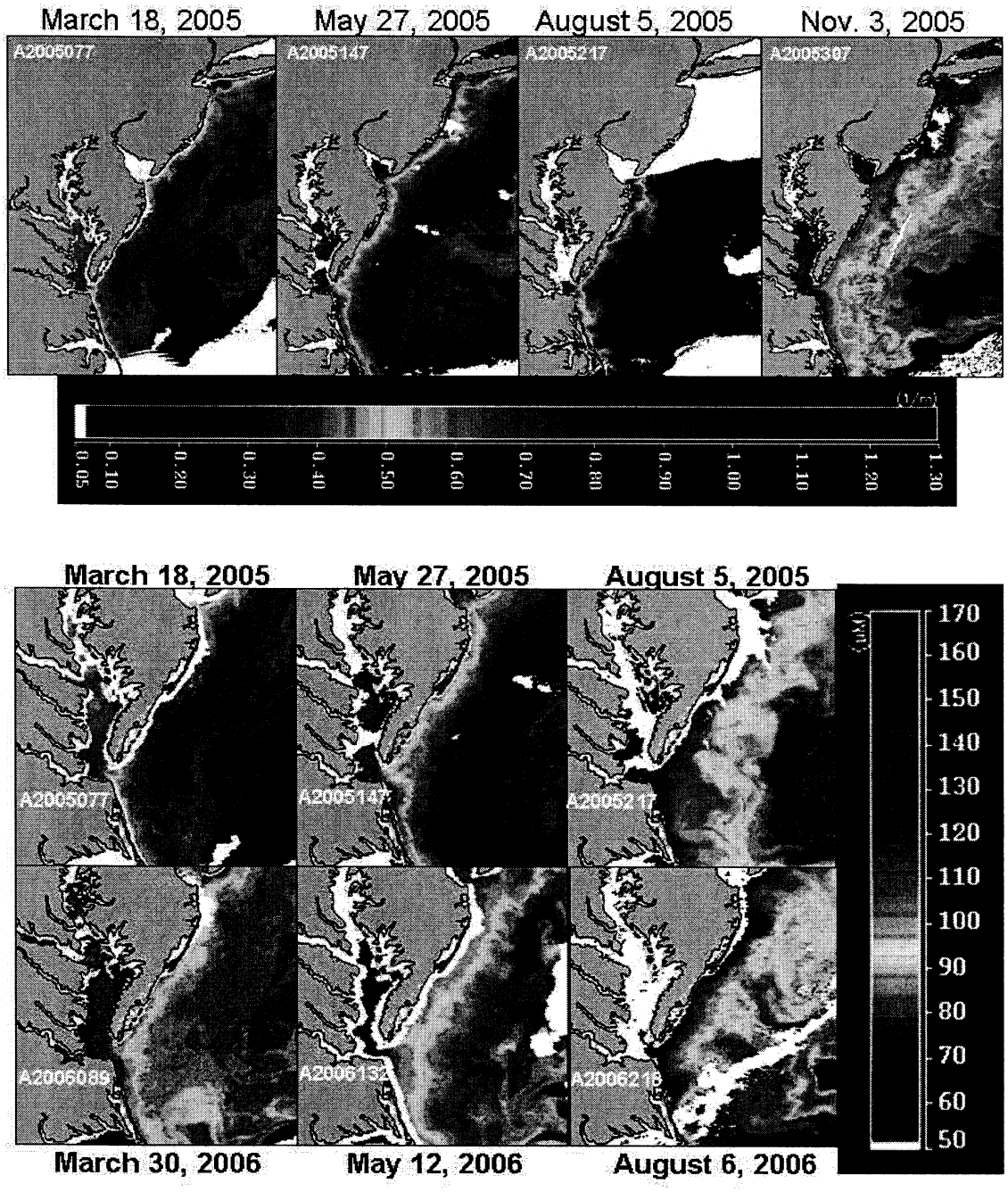
March 18, 2005
May 27, 2005
August 5, 2005
Nov. 3, 2005
A2005077
A2005147
A2005217
A2005307
(1/m)
0.05
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
1.10
1.20
1.30
March 18, 2005
May 27, 2005
August 5, 2005
A2005077
A2005147
A2005217
A2006089
A2006132
A2006216
March 30, 2006
May 12, 2006
August 6, 2006
170
160
150
140
130
120
110
100
90
80
70
60
50

Figure 10

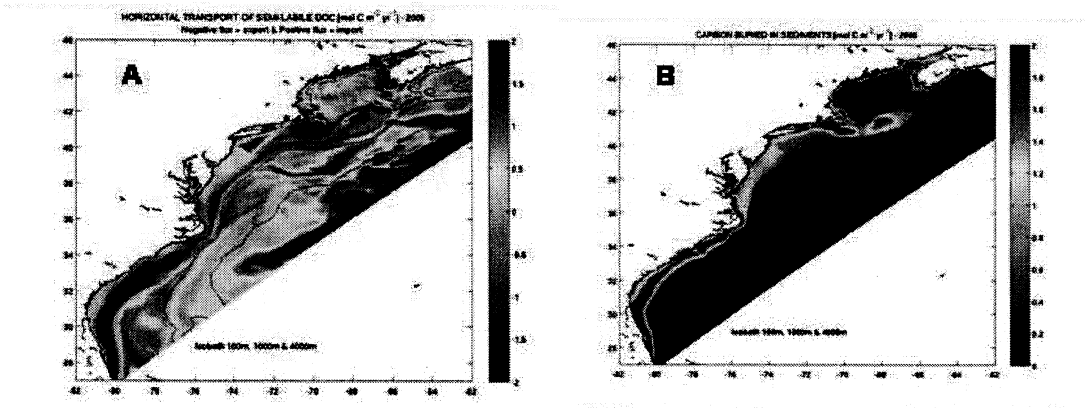

Figure 11