THE PREDICTION OF REMOTE SENSING REFLECTANCE AT LEO-15

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ABSTRACT

The prediction of spectral water leaving radiance and remote sensing reflectance from a coupled physical/ecological/optical simulation is one of the goals of the ONR Hyperspectral Coastal Ocean Dynamics Experiment (HyCODE). This goal requires coupling a high-resolution circulation model (ROMS) to provide realistic physical forcing to a dynamic ecological model that produces depth-dependent distributions of inherent optical properties (EcoSim), which are subsequently fed to a robust radiative transfer model (Ecolight) to generate the water leaving radiance and remote sensing reflectance at the sea surface. The 2001 HyCODE experiment off the coast of New Jersey provided a data rich environment that included measurements of local currents from towed ADCPs and CODAR, in situ inherent and apparent optical properties (IOPs and AOPs), sea surface remote sensing reflectance, pigment distributions, fluorescence, and ocean color remote sensing (from three different aircraft sensors and four different satellites) with which to validate a coupled numerical simulation. The predictions over the New Jersey Bight have a 300 m resolution at the LEO-15 site, encompassing a total of 250,000 grid points. The ecological simulation is initialized from estimates of historical relationships between total phytoplankton, pigments, nutrients, Color Dissolved Organic Matter (CDOM), temperature, and salinity. The mass constituents of the ecological model include specific IOP functions, which are used in a numerically fast downwelling radiative transfer model to generate the time dependent spectral photon density for the calculation of primary production, light-dependent pigment adjustments, and CDOM cycling. The resultant IOPs are then used once per simulated day to generate the Ecolight solution for spectral upwelling radiance and remote sensing reflectance. The ability to directly compare physical measurements of radiance and remote sensing reflectance to simulated estimates provides an opportunity to validate numerical simulations via photon densities, rather than through derived products such as chlorophyll concentrations.

INTRODUCTION

Ocean color is a function of the mass of optical constituents in the water column, the inherent optical properties of those constituents, and the apparent illumination of the ocean. One of the goals of ONR's Environmental Optics Hyperspectral Coastal Ocean Dynamics Experiment (HyCODE) program is to develop the forecasting ability to predict the depth-dependent optical constituents, and their impact on water-leaving radiance and water-column visibility. The satisfaction of this optical goal requires the ability to forecast the physical oceanographic environmental, such that the distribution and time-dependent change of the optical constituents can be adequately represented in a 4-dimensional framework. In pursuit of these nowcast/forecast objectives, HyCODE sought to build partnerships with ongoing research programs focused on the short-term prediction of the coastal circulation. Thus, the development an ecological and optical forecasting model was embedded into the Coastal Predictive Skill Experiments being conducted off of the coast of New Jersey during the summer of 2001. The modeling system described here is an implementation of the coupled ROMS (Regional Ocean Modeling System)/EcoSim (Ecological Simulator) model developed for ONR's HyCODE and Coastal Ocean Modeling and Observation Program (COMOP).

METHODS

ROMS is a free-surface, hydrostatic, primitive equation model initially based on the s-coordinate Rutgers University Model (SCRUM) described by (Song et al., 1994). ROMS was rewritten by the UCLA and Rutgers ocean modeling groups to improve its numerics and efficiency in single and multi-threaded computer architectures. New features include high-order advection schemes; accurate pressure gradient algorithms; several subgrid-scale parameterizations; atmospheric, oceanic, and benthic boundary layers; radiation boundary conditions; and data assimilation.

For computational economy, the momentum equations are solved using split-explicit time-stepping which requires special treatment of the coupling between barotropic (fast) and baroclinic (slow) modes. Many barotropic time steps are carried out to evolve the free-surface and vertically integrated momentum within a single baroclinic time step. To avoid aliasing errors, barotropic fields are time averaged with a centered cosine-shape filter before they replace values obtained with the longer baroclinic step. Time-stepping is constrained to maintain exactly both volume conservation and constancy preservation properties which are needed for the tracer equations (Shchepetkin et al., 1999). All time stepping uses a 3rd-order accurate predictor (leap-frog) and corrector (Adams-Molton) algorithm which is robust and stable. The enhanced stability of the scheme allows larger time steps which more than offsets the increased cost of the predictor-corrector algorithm.

ROMS employs a vertically stretched terrain-following coordinate (Song and Haidvogel, 1994) that allows increased resolution in areas of interest, such as the surface and bottom boundary layers. Pressure gradient errors can arise from splitting the pressure gradient into a terrain-following component and a hydrostatic correction, but these are minimized by a conservative parabolic spline discretization in the vertical (Shchepetkin and McWilliams, 1999). A major enhancement over related codes is a 3rd-order upstream-biased advection operator that has a velocity-dependent hyper-diffusion as the dominant truncation error (Shchepetkin et al., 1998). The scheme reduces dispersive errors and minimizes dissipation, effectively boosting the resolution on a given grid. Combined with the constancy preservation features of the time-stepping, the outcome is a dramatic improvement in the evolution of tracer fields and the simulation of mesoscale turbulence.

EcoSim is an upper ocean ecological model initially based on the differential elemental cycling model used to describe the impacts of phytoplankton ecology on oceanic carbon cycling (Bissett et al., 1999a; Bissett et al., 1999b). This initial work focused on inorganic and organic carbon cycling, and found that the dynamics of carbon cycling in the upper ocean depended on speciation of the phytoplankton community. This was not a new concept (e.g., Bissett et al., 1994; Longhurst et al., 1989), but they demonstrated the numerical extrapolation of some key ecological hypotheses relating to carbon cycling. In particular, carbon sequestration and speciation was found to be dependent on the non-stoichiometry nutrient uptake and the spectral quality of the photon density of the ambient light field. These issues had been debated and demonstrated experimentally prior to this work (e.g. Banse, 1994; Bidigare et al., 1990; Bidigare et al., 1987), but this was the first attempt at incorporating the interactions of these hypotheses in a prognostic framework. The success at the simulated interactions between light, nutrients, and phytoplankton speciation provided justification to expand the simulated phytoplankton diversity and elemental representation, as well as to incorporate the model into the three dimensional ROMS nowcast/forecast system of the Middle Atlantic Bight.

HyCODE is focused on the prediction of in situ absorption and scattering, which is mainly controlled by the vertical distribution of suspended materials in the water column. These materials include living organic matter (phytoplankton), non-living organic matter (in both dissolved and particulate phases), and suspended sediments. The ecological progress of phytoplankton growth, and resultant optical signature, on the shelf primary depends on the source and stoichiometric quality of the nutrient supply. Nutrients in the form of NO3, PO4, SiO4, and Fe supplied in abundance and in nearly "Redfield-like" proportions tend to yield phytoplankton blooms dominated by large and small diatoms; smaller nutrient supplies in Redfield proportions yield small blooms dominated by small diatoms. All species increase during these periods; however, the group that dominates the biomass drives the ecological removal of bioavailable nutrients and contaminants.

The progression of such biomass accumulations depends on the source of the nutrient supply. Upwelling events initially yield depth-dependent Case 1 type signals, where the particulates and CDOM signal co-vary at the start of the bloom. As the bloom progresses, particulate biomass is lost via grazing and/or other loss processes, and the CDOM signal increases in relative proportion. As the nutrient supplies dwindle and shift in their stoichiometric proportions (resulting from differential regeneration processes), the assemblage shifts to smaller coccoid phytoplankton and dinoflagellate populations. This classical phytoplankton succession story may be mitigated in estuarine outflow regions where the total supply of nutrients may be out of stochiometric balance compared to demand. The phytoplankton assemblage may be further impacted by the form of the nutrient supply, i.e., bioavailable nitrogen locked in Dissolved Organic Nitrogen (DON), yielding populations that are more adept at using organic molecules, e.g., dinoflagellates. In addition, the color and clarity of the water may also impact the biomass population and accumulation. CDOM will cause a shift in the spectral quality of the light field, as well as impact the total quanta density. Those populations that can alter their vertical position in the water column, as well as take advantage of the shift toward green light by alteration of their photosynthetic pigment concentration will have a competitive advantage over those phytoplankton that are non-motile.

EcoSim incorporates the non-stoichiometric nutrient dynamics of the phytoplankton population by allowing luxury uptake and non-balance nutrient growth. In addition, photosynthetic light harvesting is pigment specific and depends on growth rate, cellular nutrient content, and light history. DOM cycling includes 2 forms (labile and recalcitrant) of DOC, DON, and DOP, as well as explicit spectral description of 2 forms of CDOM. Differential regeneration of the nutrients into organic and inorganic element forms completes the non-stoichometric cycling of macro- and micro-nutrients. The current version of ROM/EcoSim for the Middle Atlantic Bight contain equations for 7 functional groups of phytoplankton (2 diatoms, 2 dinoflagellates, 2 prochlorococcus, and 1 synechococcus), but is typically run with only 4 (2 diatoms, 1 dinoflagellate, 1 synechococcus) to optimize runtime efficiency. The total numbers of independent state variables for the simulations during the ONR COMOP/HyCODE program are 62, as the description of each phytoplankton contains state equations for functional group carbon, nitrogen, silica, phosphorus, and iron, as well as state equations for each individual pigment within each functional group. Since the model tracks each state variable through mass conservative calculations, all are available for validation of the ecological forecasts. In other words, the model can be validated by measurements of DIC, NH4, NO3, PO4, SiO4, DOC, DON, DOP, POC, PON, POP, POSi, POFe, TOC, TON, TOP, TOSi, TOFe, phytoplankton counts, total chlorophyll (see Figure ROMS/EcoSim), HPLC pigments, as well as the optical measurements of spectral absorption, scattering and water-leaving radiance.

Ecolight is a version of the Hydrolight 4.1 radiative transfer model (Mobley et al., 2000a; Mobley et al., 2000b) and provides an accurate solution of the RTE for any water body, given the absorption and scattering properties of the water body, the incident sky radiance, and the bottom reflectance (for finite-depth waters). Unfortunately, the standard version of Hydrolight is computationally too intensive to be suitable for incorporating into ecosystem models where the light field must be predicted as a function of depth and wavelength for many grid points and times. Thus, Ecolight is an optimized version of Hydrolight for computational speed, has been developed for usage in the ROMS/EcoSim modeling system. Ecolight typically runs one thousand times faster than the standard versionof Hydrolight, and outputs the scalar irradiance as a function of depth and wavelength, PAR as a function of depth, and the remote-sensed reflectance, Rrs, in the nadir viewing direction.

The shared memory parallel version (using OpenMP) of the ROMS/EcoSim code that we used to produce forecasts on the New Jersey coast for ONR's COMOP/HyCODE program (Arango et al., 2002) in July 2001 required 25 hours of wall clock time to process a 31 day simulation of a 100 x 240 (horizontal) x 25 (vertical) grid when executing on 16 (out of 256) processors of the NRL Origin3800 supercomputer (neo.cmf.nrl.navy.mil). The ecological and optical state variables were initialized from an analytical relationship between the state variable and temperature and salinity on July 11, 2001, and the simulation was run until August 8, 2001.

RESULTS

The preliminary results from the coupled modeling are encouraging; however, they highlight the difficulties that will be faced in developing a prognostic simulation of IOPs. One of the major difficulties in these short term numerical experiments is the initialization of water mass constituents and numerical history of water mass properties. The initialization of the model is based on a historical analysis of the relationship between temperature and salinity and the state variables of the model. The assumption is that the system will rapidly respond to any discontinuities in the initial conditions as long as the forcing functions are accurate. However, if the forcing functions are in error, or the temperature and salinity values themselves are in error, these will have downstream consequences for the ecological and optical solutions. Figure 1 shows the estimated chlorophyll a field from SeaWiFS and the simulated total surface chlorophyll. Clearly, the simulated fields are much lower Figure 1 than those of satellite estimates. This is to be expected as the initialized fields were very low, but the beginnings are field structure is beginning to become evident. By August 8th (Figure 2) biomass as represented by simulated chlorophyll begins to show much greater accumulation as well as some coastal structures associated with upwelling features near the apex region of the NJB.

There are some spatial discrepancies, particularly around the LEO site that are related to the history of the water masses. Figure 3 shows the SST from a morning pass of AVHRR and the simulated temperature field on the July 15th. There are two simulated “hot” water features that are not evident in the AVHRR fields. These features are advected towards the shore by the 21st. While discrepancies of the simulated temperatures are reduced as time progresses, the simulated history of the water mass “remembers” the higher temperatures, as the growth and grazing processes are significantly different for the warmer waters. In this case, there is approximately a 50% increase in the growth and loss processes in the “hot” water, than would have been estimated from the actual data. The bigger impact appears to be on the loss processes as the nutrient fields are higher in the hot water mass (Figure 4), in spite of having been initialized at similar levels (Figure 5). These higher loss processes in this water mass reduce the biomass to levels that are unable to completely utilize the nutrient stocks, as well as reducing the total load of IOPs in the water column. The advection of these water mass onto the shore (see change from Figure 3 to Figure 4) alters the expected IOPs (not shown) as these are a function of the biomass growth, loss, and accumulation processes.

The hot water features appear to be artifacts of the data assimilation scheme used for temperature and salinity (Arango per. comm.). The assimilation scheme uses and interpolates field data into a three dimensional grid, and then extrapolates the data across the domain of the model. In this case, it appears that the extrapolation of interpolated field data created water mass properties, outside of the collection domain, that were unrealistic. While these values were not evident in the LEO domain during the course of the COMOP experiment, there inclusion into the larger domain impacted the ecological and optical history of the water masses that were advected into the LEO domain.

While computationally efficient, Ecolight still requires a tremendous amount of CPU time for the 4.2 x 10^8 radiative transfer calculations required to predict spectral upwelling radiance and remote sensing reflectance over the entire domain of the model once per day. Thus, for the moment, we will defer these calculations until they physical and ecological model are rectified for the conditions during the HyCODE/COMOP 2001 experiment. These should be completed by the OOXVI conference.

SUMMARY

The ROMS/EcoSim modeling system demonstrates the ability to couple a high resolution physical model to a complex ecological and optical model. This simulation shows promise in being able to deliver short term forecast of the water-column IOPs, but problems remain in the actual implementation of a nowcast/forecast solution. In particular, the initialization of the model system state variables should be as close to the actual fields as possible. In addition, the history of the water mass will be carried with it as it is advected within the model domain, thus care must be taken when using data assimilation techniques that alter the temperature and salinity of the physical solution that will have downstream effects on the ecological and optical solution.

REFERENCES

Banse, K., 1994. Uptake of inorganic carbon and nitrate by marine plankton and the Redfield ratio. Global Biogeochemical Cycles, 8(1): 81-84.

Bidigare, R.R., Marra, J., Dickey, T.D., Iturriaga, R., Baker, K.S., Smith, R.C. and Pak, H., 1990. Evidence for phytoplankton succession and chromatic adaptation in the Sargasso Sea during spring 1985. Marine Ecology Progress Series, 60: 113-122.

Bidigare, R.R., Smith, R.C., Baker, K.S. and Marra, J., 1987. Oceanic primary production estimates from measurements of spectral irradiance and pigment concentrations. Global Biogeochemical Cycles, 1(3): 171-186.

Bissett, W.P., Carder, K.L., Walsh, J.J. and Dieterle, D.A., 1999a. Carbon cycling in the upper waters of the Sargasso Sea: II. Numerical simulation of apparent and inherent optical properties. Deep-Sea Research I, 46(2): 271-317.

Bissett, W.P., Meyers, M.B., Walsh, J.J. and Muller-Karger, F.E., 1994. The effects of temporal variability of mixed layer depth on primary productivity around Bermuda. Journal of Geophysical Research, 99(C4): 7539-7553.

Bissett, W.P., Walsh, J.J., Dieterle, D.A. and Carder, K.L., 1999b. Carbon cycling in the upper waters of the Sargasso Sea: I. Numerical simulation of differential carbon and nitrogen fluxes. Deep-Sea Research I, 46(2): 205-269.

Longhurst, A.R. and Harrison, W.G., 1989. The biological pump: Profiles of plankton production and consumption in the upper ocean. Progress in Oceanography, 22: 47-123.

Mobley, C.D. and Sundman, L.K., 2000a. Hydrolight 4.1 technical documentation, Sequoia Scientific, Inc., Seattle, WA.

Mobley, C.D. and Sundman, L.K., 2000b. Hydrolight 4.1 users' guide, Sequoia Scientific, Inc., Seattle, WA.

Shchepetkin, A.F. and McWilliams, J.C., 1998. Quasi-monotone advection schemes based on explicit locally adaptive dissipation. Mon. Wea. Rev., 126: 1541-1580.

Shchepetkin, A.F. and McWilliams, J.C., 1999. The Regional Ocean Modeling System: A split-explicit, free-surface, topography-following coordinates ocean model. (in preparation).

Song, Y.T. and Haidvogel, D.B., 1994. A semi-implicit ocean circulation model using a generalized topography-following coordinate system. J. Comp. Phys., 15: 228-244.

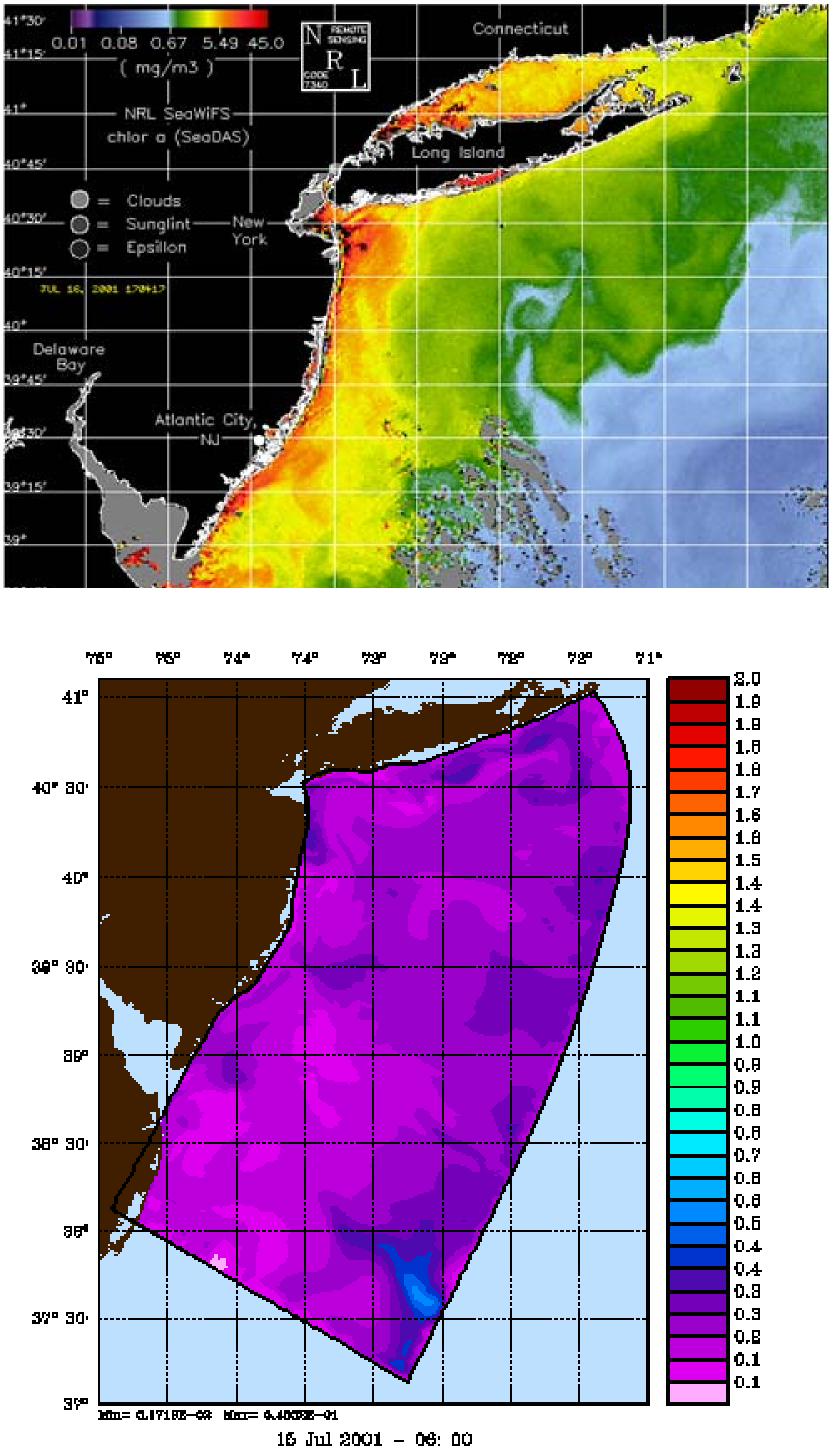

Figure 1. SeaWiFS Chlorophyll (top) and simulated Total Surface Chlorophyll (bottom) on July 15, 2001

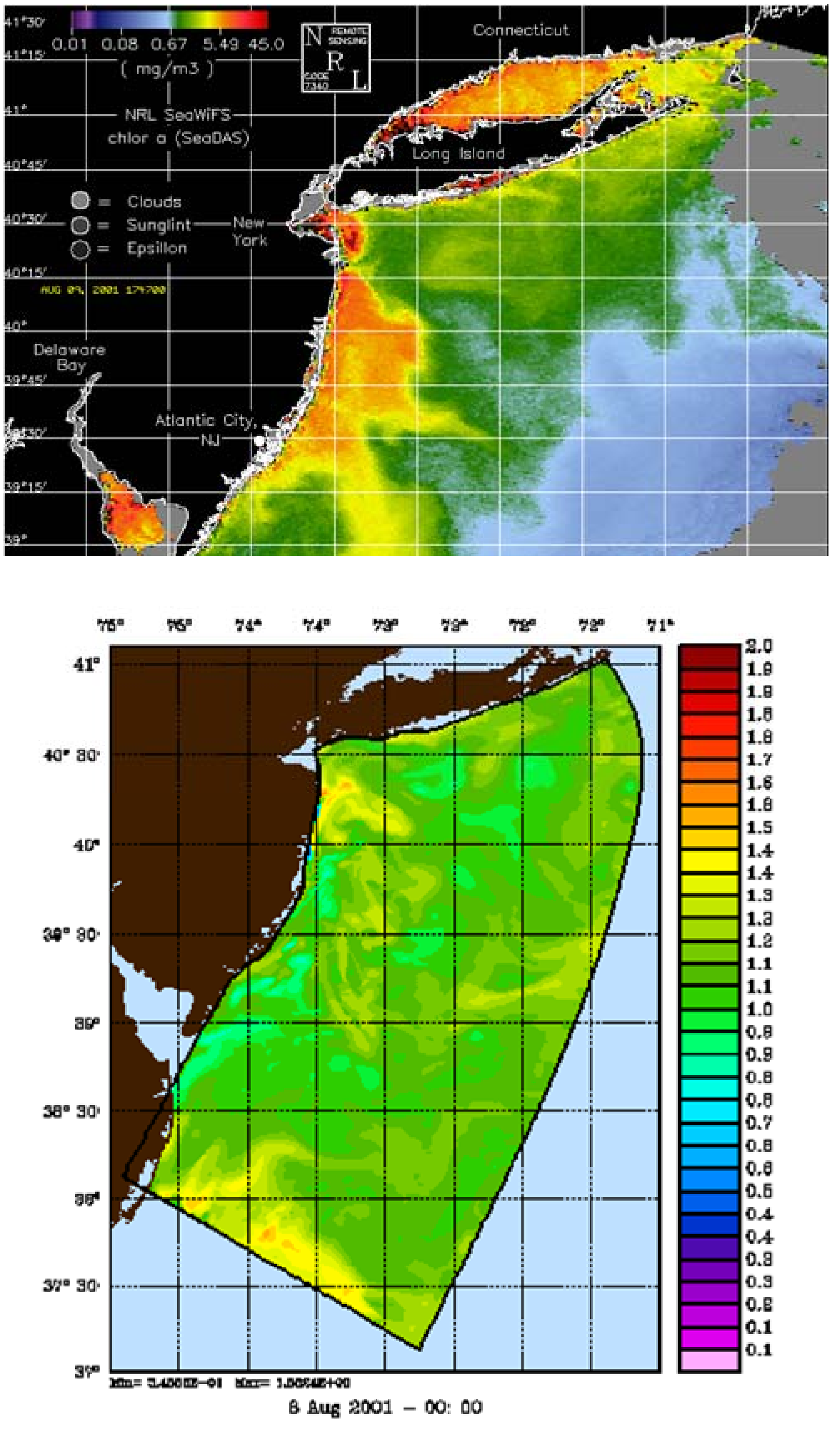

Figure 2. SeaWiFS Chlorophyll (top) and simulated Total Surface Chlorophyll (bottom) on August 8, 2001

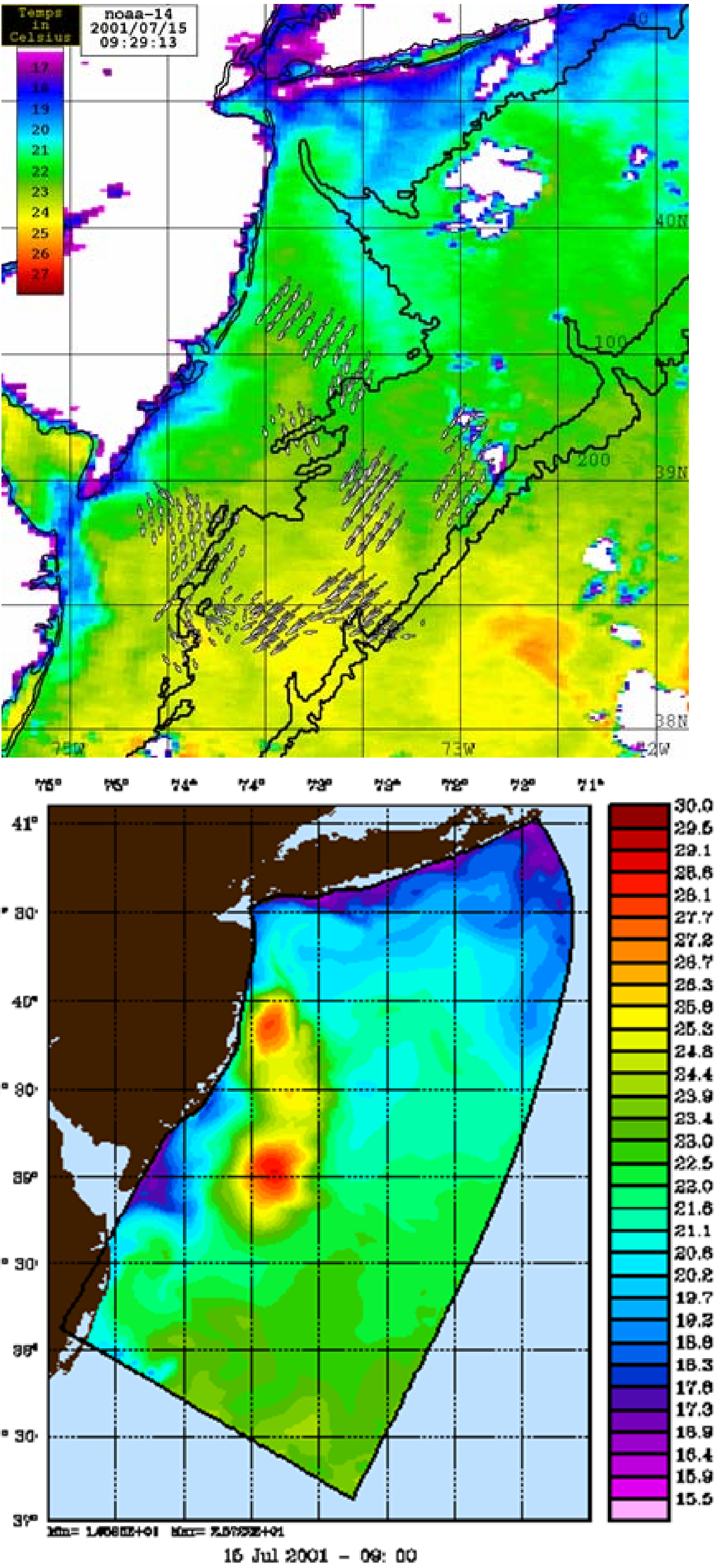

Figure 3. AVHRR SST (top) and simulated SST (bottom) on July 15, 2001

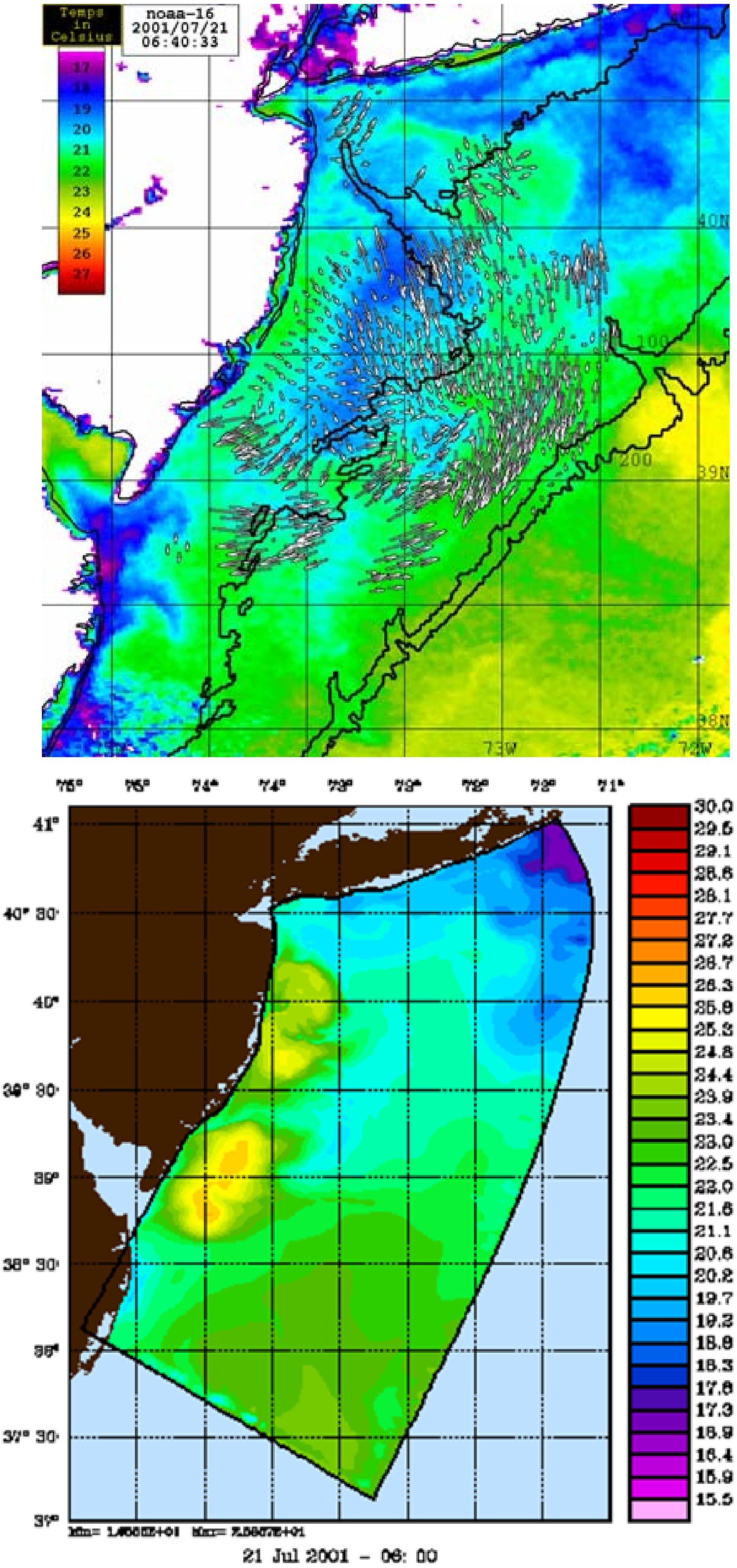

Figure 4. AVHRR SST (top) and Simulated SST (bottom) on July 21, 2001

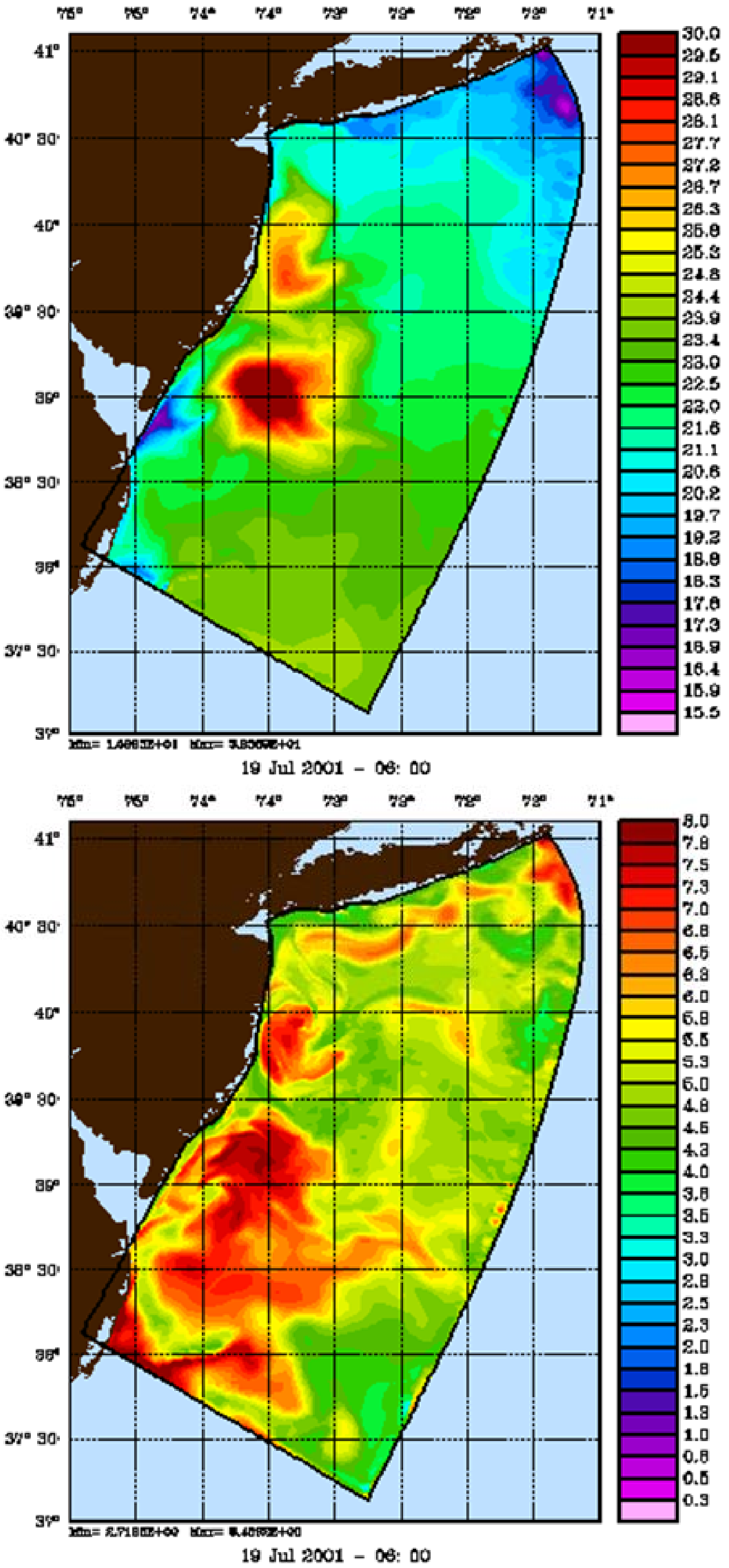

Figure 5. Simulated SST (top) and simulated NO3 (bottom) on July 21, 2001