EOS

Exploiting MODIS Data for Estimating Sea Surface Nitrate From Space

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A better understanding of the oceans' carbon cycle and a reduction in existing uncertainties in estimates of CO_2 fluxes between the atmosphere and the oceans have become central to several contemporary programs. Oceanic CO_2 fluxes are largely regulated by the "solubility pump" and the "biological pump." The solubility pump is governed by physical processes that include near-surface conditions at the air-sea interface, the partial pressure of CO_2 between the sea surface and the atmosphere, and the solubility of CO_2 in seawater.

The biological pump, in turn, is regulated by phytoplankton photosynthesis, which converts CO_2 to organic matter. The fraction of newly photosynthesized carbon exported to depth in the oceans is referred to as "export production" or "new production," and is largely dependent on exogenous nitrogeneous nutrient inputs, primarily nitrate into the euphotic zone [Eppley and Peterson, 1979].

In many oceanic regimes where the biological pump has a greater control on the distribution of CO_2 than the solubility pump, nitrate in seawater becomes critical to CO_2 flux measurements, because in most cases its concentrations determine the magnitude of carbon exported out of the euphotic zone. This is particularly true in regions where nitrogen inputs into the euphotic zone via nitrogen fixing organisms are insignificant, and trace elements such as iron are not limiting.

Despite its importance, shipboard nitrate measurements fall far short of the space and time scales required for climate research. Satellites have been suggested as a useful alternative. Although they can provide frequent, large-scale, near-surface views of several variables relevant to phytoplankton ecology such as incident radiation, chlorophyll, and sea surface temperature (SST), nutrient measurements have remained elusive as most nutrients including nitrate lack an electromagnetic signal that can be exploited from space.

Attempts have been made to estimate nitrate using proxies, one being temperature, which bears a strong inverse relationship with nitrate [Kamykowski and Zentara, 1986]. Seawater temperature and nutrient concentrations are tightly coupled because major inputs of nutrients such as nitrate and phosphate into the
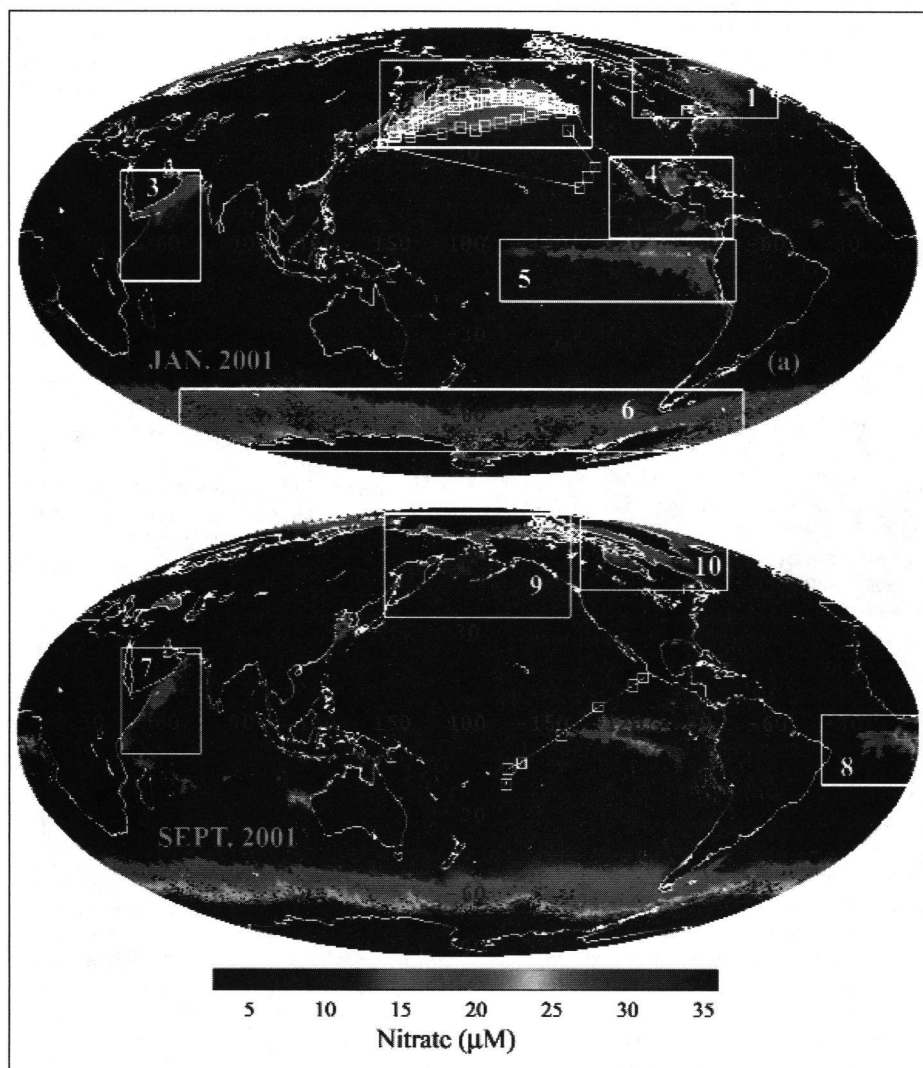

Fig. 1. Global images of surface nitrate concentrations for the world's oceans for (a) January 2001 and (b) September 2001, generated using MODIS Terra SST and chl a. Cruise tracks and stations sampled for validation the satellite-derived nitrate are shown in white open boxes. Prominent high nitrate features shown in boxes include winter convective mixing in the North Atlantic Ocean (1), North Pacific Ocean (2), and Arabian Sea (3); and upwelling off the California coast (4) in the equatorial Pacific (5) and Southern Ocean (6). Box 7 shows the Arabian Sea summer upwelling, and Box 8 shows upwelling along the northwest coast of Africa. Boxes 9 and 10 show the reduction in nitrate in the subarctic Pacific and in the North Atlantic at the end of the growth season of phytoplankton. Original color image appears at back of this volume.

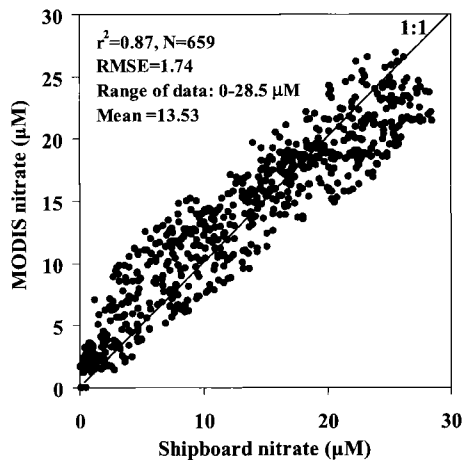BY J. I. GOES, H. DO R. GOMES, T. SAINO, C. S. WONG, AND C. W. MORDY

Fig. 2. Comparison of MODIS Terra and ship measurements of nitrate. The shipboard data were obtained during 22 trans-Pacific cruises between Canada and Japan.

euphotic zone occur when colder, nutrient-rich deeper waters are brought into the euphotic zone. However, estimation of nitrate based on T-nitrate relationships over large temporal and spatial domains has been frustrated by the time and space varying nature of these relationships [*Chavez and Service*, 1996].

One reason for these variations is that T-nitrate relationships do not account for nitrate changes that arise from phytoplankton photosynthesis and growth. In an earlier study [*Goes et al.*, 1999], it has been shown that if biologically mediated changes in the character of T-nitrate relationships are taken into account, it is possible to generate high-resolution maps of surface nitrate over much larger spatial and temporal scales than previously possible.

Development of Algorithm to Measure Nitrate from Space

An empirical algorithm to predict nitrate from SST and chlorophyll *a* (chl *a*, a major pigment necessary for photosynthesis and a measure of phytoplankton biomass) was developed using data from cruises conducted in the North Pacific from 1978 to 1996 and which covered a range of water types. Chl *a* was chosen as a predictor biological variable because of its known relationship with nitrate in the euphotic zone, and its accessibility from space in conjunction with SST.

The data were pooled together, irrespective of seasons and regions, but unlike previous studies, this analysis was restricted to surface water samples. Subsurface data were included only when the difference between SST and subsurface temperature was minimal (<0.2°C). This restriction ensured that all observations were well within the upper mixed layer. Exclusion of deep water data (where phytoplankton activity is minimal) prevented the strong signatures of T and nitrate in deeper waters from obscuring changes in the T-nitrate relationship that result from seasonal patterns in solar radiation and/or phytoplankton uptake.

Although nitrate appeared to be controlled primarily by T, the addition of chl *a* helped improve nitrate prediction, by reducing local and regional differences in the character of T-nitrate relationships resulting from phytoplankton uptake. The analyses yielded two algorithms, one for the equatorial region and the other for the nonequatorial region, both of which explained over 90% of the variation in surface nitrate concentrations.

This approach was first tested in an area off Sanriku, Japan, with local area coverage (LAC, 700-m resolution) SST and chl *a* images obtained concurrently by the multichannel sensor OCTS (Ocean Color and Temperature Sensor) on board the National Space Development Agency of Japan's ADEOS (Advanced Earth Observing Satellite) satellite. The satellite-derived nitrate values were then compared with an independent data set of shipboard measurements made over the same period during the validation exercise of OCTS.

It was observed that even when the area under investigation is small, nitrate predictions based solely on T were inappropriate, as the coefficient of determination (r^2) and the root mean square error (RMSE) based on the differences between measured and predicted values were 0.45 and 1.1, respectively, for nitrate values ranging from 2.3 to 7.8 µM. Adding chl *a* increased the r^2 to 0.94 and decreased the RMSE to about 0.39. The algorithms performed well when basin-scale estimates of nitrate for the North Pacific Ocean were generated using co-registered monthly global area coverage (GAC, 4-km resolution) SST and chl *a* images from OCTS, and compared with nitrate from 11 trans-Pacific Ocean cruises on board the MV *Skaugran* (r^2= 0.94, RMSE = 1.74, mean =11.19, range, 0–25.6 µM).

Nitrate Fields from MODIS

With the launch of MODIS (Moderate Resolution Imaging Spectroradiometer) on two NASA satellites, Terra (February 2000) and Aqua (June 2002), we are presented with another opportunity to obtain co-registered images of SST and chl *a* lost after the demise of ADEOS in June 1997. Here are presented the first basin-scale estimates of sea surface nitrate using MODIS (Terra) co-registered fields of chl *a* and SST for January and September 2001 (Figures 1a and b). MODIS level 3, chl a_2, and SST (D1) data with a spatial resolution of 4 km were used in this exercise.

Although these maps are based on algorithms developed using North Pacific Ocean data, they provide us with a synoptic view of nitrate in the world's oceans. These nitrate fields clearly show the spatial extent and magnitude of nitrate injection into the surface layer due to convective mixing in the subarctic Pacific and Atlantic Oceans in winter (January), and its consumption following the growth of phytoplankton (September).

They also depict the persistently high nitrate in the Southern Ocean and in the equatorial upwelling regions off the coasts of Peru and Northwest Africa. In January 2001, high nitrate concentrations due to upwelling along the coast of California are visible. In the northern Arabian Sea, enhanced nitrate due to winter convective mixing during the northeast monsoon (January), and coastal upwelling off the coast of Somalia during the southwest monsoon (September) are also seen.

A very large data set of nitrate measurements collected during the 2001 and 2002 trans-Pacific cruises of opportunity for different seasons and regions validated the MODIS-derived surface nitrate estimates. The results are presented in Figure 2. Strictly speaking, a comparison between the two data sets is not straightforward, as the satellite nitrate data are composites of pixels scanned on different days in one month whereas the shipboard data are point measurements. Despite this limitation, the results (r^2=0.87, RMSE=1.74, average 13.53, for a range of 0–28.5 µM) are very encouraging and show the immense promise of this method. Another comparison with an underway data set from the Gulf of Alaska yielded r^2 and RMSE values of 0.81 and 0.94, respectively, for nitrate ranging from 4.85 to 12.64, average 4.85 µM.

Accurate satellite nitrate estimates will depend on the precision of satellite-derived SST and chl *a*. The sensitivity of the algorithms to possible errors in these two satellite estimates has been addressed in detail by *Goes et al.* [1999]. The accuracy of MODIS, Terra SST (product D1) is within 0.2 K, so the maximum error in remotely derived nitrate concentrations that could arise from errors in satellite SST would be well within the 1 µM for the entire range of oceanic SSTs. Similar accuracy has been reported for MODIS Aqua SST product D1 (D. Yuan, personal communication. 2004). In the case of chl *a*, given that the overall accuracy of the MODIS Terra chl *a* products is between 20 and 65% for different water types, an error in nitrate estimates of ~1–2 µM is possible for chl *a* concentrations less or greater than 2.5 mg m⁻³. Presently the accuracy of Aqua chlorophyll is approximately 85%.

With these introductory maps, it is demonstrated for the first time the usefulness of co-registered SST and chl *a* imagery from MODIS Terra for measuring nitrate at basin to global scales. The newly calibrated MODIS Aqua now generating high-quality local and global chl *a* data presents the unique ability to map nitrate continuously and inexpensively.

The strength of this method lies in its simplicity and the ease with which the required inputs can be measured from space. The present nitrate algorithms rely solely on data from the North Pacific Ocean, and hence may not be universal in their application, as is evident, for example, off the coast of Peru, where nitrate values are slightly higher than reported in the climatological maps of *Conkright et al.* [2002].

It is believed that this approach of using chl *a* and SST to derive nitrate maps, when fine-tuned with regional and local data, would help reduce any regional biases in satellite-derived nitrate values, and it is encouraged that other investigators do so.

These nitrate maps, however, should not be considered a substitute for shipboard measurements, but rather tools that can extend ship observations and provide synoptic information on the variability in nitrate concentrations, especially at large scales. Any information from satellites over regional to basin and global scales has several obvious benefits over

conventional methods, the foremost being spatial and temporal coverage. This capability is particularly important in subpolar regions in winter, when shipboard cruises are difficult to conduct and the problem of undersampling is acute. In areas close to land masses where the physical boundaries of the water masses are more diverse and too dynamic to be understood by shipboard measurements alone, satellite data could be particularly invaluable.

Utility of Nitrate Maps

The idea of using satellite data as proxies for nitrate is not new. What is novel here is the concept of combining satellite temperature and chl a data to yield estimates of nitrate that are valid over much larger scales than attempted before. This is important particularly in studies related to climate change, as conventional methods pose the perennial problem of undersampling, such that shipboard data sets from several years have to be combined to generate maps of nitrate at the global scale. This is clearly a limitation of the conventional method if the purpose is to study interannual variations.

In previous and ongoing studies, the immense promise and potential of satellite-based nitrate maps for carbon cycling and climate change studies have been demonstrated [*Goes et al.*, 2004, and references therein]. It has been shown how satellite-derived nitrate could be exploited to estimate new production fueled by the supply of nitrate during winter convective mixing in the subarctic Pacific Ocean. These maps showed for the first time how El Niño mediated atmospheric disturbances over the North Pacific Ocean affect nutrient inputs and new production in the subarctic Pacific Ocean. In *Goes et al.* [2004], satellite-derived products aided historical shipboard

and meteorological measurements in establishing the mechanistic connections between El Niño events at the equator and carbon cycling in the North Pacific Ocean.

The inclusion of these nitrate maps in the recent report "A new vision of ocean biogeochemistry after a decade of the JGOFS study," by *Fasham et al.* [2001] on the principal achievements of the JGOFS (Joint Global Ocean Flux Studies) Program underscores the relevance of this work. The results of our ongoing studies are showcased at http://www.bigelow.org/elnino/. Presently, monthly nitrate maps for the period from 1997 to 2002 have been provided as PNG files. Further plans include providing these images on a regular basis as binary files, which will allow more flexibility to potential users.

Acknowledgments

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Author Information

Joaquim I. Goes and Helga do R. Gomes, Bigelow Laboratory for Ocean Sciences, Maine; T. Saino, Hydrospheric Atmospheric Research Center, Nagoya University, Japan, and Earth Observation Research and Application Center, Japan Aerospace Exploration Agency, Tokyo; C. S. Wong, Institute of Ocean Sciences, British Columbia, Canada; and C. W. Mordy, NOAA, Pacific Marine Environmental Laboratory, Seattle, Wash.

For additional information, contact J. Goes; E-mail: jgoes@bigelow.org

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Assessing Conceptual Models for Subsurface Reactive Transport of Inorganic Contaminants

In many subsurface situations where human health and environmental quality are at risk (e.g., contaminant hydrogeology, petroleum extraction, carbon sequestration, etc.), scientists and engineers are being asked by federal agency decision-makers to predict the fate of chemical species under conditions where both reactions and transport are processes of first-order importance.

In 2002, a working group (WG) was formed by representatives of the U.S. Geological Survey, Environmental Protection Agency, Department of Energy, Nuclear Regulatory Commission,

By J. A. DAVIS, S. B. YABUSAKI, C. I. STEEFEL, J. M. ZACHARA, G. P. CURTIS, G. D. REDDEN, L. J. CRISCENTI, AND B. D. HONEYMAN

Department of Agriculture, and Army Engineer Research and Development Center to assess the role of reactive transport modeling (RTM) in addressing these situations. Specifically, the goals of the WG are to (1) evaluate the state of the art in conceptual model development and parameterization for RTM, as applied to soil, vadose zone, and groundwater systems, and (2) prioritize research directions that would enhance the practical utility of RTM.

The WG is addressing issues related to the fate of reactive solutes in complex field systems, where spatially and temporally subsurface properties directly influence not only the physical processes of flow and transport, but also the rates and extent of biogeochemical reactions. Of particular interest is the interplay between physical and reaction processes, and how this coupling could be efficiently and

realistically accounted for in RTM. The WG has focused on the evaluation of conceptual models; improvement of numerical approaches and comparison of computer codes are outside the scope of WG activities.

The activities of the WG to date have included a literature review, internal meetings, and sponsorship of a workshop (see: www.iscmem.org for the full membership and background of the WG, and information on other interagency environmental modeling groups). The workshop included agency representatives and federal and academic specialists in model development, geochemistry, hydrology, and microbiology. This article summarizes findings of the WG to date with respect to the status of RTM for inorganic contaminants.

Technical Issues

A conceptual model for RTM represents the scientific understanding of processes controlling the movement and transformation of system components, including contaminants, for a specific water-rock system. For example, a conceptual model for a groundwater contaminant plume might include knowledge of (1)
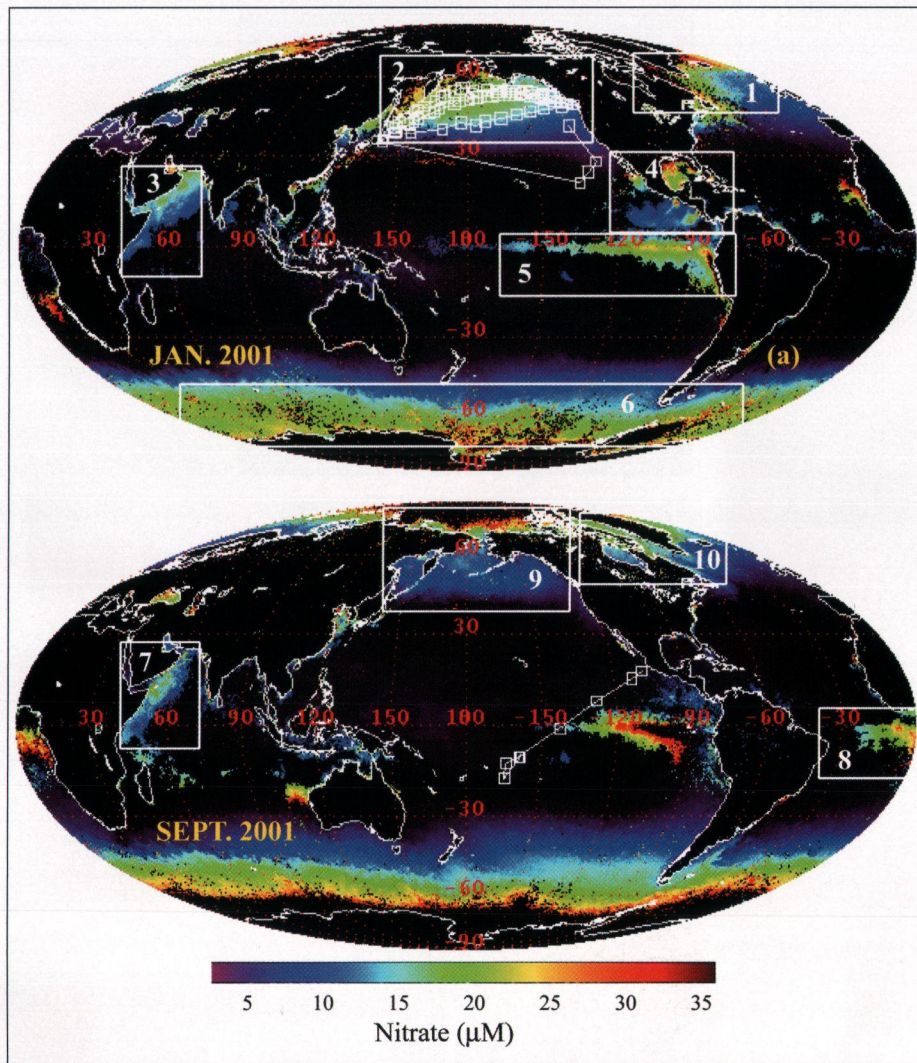
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