Semi-Annual Report for July-December, 2000
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Abstract

The activities of the second half of 2000 were concentrated on quality assurance (Q/A) for our products from the new MODIS data stream. We have updated our Case 2 chlorophyll a algorithms for MODIS using smooth functions for the transitions between different bio-domains. Two peer-reviewed papers have been submitted for publication, and three papers have been published. A number of presentations and symposium papers were presented.

Tasks Accomplished Since July 1, 2000

1. Field experiments

a. Ecology of Harmful Algal Blooms (ECOHAB) cruises- August 2-5, September 6-8, October 4-6, and November 7-10, 2000.

Jennifer Cannizzaro, Dan Otis, Jim Ivey collected remote-sensing reflectance and water samples for absorption during an ECOHAB West Florida shelf experiment. The data will be used to test and adapt the global chlorophyll and CDOM algorithms for presence of bottom-reflected radiance in SeaWiFS and MODIS data.

b. Florida Shelf Lagrangian Experiment (FSLE) cruises and PHILLS hyperspectral overflight at 10 km – July 1-10, and Nov 4-14, 2000.

Robert Steward, Jennifer Cannizzaro, David English, Daniel Otis, and Jim Ivey collected remote sensing reflectance and water samples for absorption during two FSLE experiments. The PHILLS was flown on several transects over the area with vicarious calibration measurements conducted by USF from the R/V Suncoaster. The USF slow-drop package was also deployed to collect inherent and apparent optical properties as a function of depth for an evaluation of effects of vertical structure on remote sensing spectra. These data will be used to modify MODIS algorithms for use in shallow waters.

2. Presentations & Symposiums

a. A paper named "MODIS Case 2 Ocean Color Algorithms: Use of MODIS SST to Condition the Bio-optical Domains via Nitrate-Depletion Temperatures" by K. Carder, R. Chen, J. Patch, and J. Brown will be presented at MODIS science team meeting in January at GSFC.

The chlorophyll-specific absorption coefficient at 443 nm, ${}^{*}a\_(443)$, of phytoplankton-rich particles in the ocean can change on a global basis by a factor of 8 to 10 (e.g. see Bricaud et al. 1995), making extremely difficult any accurate conversion from absorption coefficients (optical properties actually determined with MODIS) to chlorophyll *a* concentrations, [Chl *a*]. MODIS team objectives are to determine chlorophyll *a* values to better than 35% (Esaias et al. 1998), a significant task. It is only because many phytoplankton optical properties co-vary with [chl *a*] that historical pigment algorithms retrieve values within 50-100% (see O'Reilly et al 1998). For waters rich in colored dissolved organic matter, CDOM, however, or those with low pigment concentrations at high latitudes, even these co-variations disappear, requiring algorithms that distinguish between pigments and CDOM and adjust for variations in *a_(_) through an independent variable (Carder et al. 1999).

The nitrate-depletion temperature (NDT) for a given oceanic location is the temperature above which the nitrate concentration becomes negligible (Kamykowski 1987). It is indicative of a place where a major transition is occurring in the types of phytoplankton that can successfully compete for resources. Comparing the sea-surface temperature (SST; Fig. 1) to the nitrate-depletion temperature (Fig. 2) provides a means of estimating nutrient availability and allows partitioning into bio-optical domains (Fig. 3), each with much smaller ranges of *a_(_) (Carder et al. 1999). This allows the ratio of chlorophyll *a* to accessory pigments and cell optical size to change with bio-optical domain (e.g. summer versus spring in the Sargasso Sea; Bissett et al. 1999 a, b) and hence the particle absorption determined from MODIS to be more accurately interpreted in terms of chlorophyll *a* concentration. A transect from the Sargasso Sea in late spring across the Gulf Stream toward the Gulf of Maine provides a change of than 10^{o} C within less than 30 km (Fig. 1), suggesting dramatic bio-optical changes in just a short distance.

Operationally, the MODIS chlorophyll *a* algorithm (MOD_chl_a_3), released by the MODIS data archive (DAAC) in November 2000, uses weekly averaged SST values (Reynolds and Smith 1994), which were composited into 1^{o} x 1^{o} bins prior to availability of calibrated MODIS SST values. The low temporal and spatial resolution of these composites, however, caused switches between bio-optical domains to occur at locations that were not always regions of thermal gradients, implanting artificial steps in otherwise uniform chlorophyll fields (Fig. 4). While seasonal changes away from the edges of large biomes are more likely to be properly expressed with the low-resolution Reynolds SST values, transitional regions, such as those represented in Figure 1, require high-resolution synoptic SST data.

Implementation of MODIS-derived SST values for use in selection of bio-optical domains removes the effects of mismatched temporal and spatial scales between the SST and radiance fields, providing synoptic domain selection on a pixel-by-pixel basis. Developing a smooth transition rather than step-wise algorithm switches across bio-optical boundaries (Fig. 5) also mitigates striping effects due to minor inconsistencies in calibration and round-off errors among each of the 10 detector elements per band that simultaneously and contiguously view a given nominal 10-km swath of the ocean. Adjacent 10-pixel swaths at times are inconsistent due to calibration difficulties between difficult mirror sides, and the effects are evidenced in retrievals dependent upon the thermal channels (Fig. 1) or the short-wave visible channels (Fig. 6). These problems are continuing to be addressed in the calibration and validation activities by the MODIS team, but smoothing the transitions between bio-optical domains (Fig. 5) mitigates much of the effect on the chlorophyll fields as shown below.

This contribution provides a step-wise demonstration of the improvements made to the semi-analytical Case 2 chlorophyll algorithm for a region and time of year when gradients are maximal in thermal and bio-optical fields. The changes in algorithm performance are striking, especially when compared with results from the same algorithm locked in a single bio-optical domain with global packaging parameters for parameter-ization of the bio-optical model. The transition from a one-domain (Fig. 7) to a four-domain model (Fig. 8) is amazing, with lower chlorophyll values in the Gulf Stream and higher values in the Gulf of Maine for the four-domain approach. The improvements using MODIS (Fig. 8) versus Reynolds and Smith SST values (Fig. 4) are also clear, with crisp transitions at appropriate places, a wider dynamic range of chlorophyll values, and a reduction banding effects when smooth transitions between bio-optical domains are implemented.

While field values of chlorophyll *a* for May 2000 have not yet reached the major data archives, values for May in 1997-1999 for the region north of the Gulf Stream are in the 2 to 8 mg/m^3 range, consistent with Chl_a_3 values shown in Figure 8. Note that more-traditional algorithms (Chlor_modis) produce unreasonably high chlorophyll values (> 30 mg/m^3, Fig. 9) for the high-gelbstoff regions (see Fig. 6). Furthermore, values in the Gulf Stream are not low enough (note the change in the scale of the color bar).

The bio-optical domains developed using the nitrate-depletion temperature approach should also be useful in designating regimes where various species and quantum efficiencies for photosynthesis prevail. These domains could be augmented using with silica-depletion temperatures (Kamykowski 1987) to define where silica would be limiting the growth of diatoms and with phosphate-depletion temperatures to determine where phosphorus would limit the growth of nitrogen-fixing, autotrophic bacteria. These bacteria also have a higher demand for iron than other phytoplankton because of their need for making nitrogenase to fix nitrogen. Thus riverine and aeolian sources of iron also need to be considered in calculating phytoplankton growth rates and resource competition within the marine food web (Lenes et al., accepted).

The MODIS code is being updated to provide results consistent with the prototypical results shown above. Changes include a pixel-by-pixel domain selection using MODIS SST values and a linear smoothing function implemented to provide for transitions between bio-optical domains (Fig. 5). This includes an additional hyper-packaged domain to address high-latitude phytoplankton regimes such as encountered by Mitchell and Hansen (1991) near the Antarctic. The thermal contrast in the scene is caused by the warm Gulf Stream with tiny, subtropical phytoplankton juxtaposed with the cold Labrador Current with large, diatom-rich assemblages. Icebergs are still prevalent in May in the Labrador Current, which feeds into the region north of the Gulf Stream, and it is a region of fairly high gelbstoff (Walsh et al. 1992). Rivers also provide nutrients to the coastal waters of the region, gelbstoff and diatoms, requiring an algorithm that separates phytoplankton absorption spectra from gelbstoff spectra, and characterizes the phytoplankton absorption in terms of chlorophyll *a* concentration through an adaptable chlorophyll-specific absorption coefficient. The Chl_a_3 algorithm does this, while others do not.

The absorption coefficient at 400 nm due to gelbstoff (a_g[400]) (Fig. 6) is more sensitive to striping than is Chl_a_3 as it is more dependent upon the stripe-rich 412 nm channel of L_w. While not too severe on the right-hand sides of imagery, L_w values at 412 and 443 nm are especially sensitive to striping on the left-hand sides of images (e.g. Fig. 10). Until calibration consistency is achieved among the 10 elements and two mirror sides of Terra, the ability to separate the effects due to gelbstoff from those due to phytoplankton using the 412 and 443 nm channels will be severely limited. Over-estimates of chlorophyll *a* by as much as 5-fold for gelbstoff-rich, spring, high-latitude waters will not be unusual if we are forced to use only the longer-wavelength (> 443 nm) channels because of the striping problems of Terra.

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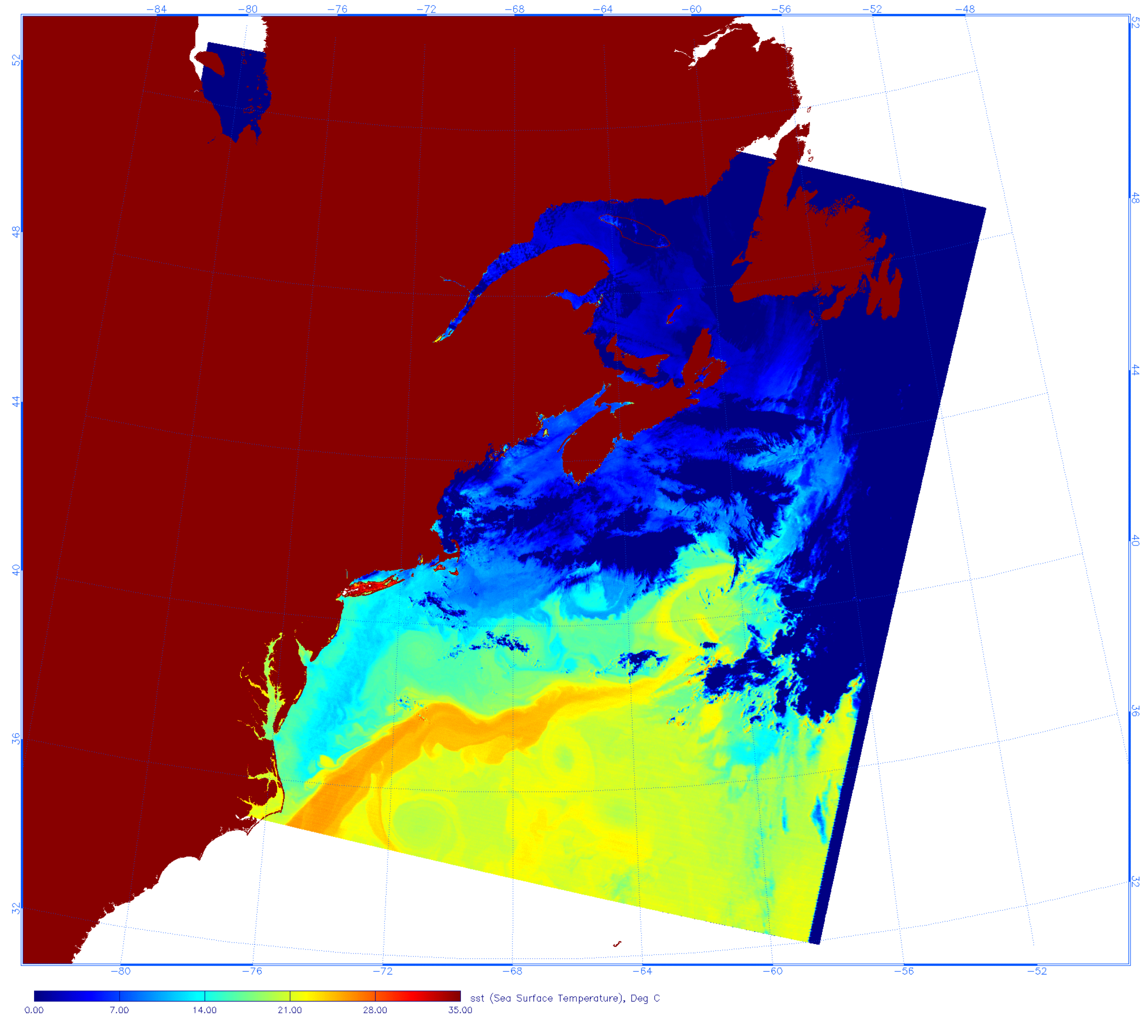

Figure 1 Sea-surface temperature (SST) retrieved from MODIS for Julian Day JD129, 2000.

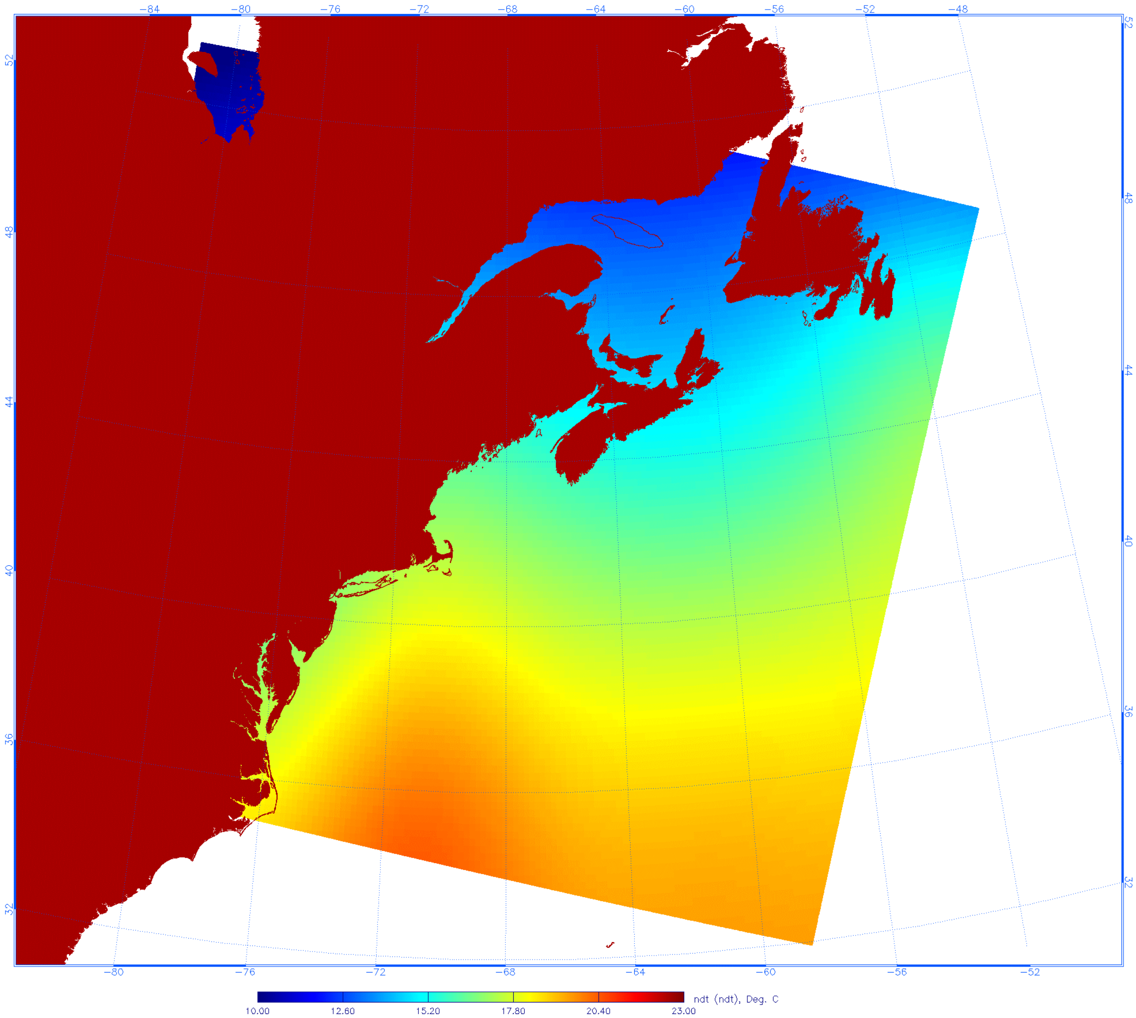

Figure 2 Nitrate-depletion temperature (NDT) variation for the study area.

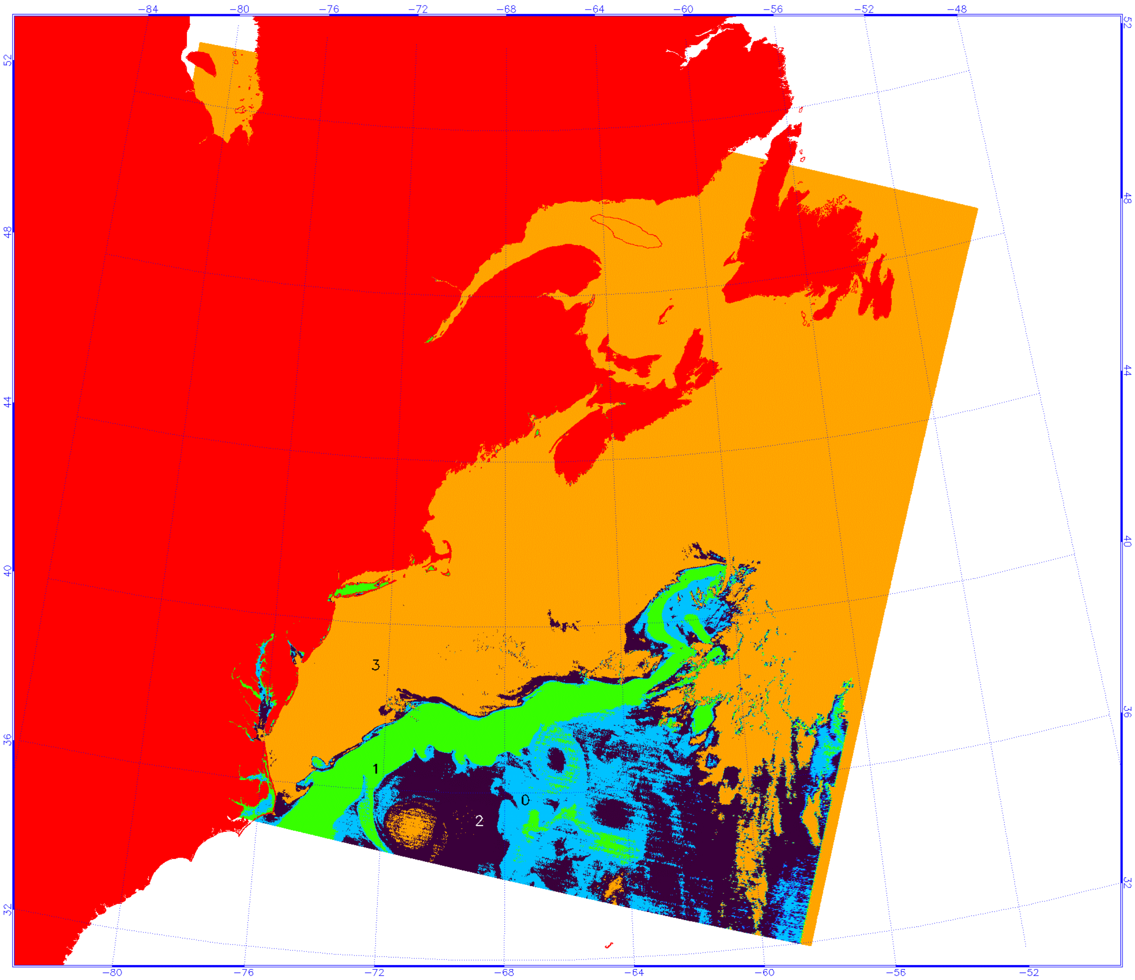

Figure 3 Bio-optical domains for JD129 from MODIS SST-NDT values sorted as shown in Fig. 5.

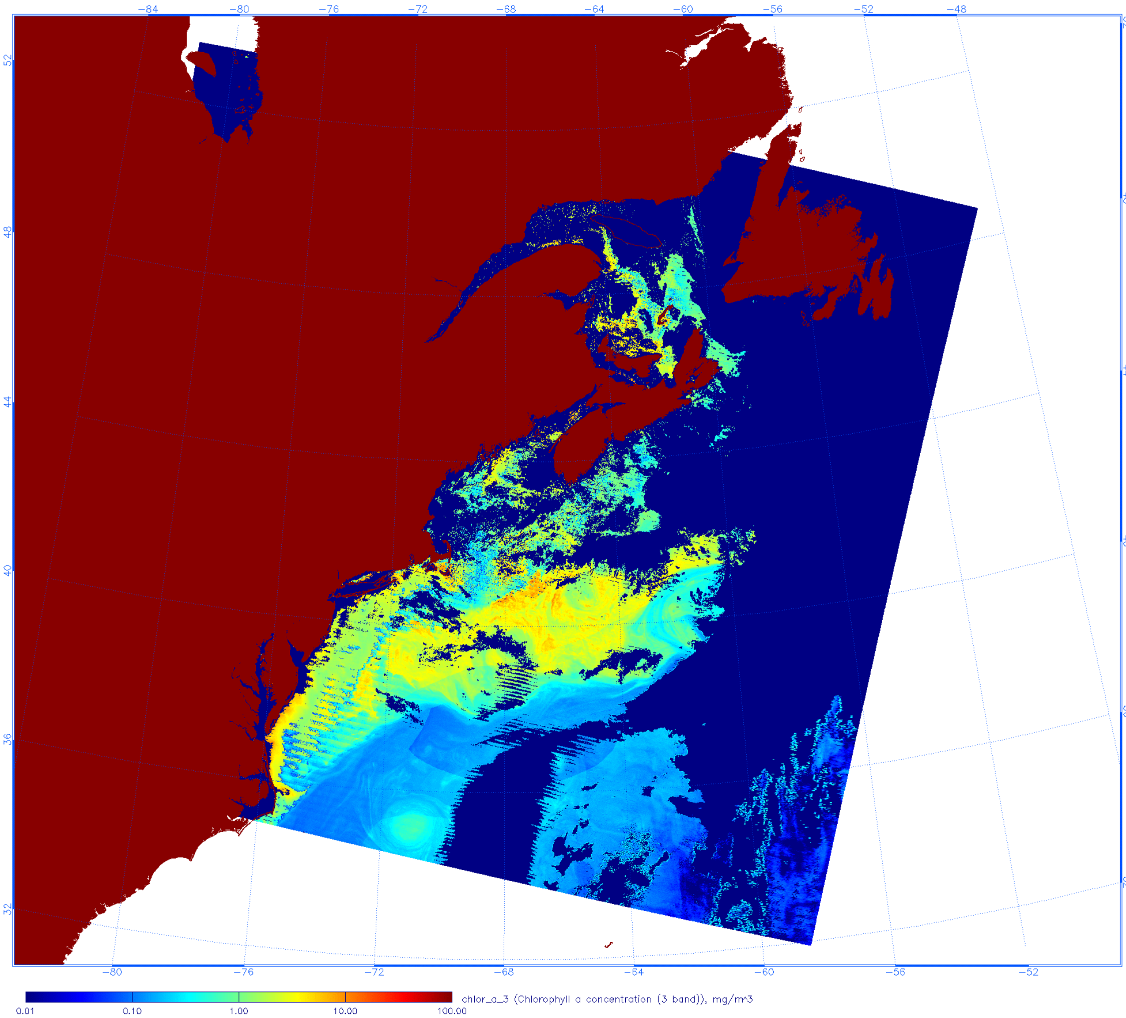

Figure 4 Chlorophyll *a* concentrations derived using the Carder et al. (1999) algorithm with MODIS water-leaving radiances, but Reynolds and Smith (1994) weekly-composited (1^o x 1^o) SST values were used for selecting bio-optical domains. Note the odd chlorophyll gradient in the Gulf Stream, the non-circular cold-core eddy, and the step-gradient parallel to but north of the north wall of the Gulf Stream resulting from coarse-resolution and one-week composit of SST data.

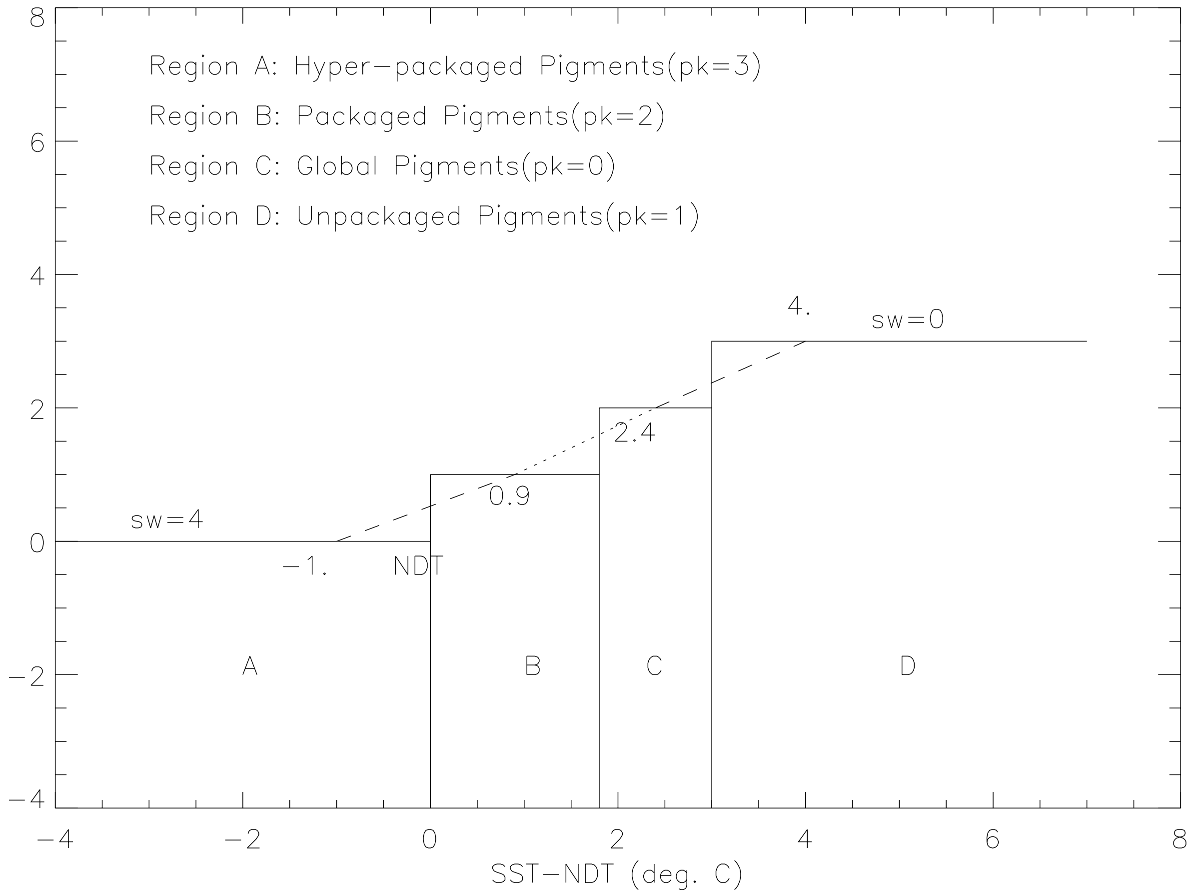

Figure 5 Sorting schematic for bio-optical domains using SST-NDT: pk0 = global; pk1 = unpackaged; pk2 = packaged; and pk3 = hyper-packaged. Once the domains are established, the transitions between domains result from mixing of derived chlorophyll values for each domain weighted according to the dotted gradient lines.

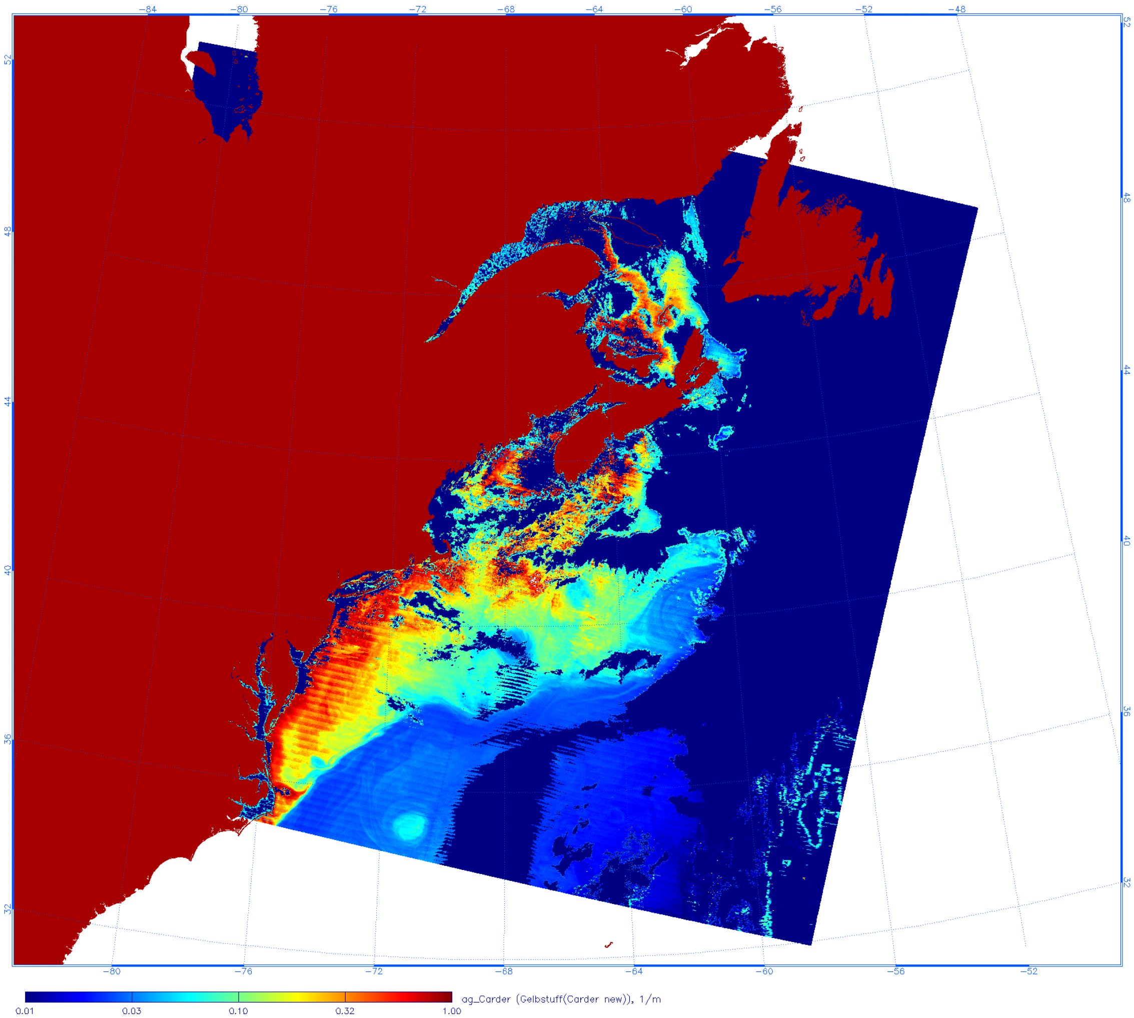

Figure 6 Absorption coefficient due to gelbstoff at 400 nm. This algorithm is especially dependent on good calibration of the 412 nm and 443 nm channels (see Carder et al. 1999).

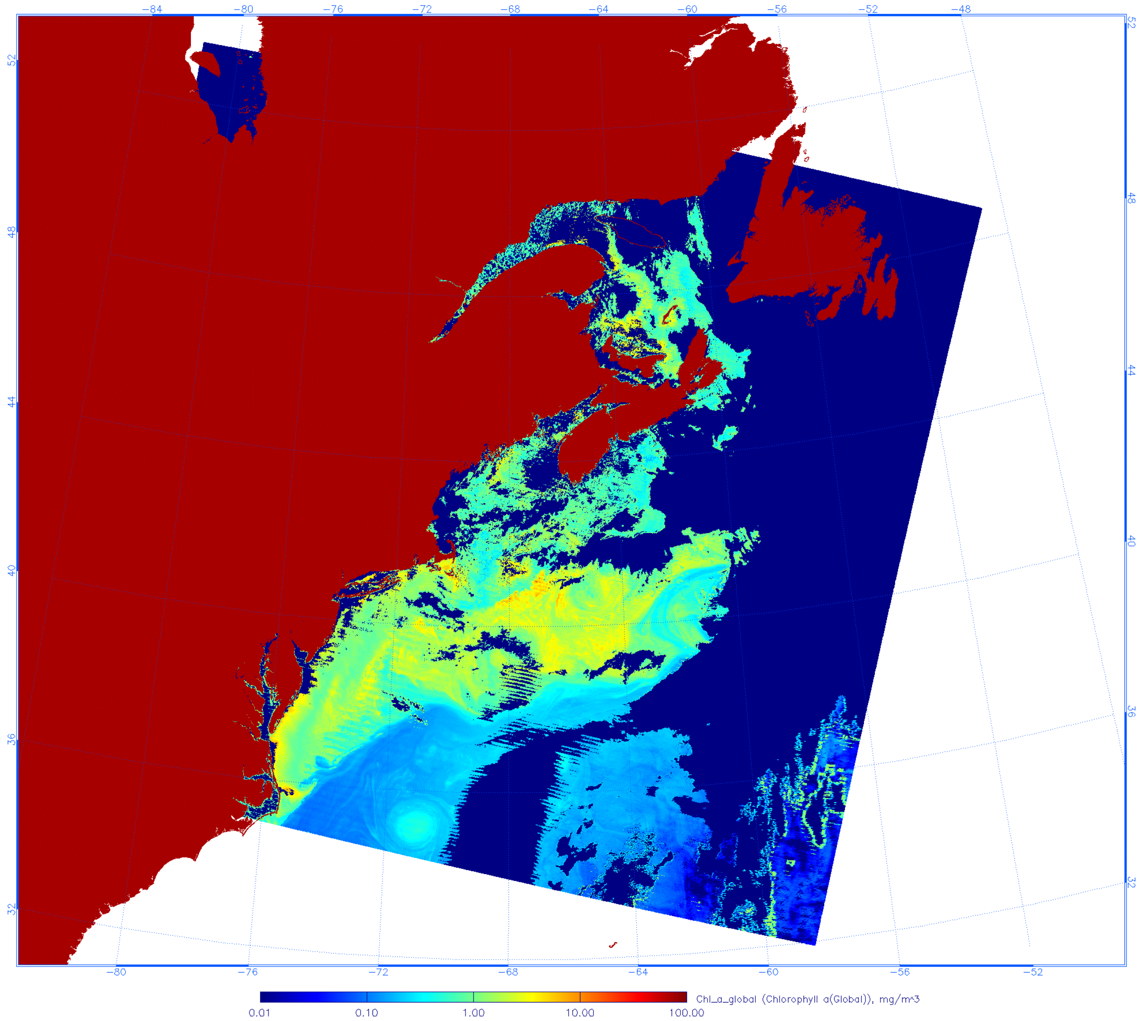

Figure 7 Chlorophyll *a* concentrations derived using the Carder et al. (1999) algorithm with MODIS water-leaving radiance values, obtained using a fixed, global parameterization of the package effect (pk=0; see Fig. 5) rather than using four different domains.

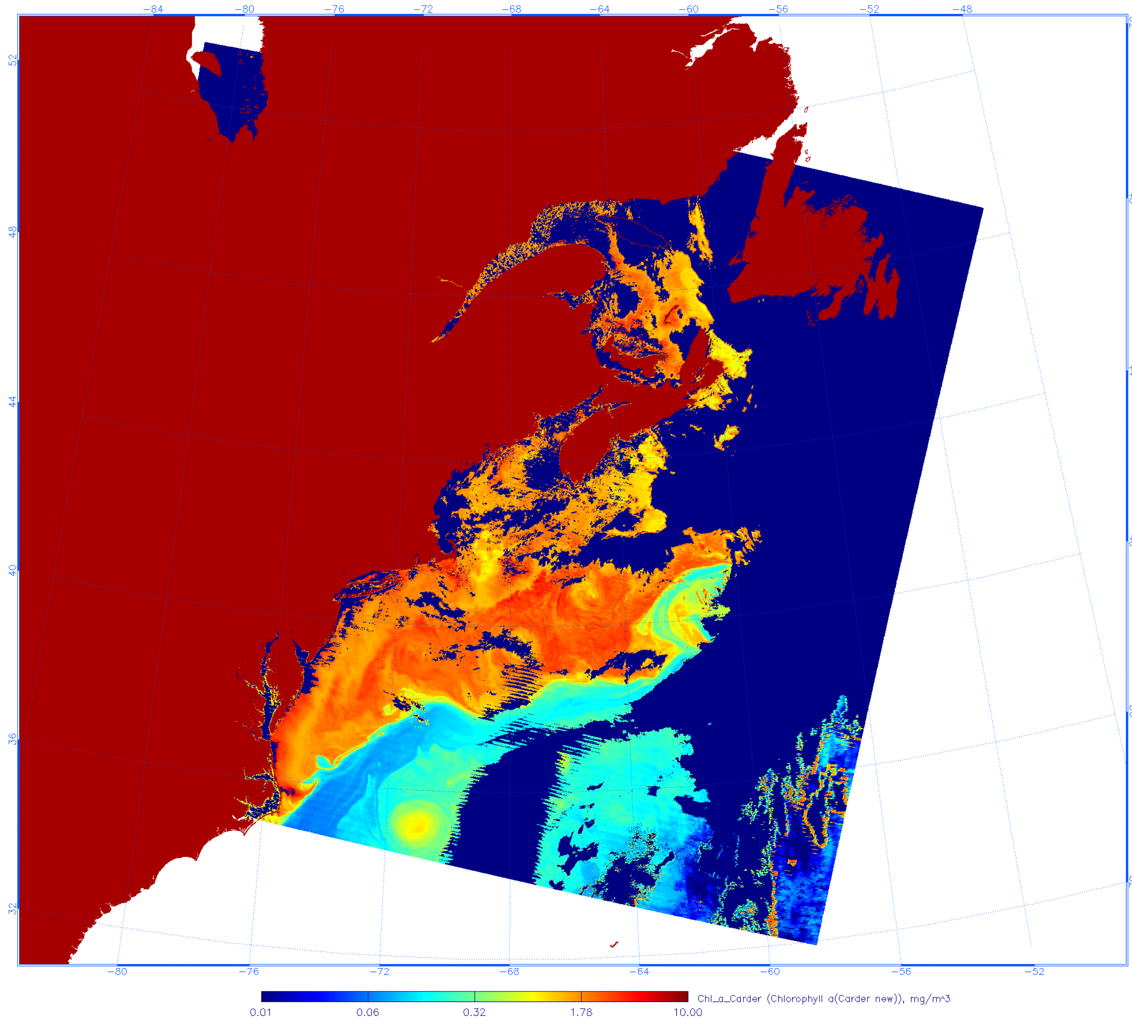

Figure 8 Chlorophyll *a* concentrations derived using the Carder et al. (1999) algorithm with MODIS water-leaving radiance values, obtained using the four different domains with smooth transitions as shown in Figure 5.

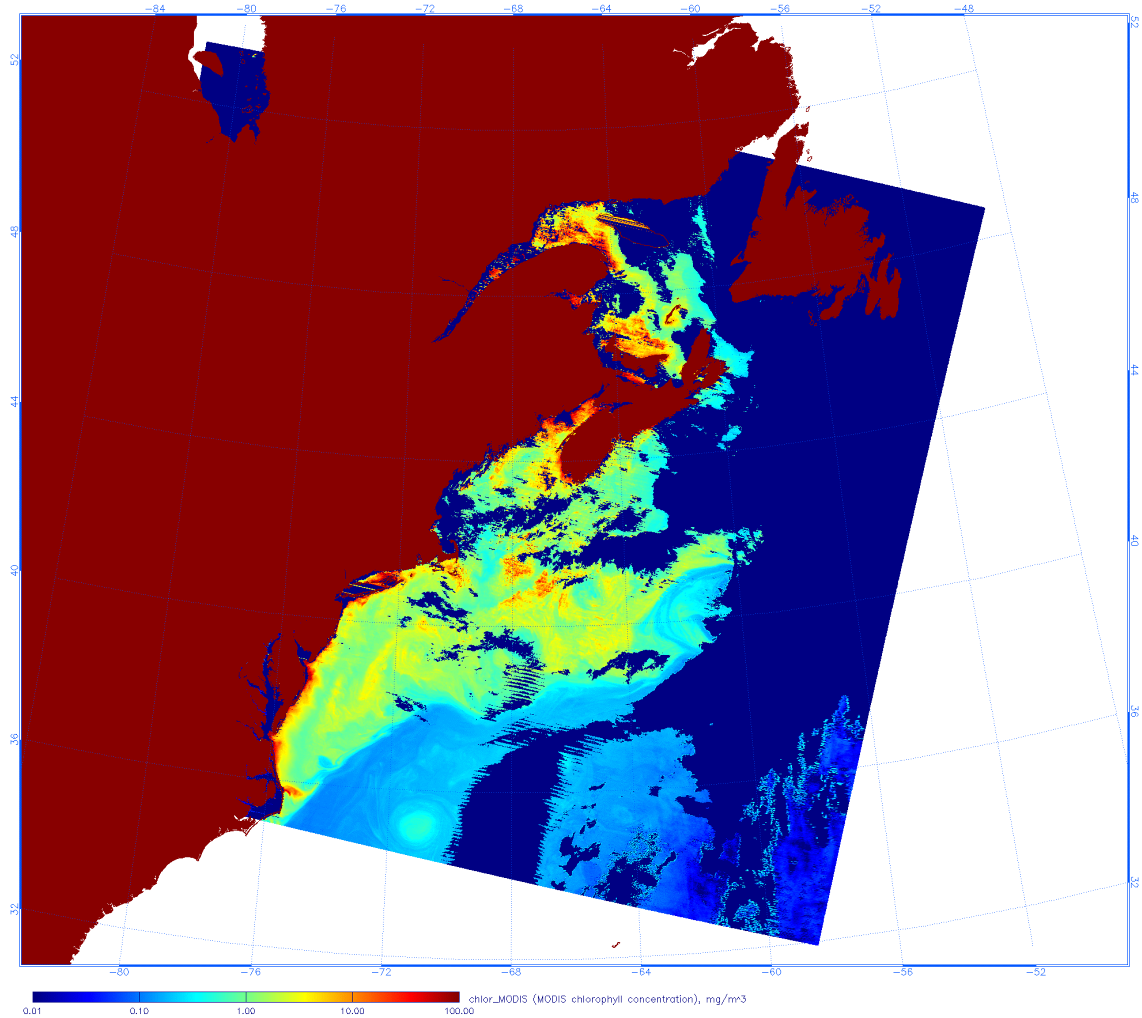

Figure 9 Chlorophyll *a* concentrations derived using the Chlor_MODIS band-ratio algorithm with MODIS water-leaving radiance values.

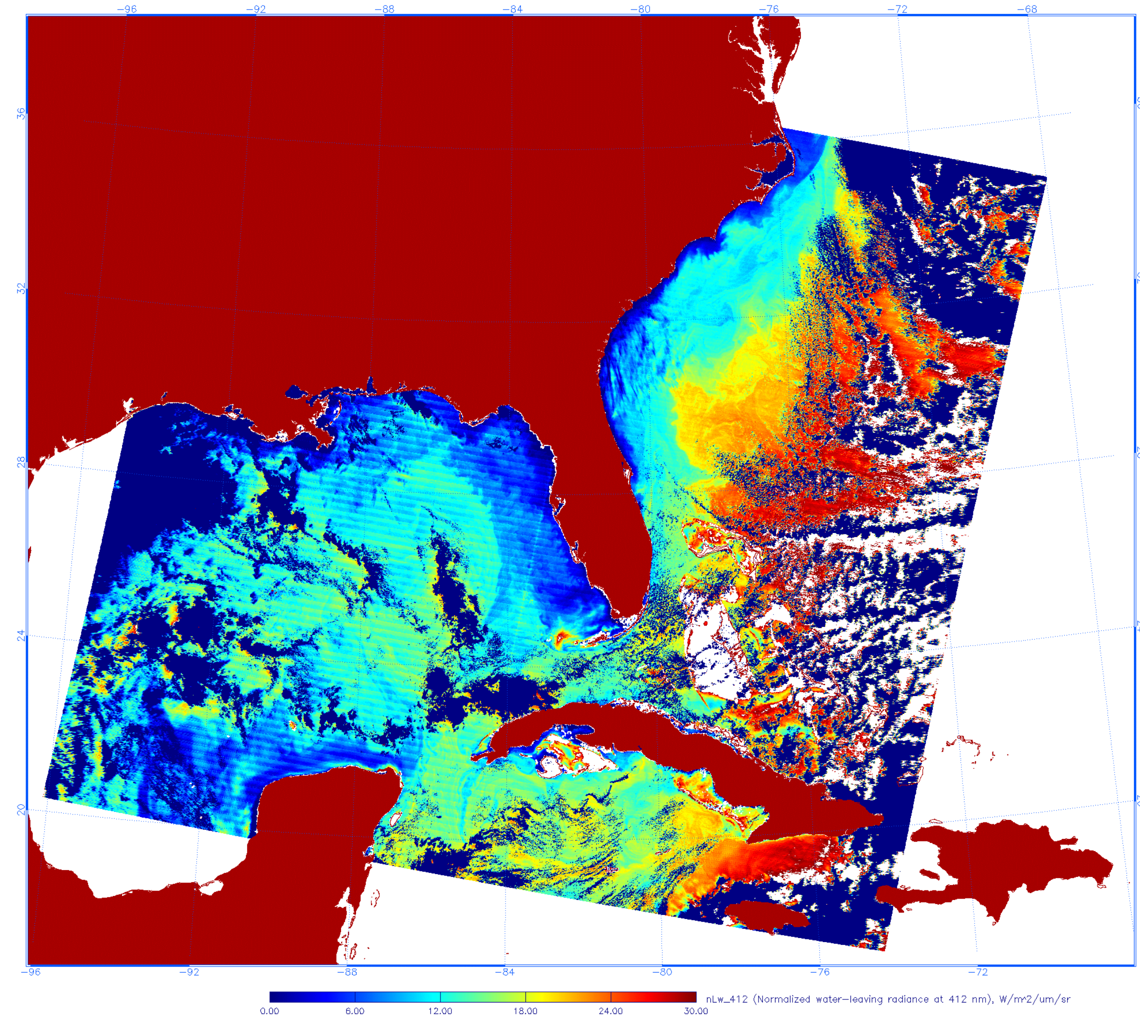

Figure 10a Normalized water-leaving radiance values at a) 412 nm and b) 443 nm for the Gulf of Mexico on Julian Day 306 2000. Note the most severe striping occurs on the west sides of the image.

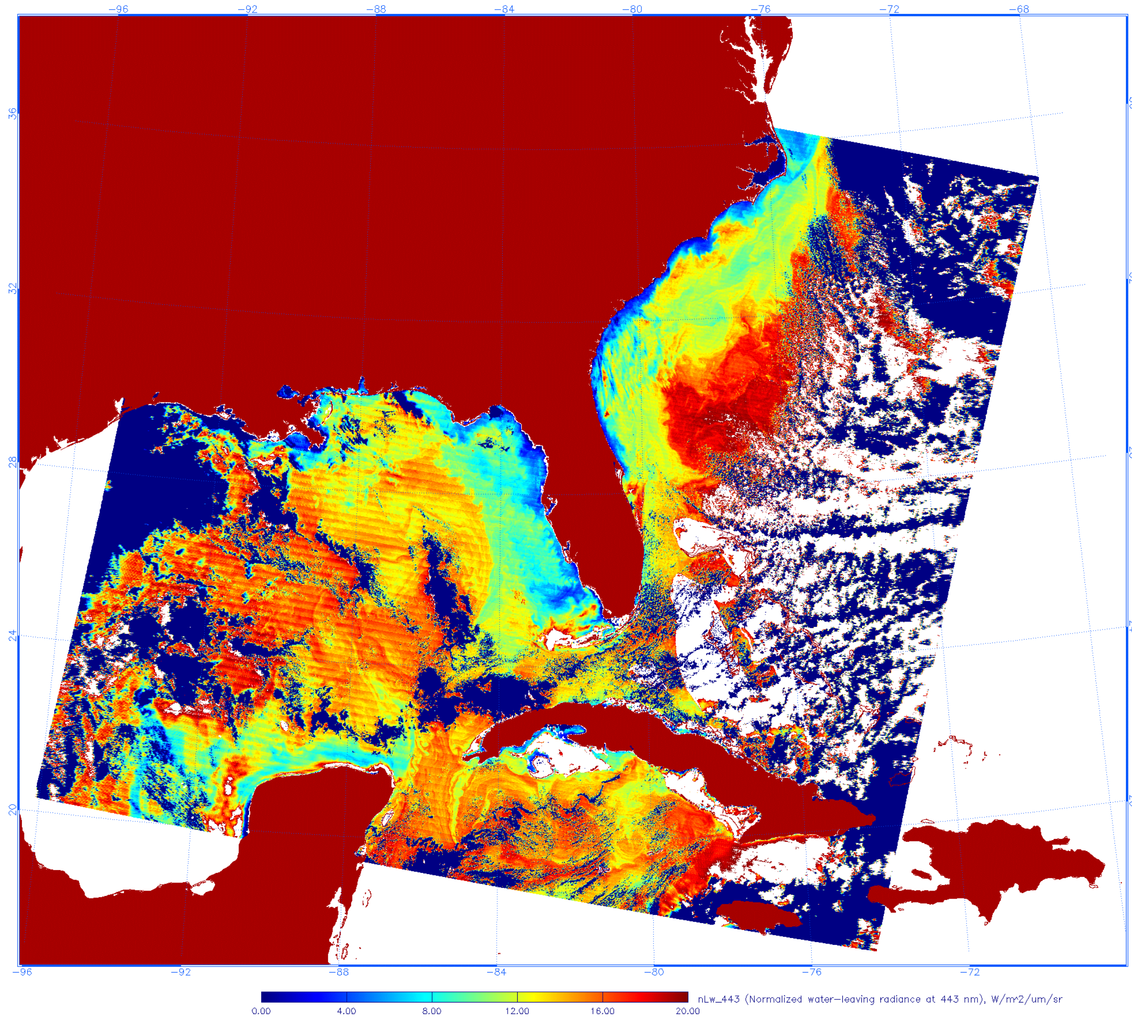

Figure 10b Normalized water-leaving radiance values at a) 412 nm and b) 443 nm for the Gulf of Mexico on Julian Day 306 2000. Note the most severe striping occurs on the west sides of the image.

b. Paper entitled "HYPERSPECTRAL REMOTE SENSING OF SHALLOW WATER ENVIRONMENTS: A REVIEW" by Zhongping Lee and Kendall L. Carder was presented at *Remote Sensing of the Atmosphere, Environment and Space* conference in Sendai, Japan, October, 2000, and it appears in the Symposium volume.

In this study, we show an advanced technique that can be used to retrieve properties from images of shallow coastal areas. To test this technique, we applied it to a recently collected AVIRIS image over Tampa Bay (Florida). It is found that information about the properties of the water column and bottom can be adequately retrieved. The derived properties include bottom depth, bottom albedo, water absorption coefficients, and particle backscattering coefficients. The derived bottom depths were compared with bathymetry charts and found to agree very well. Also, the derived image of bottom albedo shows distinct bottom patterns, with albedo end-members consistent with sand and seagrass. The images of absorption and backscattering coefficients indicate that the water-column properties were not horizontally uniform, though with much less variation than bottom depth or bottom albedo. There were no apparent co-variances among the retrieved variables. The data used in the retrieval process were obtained from AVIRIS, with no need for *in situ* data from the water required for the retrievals.

c. Paper entitled "PURE WATER ABSORPTION COEFFICIENT AROUND 400NM: LAB MEASURED VERSUS FIELD OBSERVED" by *Zhongping Lee, James E. Ivey, Kendall L. Carder, Robert G. Steward, and Jennifer S. Patch* was presented in SPIE, Ocean Optics 2000 in Monaco, France, October, 2000.

From numerical studies, it has been found that remote-sensing reflectance (or irradiance reflectance) of optically deep waters is a function of the ratio of the backscattering coefficient to the absorption coefficient (or the sum of absorption and backscattering coefficients), when there is no contribution from in-elastic scattering such as Raman scattering and fluorescence. In general, reflectance can be well explained (or modeled) using known absorption and backscattering coefficients of pure water, plus measured pigment absorption coefficients and bio-optical models regarding the absorption coefficient of gelbstoff and backscattering coefficient of particles. Recently, we found that there are some residual distinct mismatches near 400nm for clear waters. Checking literature values of the absorption coefficients of pure waters, it is found that there are wide variations from measurement to measurement, especially at blue-green wavelengths. For the consistent mismatch observed for various clear waters, we suspect that one possible source may be the uncertainty of reported pure-water absorption values, since pure-water absorption plays a larger role for clear waters. For coastal waters, the mismatch was not as apparent. To compare various pure-water absorption curves, we spectrally decomposed remote-sensing reflectance into spectra for absorption coefficients of pigments, water and gelbstoff and backscattering of particles, and assign the residual differences between measured and modeled R_{rs} to pure-water absorption coefficients.

When comparing the derived a_w values with lab-measured values [Pope and Fry, 1997], it is found that 1) there is a substantial, high-resolution curvature difference around 400nm, and 2) the values could differ by as much as 20% from 380 to 420nm. The derived values, however, were more consistent with those from in-water diffuse attenuation measurements, but it is not clear yet what could be the possible reasons for the mismatch between the lab values and various field observations. Other than the wide variations among the reported pure-water absorption values, possible explanations are that absorption by gelbstoff and backscattering by particles may not be smooth functions of wavelength as are commonly used, and that bacteria may be a perturbing factor near 400nm.

d. Paper entitled "SATELLITE PIGMENT RETRIEVALS FOR OPTICALLY SHALLOW WATER" by Kendall L. Carder, *Zhong Ping Lee and F. Robert Chen* was presented at SPIE, Ocean Optics XV in Monaco, France, October, 2000 and appears in the symposium volume CDROM as paper 1134.pdf, 9pp.

The inner continental shelves of the world ocean play important roles in terms of transitioning riverine water, carbon, and nutrients to the ocean. This region provides cover for larval fish and other larvae as well as food for grazers, with major phytoplankton blooms typically found at the mouths of estuaries. The inner shelf supports primary production by phytoplankton, macrophytes, benthic micro-flora (e.g. benthic diatoms), and by recycling nutrients through the benthic community, providing annually up to 2800 g C m^{-2} for kelp forests and from 120 to 1000 g C m^{-2} for other macrophytes (Lalli and Parsons 1993), and as much as 892 g C m^{-2} by benthic microflora (Grontved 1962). In fact for oligotrophic shelves, there are usually higher areal chlorophyll concentrations and primary productivity in the sediments than found in the overlying water column, sometimes by as much as 4 to 6 fold (Cahoon and Cooke 1992).

In order to retrieve the bottom depth, the water-column contributions and optical properties of the water column must be known or derived. Similarly, to retrieve water-column properties, the bottom contribution must be known or derived. Historically, values for water-column contributions were approximated from values of adjacent deep waters [e.g., Polcyn et al. 1970; Lyzenga 1978, O'Neill et al. 1989], and light-attenuation values were assumed known *a priori* [e.g., Polcyn et al. 1970, Paredes and Spero 1983], or they were empirically derived from an image by regression using a few known depths provided by LIDAR or on-site ship measurements [Lyzenga 1985, Philpot 1989]. All of these methods require knowledge of a few actual depths or accurate attenuation values.

To be able to derive properties of shallow-water environments routinely, it is desired to ***simultaneously*** derive bottom depth and albedo and the optical properties of the water column. The model-driven optimization technique developed by Lee et al. [1999] demonstrated that most of the underwater information could be derived from hyperspectral, measured remote-sensing reflectance, and Lee et al. [accepted] have derived accurate bathymetry and water-column properties for turbid Tampa Bay

($1<c<2.5$ m^{-1}) using Airborne Visible Infra-Red Imaging Spectroradiometer (AVIRIS) data. AVIRIS data has 20-m pixels and 10-nm spectral resolution from 400 to 2400 nm, appropriate for bays and estuaries, but not for repeatedly examining large areas such as the west Florida shelf. By binning pixels and spectral channels, however, AVIRIS data provides a means of simulating the performance of several different sensors such as MODIS.

AVIRIS data are used to simulate the utility of MODIS or SeaWIFS data to remove bottom effects from shallow-water imagery for the WFS collected from space. The primary-modal chlorophyll values (Fig. 2a) corrected for bottom effects using methodologies developed by Lee et al. [1999] are consistent with historical data for the region. The uncorrected values (Fig. 2b) and those under the secondary peak for the "corrected" histogram, however, are higher by perhaps 75% and 26%, respectively. Although the secondary chlorophyll mode for corrected data is higher than the primary mode by about 26%, suggesting incomplete removal of the bottom effects over bright pixels, it still falls within the 35% accuracy objectives of the SeaWiFS Project [Hooker et al. 1992] relative to a "true" value of about 0.40 mg m^{-3}. Comparison with retrievals using hyperspectral data suggest that addition of a channel at about 610 nm would have a significant positive impact on improving the accuracy of retrievals of water-column and bottom properties for shallow waters [Lee and Carder 1999]. Correction for bottom effects is absolutely required to achieve chlorophyll-accuracy goals for shallow waters.

e. Paper entitled "Phase function and albedo of mineral dust determined from ground-based sky measurements in the Florida Keys" by C. Cattrall and K.L. Carder was presented at AGU Meeting, San Francisco CA, Dec 15-19, 2000

The absorption and scattering properties of dust are of interest to both radiative transfer studies and climate system modelling. Direct measurement of the single-scattering albedo and scattering phase function are suitable for specific investigations but not practicable for extended periods of monitoring. Indirect measurements of the scattering phase function and single-scattering albedo can be achieved using the sky radiance to infer aerosol optical properties (Nakajima et al 1989; Devaux et al. 1999; Dubovik et al. 2000). In this study we determine the single scattering albedo and phase function of mineral dust by inverting principal plane measurements of sky radiance. The data are collected with a well-calibrated, portable, 512-channel spectrometer possessing a 2.2° field-of-view and 2.3 nm FWHM. The inversion algorithm iteratively solves for the wP(Q) product which, when inserted into the radiative transfer equation, yields the measured sky radiance.We present here the results of measurements collected during two Saharan dust events in the Florida Keys during July, 1998. Data are shown at 9 selected wavelengths spanning the visible spectrum (400-900 nm), but these calculations may be performed at any wavelength sufficiently free of absorption by water vapour, oxygen, and other trace gases. The single-scattering albedos obtained ranged as low as 0.85 at 400 nm, due largely to the iron content or coatings on the particles. This relates to the Lenes et al. paper discussed below.

3. Peer-reviewed Publications

a. A paper entitled Properties of the water column and bottom derived from AVIRIS data by ZhongpingLee, Kendall. L. Carder, Robert F. Chen and Thomas G. Peacock is accepted by *J. Geophys. Res* for publication.

Using AVIRIS data as an example, we show in this study that the optical properties of the water column and bottom of a large, shallow area can be adequately retrieved using a model-driven optimization technique. The simultaneously derived properties include bottom depth, bottom albedo, and water absorption and backscattering coefficients, which in turn could be used to derive concentrations of chlorophyll, dissolved organic matter, and suspended sediments. The derived bottom depths were compared with a bathymetry chart and a boat survey and were found to agree very well. Also, the derived bottom-albedo image shows clear spatial patterns, with end members consistent with sand and seagrass. The image of absorption and backscattering coefficients indicates that the water is quite horizontally mixed. These results suggest that the model and approach used work very well for the retrieval of sub-surface properties of shallow-water environments even for rather turbid environments like Tampa Bay, Florida.

b. Paper entitled “Band-ratio or spectral-curvature algorithms for satellite remote sensing?” by Zhongping Lee and Kendall L. Carder is published in Applied Optics, vol. 39, No. 24, 2000.

For the retrieval of chlorophyll concentrations or the total absorption coefficients of oceanic waters based on water color, there are algorithms using either band ratios or spectral curvature of remote-sensing reflectance or water-leaving radiance. In this short note, we show that band-ratio algorithms have the potential to be applied to a wider dynamic range of oceanic waters, while spectral-curvature algorithms show stable performance as long as the data set falls in a narrower but appropriate range.

c. A paper entitled Atmospheric correction of SeaWiFS imagery: assessment of the use of alternative bands, by Hu, C., Carder, K. L., and Muller-Karger, F. E. is published in Appl. Opt. 39:3573--3581, 2000.

d. A paper entitled Atmospheric correction of SeaWiFS imagery over turbid coastal waters: a practical method by C. Hu, K. L. Carder, and F. E. Muller-Karger is published in Remote Sensing of the Environment, 74:195-206(2000).

The current SeaWiFS algorithms frequently yield negative water-leaving radiance values in turbid Case II waters primarily because the water-column reflectance interferes with the atmospheric correction based on the 765 and 865 nm spectral bands. Here we present a simple, practical method to separate the water-column reflectance from the total reflectance at 765 and 865 nm. Assuming the type of aerosol does not vary much over relatively small spatial scales (~50-100 km), we first define the aerosol type over less turbid waters. We then transfer it to the turbid area by using a "nearest neighbor" method. While the aerosol type is fixed, the concentration can vary. This way, both the aerosol reflectance and the water-column reflectance at 765 and 865 nm may be derived. The default NASA atmospheric correction scheme is subsequently used to obtain the aerosol scattering components at shorter wavelengths. This simple method was tested under various atmospheric conditions over the Gulf of Mexico, and it proved effective in reducing the errors of both the water-leaving radiance and the chlorophyll concentration estimates. In addition, in areas where the default NASA algorithms created a mask due to atmospheric-correction failure, water-leaving radiance and chlorophyll concentrations were recovered. This method, in comparison with field data and other turbid-water algorithms, was tested for the Gulf of Maine and turbid, post-hurricane Gulf of Mexico waters. In the Gulf of Maine it provided more accurate retrievals with fewer failures of the atmospheric-correction algorithms. In the Gulf of Mexico it provided far fewer pixels with atmospheric-correction failure than the other methods, did not over-estimate chlorophyll as severely, and provided fewer negative water-leaving radiance values.

e. Paper entitled "Comparison of ship and satellite bio-optical measurements on the continental margin of the NE Gulf of Mexico" by Hu, at el has been accepted for publishing by International Journal of Remote Sensing.

4. Science Meetings

MODIS Science Team, January 21-25, 2001.