Quarterly Report for July - September, 1997
Kendall L. Carder, University of South Florida
NAS5-31716

Abstract

The algorithm-development activities at USF during the third quarter of 1997 have concentrated on data collection and theoretical modeling. Three papers were submitted to JGR and Applied Optics for publication.

Tasks Accomplished:

1. Two cruises were completed.

    a. Red Tide Cruise #1

        1) August 20 – September 4, 1997

        2) Florida DEP-funded boat time

        3) Transects from the west and northwest Florida Shelf

        4) Chlorophyll *a* (Chl), particle absorption coefficients (ap), detritus absorption coefficients (ad), gelbstuff absorption coefficients (ag), remote sensing reflectance (Rrs) were collected at station locations, while chlorophyll fluorescence, attenuation coefficients (c), salinity, and temperature were collected underway.

2. A paper entitled ‘Satellite-Sensor Calibration, Verification Using The Cloud-Shadow Method’ by P. Reinersman et al. was submitted to Applied Optics for publishing.

An atmospheric-correction method which uses cloud-shaded pixels together with pixels in a neighboring region of similar optical properties is described for use with high-resolution(e.g.

30m pixels) satellite or aircraft data. This cloud-shadow method uses the difference between the total radiance values observed at the sensor for these two regions, thus removing the nearly identical atmospheric radiance contributions to the two signals(e.g. path radiance and Fresnel-reflected skylight). What remains is largely due to solar photons backscattered from beneath the sea to dominate the residual signal. Normalization by the direct solar irradiance reaching the sea surface and correction for some second-order effects provides the remote-sensing reflectance to the ocean at the location of the neighbor region, providing a known “ground target” reflectance spectrum for use in testing the calibration of the sensor.

A similar approach may be useful for land targets if horizontal homogeneity of scene reflectance exists about the shadow. Monte Carlo calculations have been used to correct for adjacency effects and to estimate the differences in the sky light reaching the shadowed and neighbor pixels.

3. A paper entitled ‘Semi-Analytic MODIS Algorithms for Chlorophyll *a* and Absorption with Bio-Optical Domains Based on Nitrogen-Depletion Temperatures’ by K. L. Carder, F. R. Chen, Z. P. Lee, S. Hawes , and D. Kamykowski was submitted to the JGR MODIS special issue for publication.

This work describes MODIS algorithms for chlorophyll *a* concentration and phytoplankton and gelbstoff absorption coefficients. The algorithms are based on a semi-analytical, bio-optical model of remote-sensing reflectance, $R_{rs}(\lambda)$, where $R_{rs}(\lambda)$ is defined as the water-leaving radiance, $L_w(\lambda)$, divided by the downwelling irradiance just above the sea surface, $E_d(\lambda,0^+)$. The $R_{rs}(\lambda)$ model has two free parameters, the absorption coefficient due to phytoplankton at 675 nm, $a_{\varphi}(675)$, and the absorption coefficient due to gelbstoff at 400 nm, $a_g(400)$. The R_{rs} model has several other parameters which are fixed, or can be specified based on the region and season of the MODIS scene. R_{rs} is modeled using these parameters at each of the visible-range MODIS wavelengths, λ_i, $R_{rs}(\lambda_i)$ is derived at each pixel from the normalized water-leaving radiance, $L_{wn}(\lambda_i)$, measured by MODIS. These $R_{rs}(\lambda_i)$ values are put into the model, the model is inverted, and $a_{\varphi}(675)$ and $a_g(400)$ are computed. Chlorophyll *a* concentration is then derived simply from the $a_{\varphi}(675)$ value. For waters with high chlorophyll *a* concentrations where $R_{rs}(412)$ and $R_{rs}(443)$are very low and the algorithm is insensitive, an empirical algorithm with $R_{rs}(488)$ and $R_{rs}(551)$ is used to estimate chlorophyll *a*. The algorithm also outputs both the total absorption coefficients, $a(\lambda_i)$, and the phytoplankton absorption coefficients, $a_{\varphi}(\lambda_i)$, at the visible MODIS wavelengths. Since absorption per unit chlorophyll varies by a factor of five or more for the global ocean due to accessory pigment-to-chlorophyll variations and pigment packaging or self-shading, to derive accurate chlorophyll *a* concentrations based upon MODIS estimates of absorption, the MODIS algorithms are parameterized for three different bio-optical domains: 1) unpackaged; 2) transitional; and 3) packaged. These provide a variation in domain type from high-light, warm conditions to lower-light, cool conditions and can be identified from space by comparing sea-surface temperature to nitrogen-depletion temperatures(NDTs) for each domain. Algorithm errors of more than 45% are reduced to errors of less than 30% with this approach, with the greatest effect occurring at the eastern and polar boundaries of the basins.

To partition the data into one for regions where little pigment packaging is to be expected but high photoprotective pigments are found (e.g., high-light, non-upwelling locations in warm, tropical and subtropical waters), versus locations with more packaging and little photoprotective pigments(e.g., eastern boundary upwelling, and non-summer, high latitude sites) two numerical filters were used.

The first numerical filter compares regional field data sets to the CZCS chlorophyll pigment algorithm ($C = 1.14\ [r_{25}]^{-1.71}$, $r_{25} = R_{rs}(443)/R_{rs}(551)$) to check for consistency with this classical algorithm for Case 1 waters, which was developed with largely subtropical and summer temperate data.

The second numerical filter uses the ratios $r_{12}(= R_{rs}(412)/R_{rs}(443))$ and r_{25}. For waters with unpackaged pigments, the line $r_{12} = 0.95\ [r_{25}]^{0.16}$ was used to separate high-gelbstoff data points from the Case 1 data. Based upon the measured a_g data, the gelbstoff-rich Case 2 data had $a_g(400)$ values typically in excess of the relationship $0.12\ [\text{chl } a]^{0.7}$.

Those data sets generally found to be consistent with the CZCS algorithm line as well as occurring above the line $r_{12} = 0.95\ [r_{25}]^{0.16}$ for points where $r_{25} > 3.0$, were classified as “unpackaged”, and these consisted of tropical and subtropical data away from eastern-basin boundaries.

There are 287 data points in this ensemble data set: 134 USF data points and 37 EqPac equatorial Pacific points, all measured above-surface and processed using the Lee et al. (1996) protocols; and 126 EqPac points, all measured below-surface using the Mueller and Austin (1995) protocols.

There are 326 points in an ensemble of multi-year, multi-season data sets from the California Current which we label as "packaged." These consist of CalCOFI (n=303) and Cal9704 (n=23) data. The CalCOFI R_{rs} data were subsurface while the Cal9704 data were above-surface collections. The algorithm yielded RMS1 (log fractional) and RMS2 (linear) errors for chl *a* retrieval of 0.111 and 0.268, respectively when tested with this data set. The Type II RMA slope and intercept was 0.999, the bias was -0.006, and the r^2 value was 0.917

To generate an algorithm to transition between regions and periods with packaged and unpackaged pigments, we developed a global data set combining the "packaged", "unpackaged", and other mixed data sets from SeaBASS. This data set has 976 data points and the algorithm yielded RMS1 and RMS2 errors in algorithm-derived chl *a* of 0.176 and 0.446, respectively.

While algorithms appropriate for regions with packaged or unpackaged pigments can reduce the uncertainty in chlorophyll-a concentration from perhaps 45-50% to less than 30%, methods based upon space-derived data to determine when and where to apply the appropriate parameterization are still under development. A numerical filter has already been discussed, but it is only definitive for waters where $r_{25} > 3.0$ and when no uncertainty in atmospheric correction exists. Also, stations with high gelbstoff concentrations can cause confusion with this method. For offshore oligotrophic to mesotrophic waters, however, it is a very useful diagnostic tool.

A second space-based approach uses the fact that unpackaged pigments are usually found in high-light, nutrient-poor waters where small-diameter phytoplankton cells predominate. Since dissolved nutrients cannot be detected from space, a nutrient surrogate was sought.

Kamykowski (1987) developed a model that explained much of the global covariance observed between upper-layer temperatures and nitrate concentrations. Kamykowski has since developed nitrate-depletion temperatures (NDTs) for the north Atlantic Ocean. These NDTs provide a means to observe from space a variable that indicates when and where nitrate may be limiting phytoplankton growth, and where upper-layer production is dependent upon recycled nitrogen. Such phytoplankton are typically small with unpackaged pigments and with high photoprotective-chlorophyll pigment ratios.

To delimit regions of the north Atlantic Ocean with unpackaged pigments, we have compared sea-surface temperatures to Kamykowski's NDTs. Fig ure 1 shows annual trends in sea-surface temperature (SST), CZCS pigment, and NDTs for the Gulf of Maine, Bermuda, and Barbados. The temperatures and pigments are four-year (1982-85) monthly averages from the AVHRR and CZCS sensors.

Clearly, the Gulf of Maine is a lower-light, higher-nutrient environment than are Bermuda and Barbados, so the degree of packaging there is likely to be much higher, and the chlorophyll-specific absorption coefficient much smaller. By analyzing bio-optical data in the SeaWiFS SeaBASS archive, some preliminary functional relationships between the NDTs and pigment-packaging classifications for the north Atlantic Ocean were empirically derived using sea-surface temperature (SST) derived from the AVHRR satellite sensor:

<u>DOMAIN</u>:

1. Unpackaged: SST $> NDT + 3.0^{o}$ C

2. Transitional or global: NDT $+1.8^{o}$ C < SST < NDT + 3.0^{o} C

3. Packaged: SST < NDT + 1.8^{o} C

These domains for the months of May and August are shown in Figure 11 from the manuscript, based upon climatological sea-surface temperatures.

Using AVHRR SST data from the physical-oceanographic data archive, bio-optical data were sorted into domains using NDTs. Data for the transition period from spring to summer from the NASA SeaBASS archive for the cruises MLML2, AMT4, GOMEX1, GOMEX2, and the North Sea were sorted into the three bio-optical domains, and the appropriate algorithm parameterization was applied to derive chlorophyll *a* values. Atlantic Meridional Transect (AMT 4) data along 20^{o} W longitude collected in May, North Sea data and MLML2 data collected in July, and GOMEX1 and GOMEX2 data collected in April and June provide a diverse set of north Atlantic observations that were sorted by the NDT filter and processed. The results are compared to those obtained by simple use of the global (transitional) algorithm. The RMS1 and RMS2 errors for this diverse data set were 0.153 and 38%, respectively, for domain-sorted data, while the errors grew to 0.186 and 50%, respectively, when processed using global or transitional parameterization for the algorithm without sorting by domain.

In summary a semi-analytical algorithm was tested using a total of 976 global data points from regions where the pigments were typically unpackaged, transitional or packaged with appropriate algorithm parameters applied for each data type.

The semi-analytical algorithm performed superbly on each of the data sets after classification, resulting in RMS1 errors of 0.102 and 0.111 (e.g. 0.10 log unit), for the unpackaged and packaged data classes, respectively, with little bias and with slopes near 1.0. RMS2 errors for the algorithms were 24% and 28%, respectively.

For the difficult transition period between spring and summer, a data set was tested that included the eastern-boundary upwelling region of the north Atlantic. The nitrogen-depletion temperature was used with AVHRR-derived sea-surface temperature to sort stations into “packaged”, “unpackaged”, and transitional domains. RMS2 errors dropped from 50% to 38% as a result of this data-sorting exercise. Since large regions of the subtropical Atlantic and Pacific oceans remain in the “unpackaged” bio-optical domain during all seasons and provide rather stable data with accuracies from 24% to 28%, it seems reasonable to expect that use of an NDT-based sorting algorithm with MODIS sea-surface temperatures to separate data into appropriate bio-optical domains will result in accuracies for the MODIS semi-analytical chlorophyll *a* algorithm that are significantly lower than our target value of 35%.

This study is being expanded to include all oceans and a model parameterization for hyperpackaged pigments found in low-light, high-latitude environments has been developed for addition to the algorithm.

4. A paper entitled ‘Empirical Ocean Color Algorithms for Absorption Coefficients of Optically Deep Waters’ by Z.P. Lee, K.L. Carder, R.G. Steward, T.G. Peacock, C.O. Davis and J.S. Patch has been submitted to JGR for publishing.

Since the late 1970’s, many empirical algorithms have been developed for chlorophyll-a or pigment concentrations for waters from open ocean to coastal environments, but only a few algorithms have been developed for optical properties of the water. Applying a specific optical property (e.g., specific absorption coefficient), those concentrations can however be converted to absorption and/or attenuation coefficients. As demonstrated, in-water optical properties can be empirically derived from ratios of water-leaving radiance or ratios of remote-sensing reflectance in one step. To extend our early studies, total absorption coefficients at 440 nm ($a_t(440)$, see Notation for symbols used in this text) for the ocean, and those for surface pigment and for gelbstoff are empirically related to the ratios of remote-sensing reflectance at the SeaWiFS bands, which provide alternatives to the pigment-concentration algorithms for deriving in-water optical information.

The total absorption coefficient of surface water, which dominates the variance of both remote-sensing reflectance and the diffuse attenuation coefficients, is important to many aspects of oceanography (e.g., water-type classification, subsurface light intensity, heat flux, etc.).

Empirical algorithms, based on in-water measurements, have been developed for the derivation of the diffuse attenuation coefficient, which closely related to the total absorption coefficient. As the relationship between remote-sensing reflectance and absorption only weakly depends on the solar elevation, the spectral ratios of remote-sensing reflectance data should then be almost independent of solar and/or view angles. This suggests that inherent optical properties such as the total absorption coefficients might be derived from the ratios of remote-sensing reflectance. Based on smaller data sets than the present one, Carder et al. [1992] and Lee [1994] proposed an $a_t(490)$ algorithm using the ratio of remote-sensing reflectance at 520 and 560 nm. Since pigment absorption peaks near 440nm, the values of $a_t(440)$ are instead empirically related to various spectral ratios of remote-sensing reflectance in this study. Actually, field data show that optical properties at 440 and 490nm (e.g., $K_d(440)$ and $K_d(490)$, c(440) and c(490)) are all highly correlated.

The pigment absorption coefficient is important for the calculation of light harvesting by phytoplankton pigments for use in primary production models and for determination of the chlorophyll-a/pigment concentration. Traditional remote sensing methods have estimated pigment absorption using two steps: 1) derive chlorophyll-a or pigment concentration from empirical remote-sensing algorithms; and 2) convert the concentration values to absorption values using known or assumed chlorophyll-specific absorption coefficients. That perhaps accounts for the different empirical and semi-analytical algorithms developed for remote sensing of pigment concentrations. We may, however, get the pigment absorption coefficients directly from the remotely measured data as briefly indicated in Lee et al. [1996a]. This type of algorithm may be applied to a wider range of oceanic environments than the two-step algorithms, since the chlorophyll specific-absorption coefficient is not involved, which varies widely from place to place.

Gelbstoff absorption coefficients can be used as a tracer of land runoff for coastal environments. No simple remote-sensing algorithm yet exists for gelbstoff absorption coefficient, but more complex analytical and semi-analytical approaches have been used.

An analytical method has been developed for the derivation of oceanic absorption coefficients from above-surface remote-sensing reflectance. The method uses an optimization approach with hyperspectral data, which would take a rather long calculation time for processing of a satellite image. It is, however, more accurate in decomposing the total absorption coefficients into those of pigment and gelbstoff. For image processing purposes, more rapid algorithms are needed, though they may be less accurate. Recently, Hoge and Lyon [1996] suggested a matrix inversion technique. The technique requires, however, pre-knowledge of the spectral models of the inherent optical properties, and the method has not been tested with field data.

In this study, empirical algorithms are developed for quickly estimating the coefficients at 440nm for total absorption, pigment absorption, and gelbstoff absorption by directly relating them to the ratios of remote-sensing reflectance at two or three of the SeaWiFS wavelength bands. We adopt a formula of cubic polynomials using two spectral ratios. With derived absorption coefficients at 440 nm, the absorption spectrum of the total, the pigment, and the gelbstoff in the visible domain can be constructed using the approaches of Austin and Petzold [1986], Lee [1994], Bricaud et al. [1981], and/or Carder et al. [1991].

Publications:

1. Bissett, W.P., J.S. Patch, K.L. Carder, and Z.P. Lee, 1997 "Pigment Packaging and Chlorophyll a-Specific Absorption in High-Light Oceanic Waters," *Limnol. Oceanogr.*, 42(5), pp. 961-968.

Anticipated Activities:

1. The relationships between temperature anomalies and nutrients in regard to the packaging effect will be explored in order to reduce uncertainty in the chlorophyll algorithm using Bering Sea data and upwelling data from the Arabian Sea , Monterey Bay, Southern California Bight, and the East China Sea.

2. Research expeditions to be completed:

a. Florida Bay Cruise

1) October 2-4, 1997

2) NESDIS and NRL-funded ship time

3) Transects inside Florida Bay

4) Rrs, ap, ag, chl, c, salinity, and temperature were collected. NESDIS overflew the bay with the VIMS Beaver equipped with the Scanning Low-Frequency Radiometer (SLFMR), and the Satlantic SeaWiFS Airborne Surveyor (SAS).

b. Lake Okeechobee

1) January 13, 1998

2) SIMBIOS funded

3) Transects in Lake Okeechobee

4) Determining stray light effects on SeaWiFS and a "dark target" evoluation of

aerosol radiance at 412 nm.

c. Florida Bay cruise

1) January, 1998

2) NOAA funded ship time

3) Transects inside Florida Bay, SLFMR overflight.

d. Calibration:

1) March, 1998

2) At U. of Arizona and Mt. Lemmon

3) Calibrating the handheld Spectrix spectrometers, Microtops II, Reagan radiometers, and the Spectralon targets in the field and in the lab.

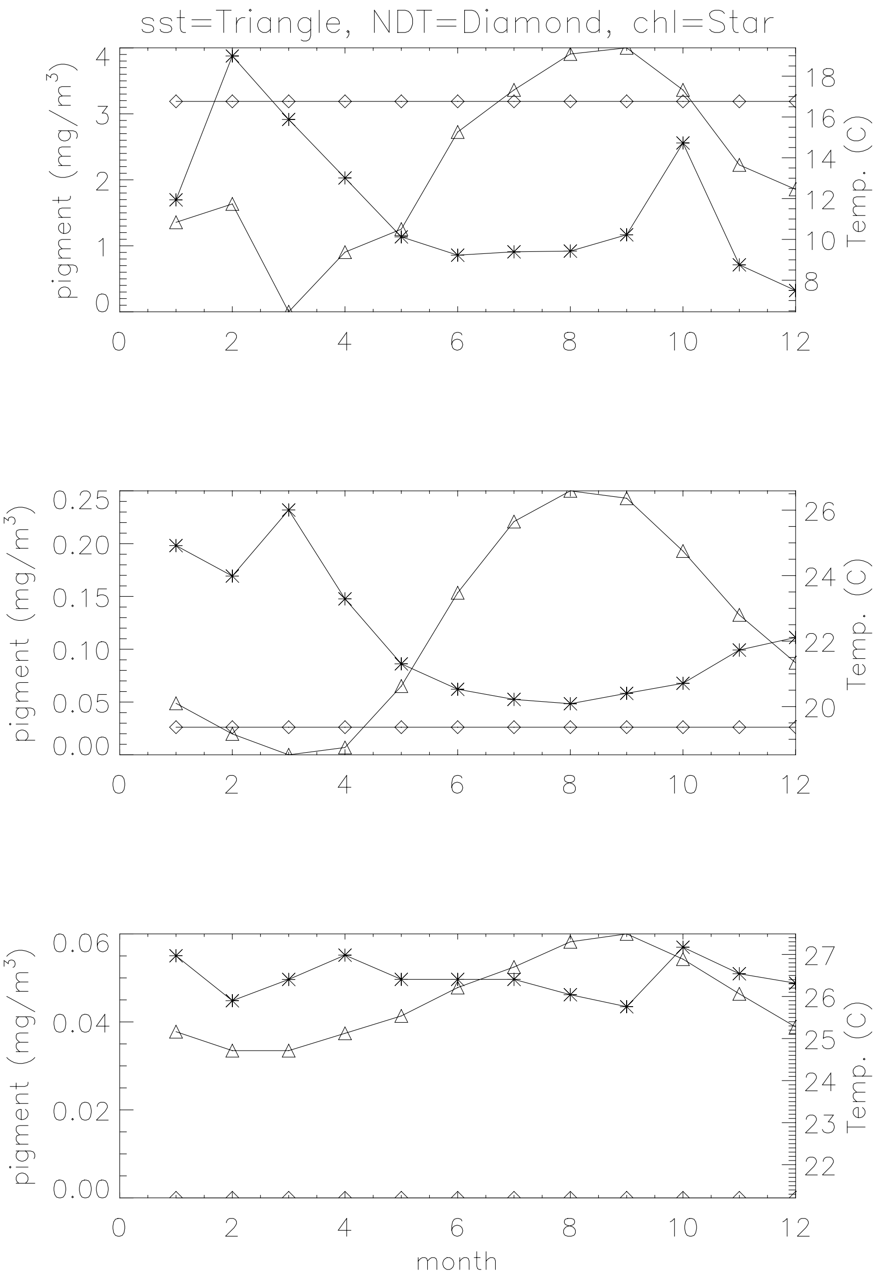
e. Tongue of the Ocean cruise

1) April 1 – 7, 1998

2) SIMBIOS and ONR funded ship time

3) Transects along shallow banks of Tongue of the ocean in Bahamas

4) Assessing atmospheric adjacency effects and stray light of bright/dark targets on SeaWiFS data.


sst=Triangle, NDT=Diamond, chl=Star
pigment (mg/m3)
Temp. (C)
month