Semi Annual Report

(January 1 — June 30, 2001)

Contract Number NAS5—31363

OCEAN OBSERVATIONS WITH EOS/MODIS:

Algorithm Development and Post Launch Studies

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Preamble

This document describes our progress thus far toward completion of our research plans regarding two MODIS Ocean-related algorithms.

A. Retrieval of the Normalized Water-Leaving Radiance (Atmospheric Correction).
B. Retrieval of the Detached Coccolith/Calcite Concentration

Our plans for Fiscal Year 2001 are included in this report as **Appendix I**. [In this report, we have combined items 2 (*Implement the Initial Algorithm Enhancements*) and 3 (*Study Future Enhancements*) from Appendix I into item "2 and 3" (*Algorithm Enhancements*).]

Fiscal Year 2001 was to be heavily focused on validation of MODIS-derived products. Unfortunately, the unexpected difficulty in calibrating MODIS required modification of out initial plan. In addition, as we already know that there are certain situations in which the algorithms are unable to perform properly, or that there are items that have not been included in the initial implementation, a portion of our effort was directed toward algorithm improvement. Thus, we break our effort into two broad components for each algorithm:

- Algorithm Improvement/Enhancement;
- Validation of MODIS Algorithms and Products.

Of course, these components will overlap in some instances.

RETREIVAL OF NORMALIZED WATER-LEAVING RADIANCE (ATMOSPHERIC CORRECTION)

Algorithm Improvement/Enhancement

1. Evaluation/Tuning of Algorithm Performance

Task Progress:

As indicated in our last Semiannual Report, considerable effort has been expended by R. Evans and co-workers toward removing the instrumental artifacts from MODIS ocean imagery. Examples of such artifacts are severe striping, mirror side difference effects the variation of the instruments response as a function of scan angle, and the "zipper." Much progress has been made along these lines, but much more needs to be done, especially following the shift from the "A-side" to the "B-side" electronics, that modifies the artifacts and requires a re-initialization of the sensor. However, the "zipper" effect has now been removed.

The "zipper" was an artifact in the imagery that resembles a zipper running along the nadir track through MODIS imagery. An example is shown in Figure 1 on the next page. The zipper was intensely studied for ~ two months before we determined that it was placed in the imagery by the correction for residual MODIS polarization sensitivity. This correction assumed that the polarization of the radiance measured by MODIS is the same as would obtain in a pure Rayleigh-scattering atmosphere. When the correction algorithm was written, it was incorrectly assumed that, for a given scan, all 10 pixels at the center of the scan (pixel 678) were actually viewing at nadir. Or equivalently, it was assumed that the scan planes of all ten lines in a single MODIS scan contained the normal to the surface of the ocean, and were therefore coincident with the same reference plane as that describing the polarization of the radiance. In reality, only one pixel (the center of the 10) was viewing at nadir, the other 9 having a nonzero nadir-view angle. Thus, the reference plane for polarization of the radiance and the reference plane describing the polarization sensitivity of the sensor intersected at an angle that became large near the scan center, where the viewing azimuth angle changes rapidly with pixel number. This angle was originally assumed to be zero. A simple rotation of the Stokes vector of the radiance from the earth-based reference to the MODIS-based reference, completely removed the zipper. To effect the rotation, we needed a vector normal to the MODIS scan. This was computed inside the MODIS code using the latitude and longitude data for each pixel along a given scan.

On the positive side, the MODIS imagery shows considerably more detail than SeaWIFS. An example of this is shown in Figure 2 in which water backscattering at 550 nm from SeaWiFS (upper image) and MODIS (lower image), acquired ~1.5 hours apart, are compared. In this example, we have applied the algorithm developed by Gordon et al.

Total Radiance - Rayleigh Radiance @412 nm MODIS 2000346.2215

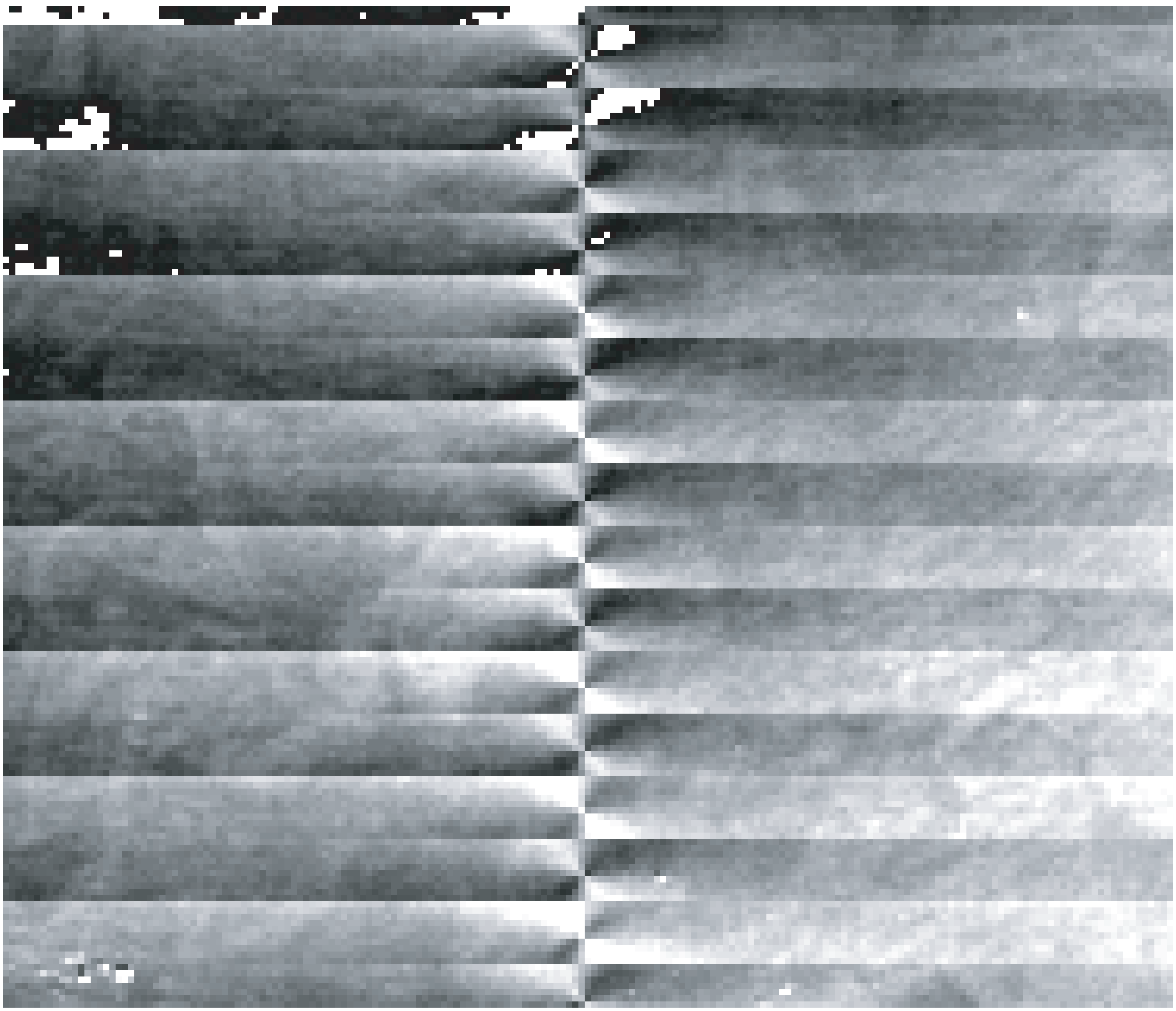
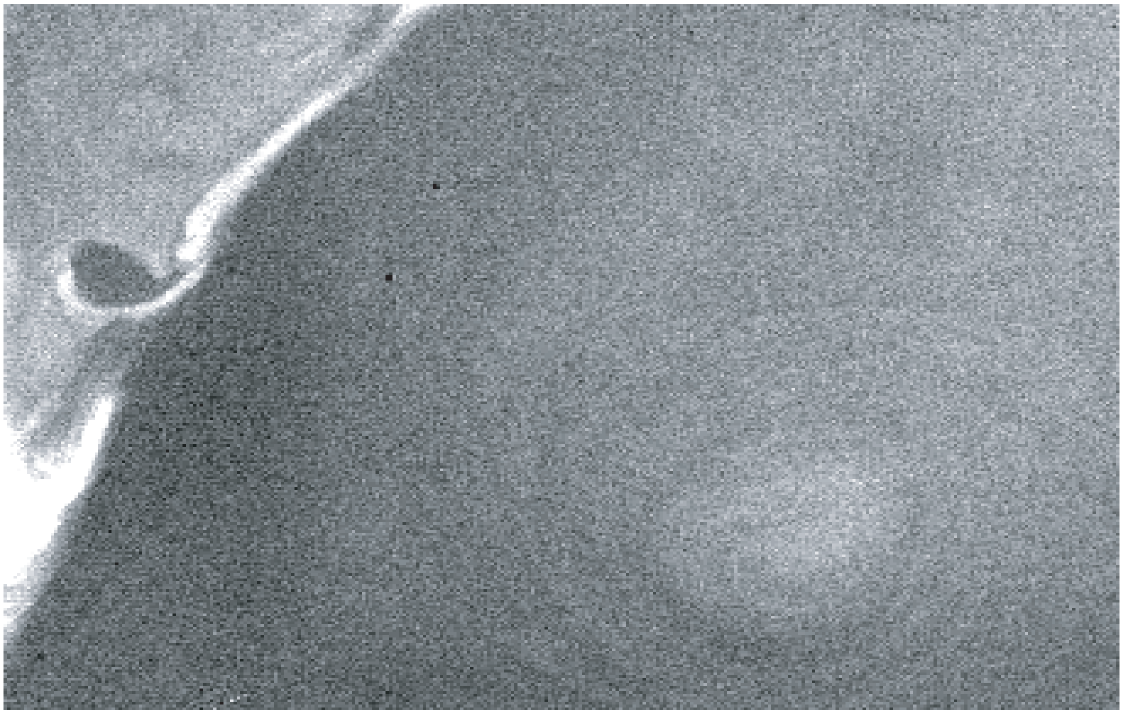


Figure 1

SeaWiFS 2000-129



MODIS 2000-129

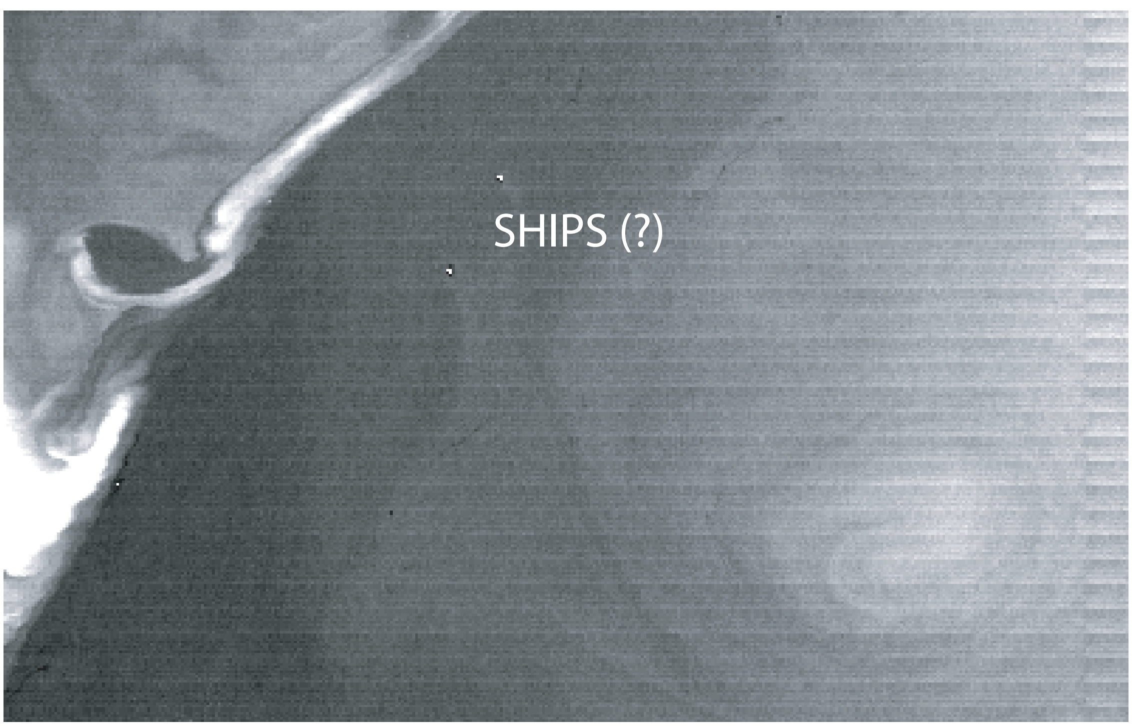


Figure 2

(H.R. Gordon, G.C. Boynton, W.M. Balch, S.B. Groom, D.S. Harbour, and T.J. Smyth' Retrieval of Coccolithophore Calcite Concentration from SeaWiFS Imagery, *Geophys. Res. Lett.* **28**: 1587—1590, 2001) to compute the backscattering coefficient. The algorithm uses the MODIS bands at 667, 749, and 869 nm and/or the SeaWiFS bands at 670, 765 and 865 nm. The MODIS imagery was obtained on Day 129 of 2000 using the "A-side" electronics. Although artifacts such as horizontal striping and the "zipper" are evident in the MODIS image, a significant reduction in noise from SeaWiFS to MODIS is apparent. The two sensors yielded backscattering values that differed by < 10%.

Unfortunately, MODIS imagery sometimes shows significant asymmetry between adjacent orbits (i.e., close to overlap) where one would not expect it. This asymmetry needs to be understood, and corrected, in order to provide a consistent data set.

<u>Anticipated Future Actions</u>:

We will continue the evaluation of MODIS imagery, and work closely with R. Evans on removing the artifacts, especially east-west asymmetry, from the imagery. We will compare the BRDF effects with the MODIS asymmetry to see if that can be ruled out. Other possibilities for this asymmetry that we will examine include a lack of understanding of the MODIS response-versus-scan-angle variability or error in the polarization-sensitivity correction.

2. and 3. Algorithm Enhancements

There are two important issues we are examining for inclusion into the MODIS algorithm: effecting atmospheric correction in the presence of strongly absorbing aerosols and/or Case 2 waters; and including the influence of the subsurface upwelling BRDF on water-leaving radiance. The BRDF influence may be important in the MODIS scan asymmetry.

Strongly Absorbing Aerosols

The first of the two enhancements we have been considering concerns absorbing aerosols. Although success with SeaWiFS has shown that the MODIS algorithm performs well in ~ 90% of Case 1 water situations, it does not perform adequately everywhere; most notably in atmospheres containing strongly absorbing aerosols. Strongly absorbing aerosols constitute a previously unsolved atmospheric correction issue for Case 1 waters, and have a significant impact in many geographical areas. Two important situations in which absorbing aerosols make an impact are desert dust and urban pollution carried over the oceans by the winds. In the case of urban pollution the aerosol contains black carbon and usually exhibits absorption that is nonselective, i.e., the imaginary part of the refractive index (the absorption index) is independent of wavelength. In contrast, desert dust absorbs more in the blue than the red, i.e., the absorption index decreases with wavelength.

Task Progress:

We have applied the spectral optimization algorithm [R.M. Chomko and H.R. Gordon, Atmospheric correction of ocean color imagery: Test of the spectral optimization algorithm with SeaWiFS, *Applied Optics*, **40**, 2973—2984, 2001] with the Garver and Siegel reflectance model ["Inherent optical property inversion of ocean color spectra and its biogeochemical interpretation: 1 time series from the Sargasso Sea," *Geophys. Res.*, **102C**, 18607—18625, 1997] to Case 2 waters. Unlike Case 1 waters, in which phytoplankton and their immediate detritus control the optical properties, in Case 2 waters phytoplankton play a lesser role. For example, in coastal regions resuspended sediments from the bottom and/or sediments and dissolved organic material can be carried to the coasts by rivers, etc., may control the water's optical properties. These Case 2 waters are difficult to atmospherically correct because the water-leaving reflectance in the NIR is often not negligible. We have modified the spectral optimization algorithm so that we no longer employ the simplifying assumption of negligible marine reflectance in the NIR. Such a modification enables use of spectral optimization algorithm in waters with moderate sediment concentrations. This modification has been applied to imagery of Chesapeake Bay; although, the Garver-Siegel reflectance model is not correct for such waters. With the Case 2 modification, the algorithm appeared to function properly.

Anticipated Future Actions:

We will continue to evaluate the performance of the absorbing aerosol algorithms for possible inclusion in the MODIS processing software, as we believe they are the most versatile. However, we need to (1) be sure they perform as well as experiments thus far indicate, and (2) optimize their performance to decrease processing time. We are looking for an example where algorithms of the Garver-Seigel type have been tuned to specific Case 2 waters. We will then apply our Case 2 algorithm with the tuned water model to examine the efficacy in Case 2 waters.

The subsurface upwelling BRDF

The subsurface BRDF issue revolves around the fact that nearly all measurements of the upwelled spectral radiance (used for bio-optical algorithm development, sensor calibration and product validation of all ocean color sensors) are made in the nadir-viewing direction, while the water-leaving radiance estimate from the signal at the remote sensor is for a particular viewing geometry that is rarely nadir. Thus, we need to understand the BRDF of the subsurface radiance distribution to reconcile these measurements. Our approach is to directly measure the BRDF as a function of the chlorophyll concentration and to develop a model that can be used for MODIS.

Task progress:

We have been collecting upwelling radiance data on each of the last several MOCE cruises. The MOCE-5 in the Gulf of California provided a wide range of chlorophyll *a* concentrations, thus allowing our modeling efforts to have a validation data set for a wide range of water properties. We are currently trying to model these results. The other MOCE cruises (MOCE 6-8, to date) were in the vicinity of Hawaii, so were limited to low chlorophyll cases, but provide data with various solar zenith angles, for correction of the MOBY data and the specific MOCE cruise data. For each of these cruises, we have provided BRDF data specific to the cruise/satellite geometry. For example Figure 3 shows the correction factor relating Nadir radiance (measured by the in-situ instruments, for the most case) and the satellite viewing radiance for the MOCE-7 cruise. As can be seen the corrections vary depending on the specific geometry, but can be as large as 15-20%. To make this correction for all satellite viewing geometry's/locations will require a validated model as there are just too many variables to consider (chlorophyll, satellite viewing angles, incident irradiance angles). Thus we are currently collecting the data for specific cruise applications, and to use in the modeling exercises.

In addition to the MOCE cruises, we participated in a regular buoy exchange cruise in early June. The hope was to get a time series, when the sun reached near zenith at solar noon, of the BRDF at the MOBY site. Unfortunately the power supply for RADS-II was destroyed during a power surge on the ship, so no data was obtained with this instrument. However, we have been working with Dennis Clark on his WARS instrument. This instrument does not measure the whole radiance distribution, but does measure much of the important portion. The radiometric accuracy is not as great as with RADS, but it gives a reasonable measurement of the BRDF relevant to the satellite problem and can be operated autonomously on the MOBY buoy. During this cruise, a single one-day data set was collected with WARS, and we have been working with this data.

One aspect which we feel is interesting is the idea that, because MODIS/Terra is in a specific orbit that repeats frequently, correcting MOBY (a single location) data for the BRDF effect throughout the year can be done with experimental data. This is reasonable because the chlorophyll concentration at MOBY does not change significantly and there is a specific subset of satellite viewing geometries that are required. Thus while the relative solar-satellite azimuth angle and solar zenith angle will vary through the year, the other variables (chlorophyll level, satellite viewing zenith angles, and satellite measuring time) are constrained to specific values. There are 14 sets in all, but only 5 significantly different cases. These cases (labeled A-E) are provided in Table 1, which shows the measurement times, view zenith, annual solar zenith range for the MOBY site at that measurement time, and annual relative azimuth range between MOBY and MODIS.

As an example of this type of analysis Figure 4 shows three contour graphs of the BRDF correction, derived from the WARS data for the MOBY site in configuration E (from Table 1, corresponding to satellite viewing zeniths of 36-38 degrees and measurement times at 21:02 and 21:45 (GMT). With graphs such as these, the BRDF correction can be determined for any period through the year, in this geometry. We are working to try to improve this analysis technique, but this also helps us to see how large the BRDF correction is for MOBY in the various geometries.

Table 1: The 14 viewing geometries available at the MOBY site.
All angles are in degrees.

Configuration #	Time	view zenith	solar zenith range	delta azimuth	final 5
1	2121	3	15-47	0-59	none
2	2204	53	5-45	180-109	A
3	2109	27	17-48	0-45	B
4	2151	44	8-45	180-113	C
5	2056	42	21-50	0-53	C
6	2139	30	11-46	180-117	B
7	2044	52	24-52	0-50	A
8	2127	8	13-47	180-120	none
9	2116	16	16-48	0-58	D
10	2157	49	6-45	180-112	A
11	2102	36	19-49	0-56	E
12	2145	38	9-45	180-114	E
13	2050	48	22-50	0-51	A
14	2133	20	12-46	180-119	D

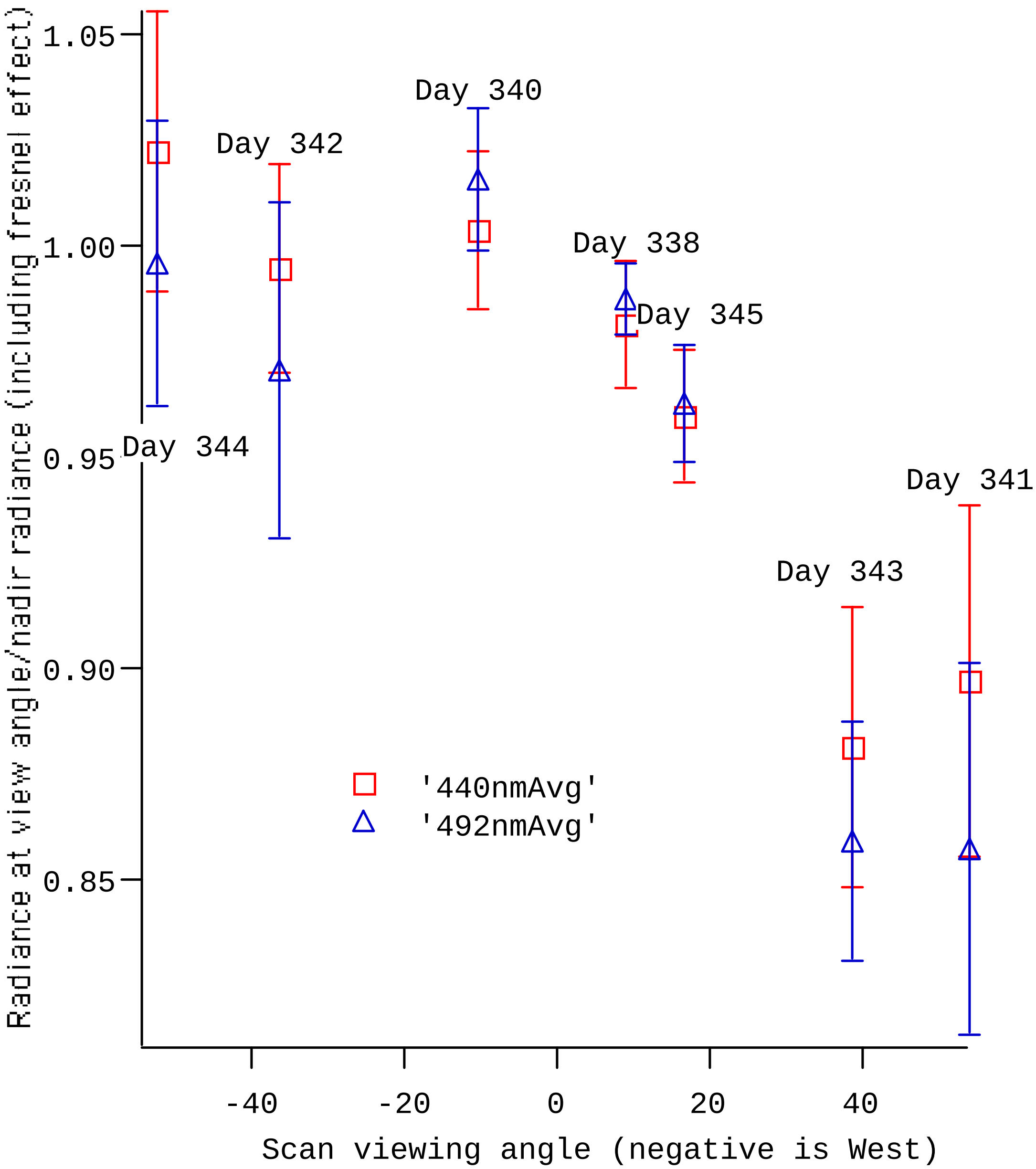


Figure 3: Radiance (Viewing)/Radiance(Nadir) at the MOBY site.
"Day" refers to day-of-the-year 2000.

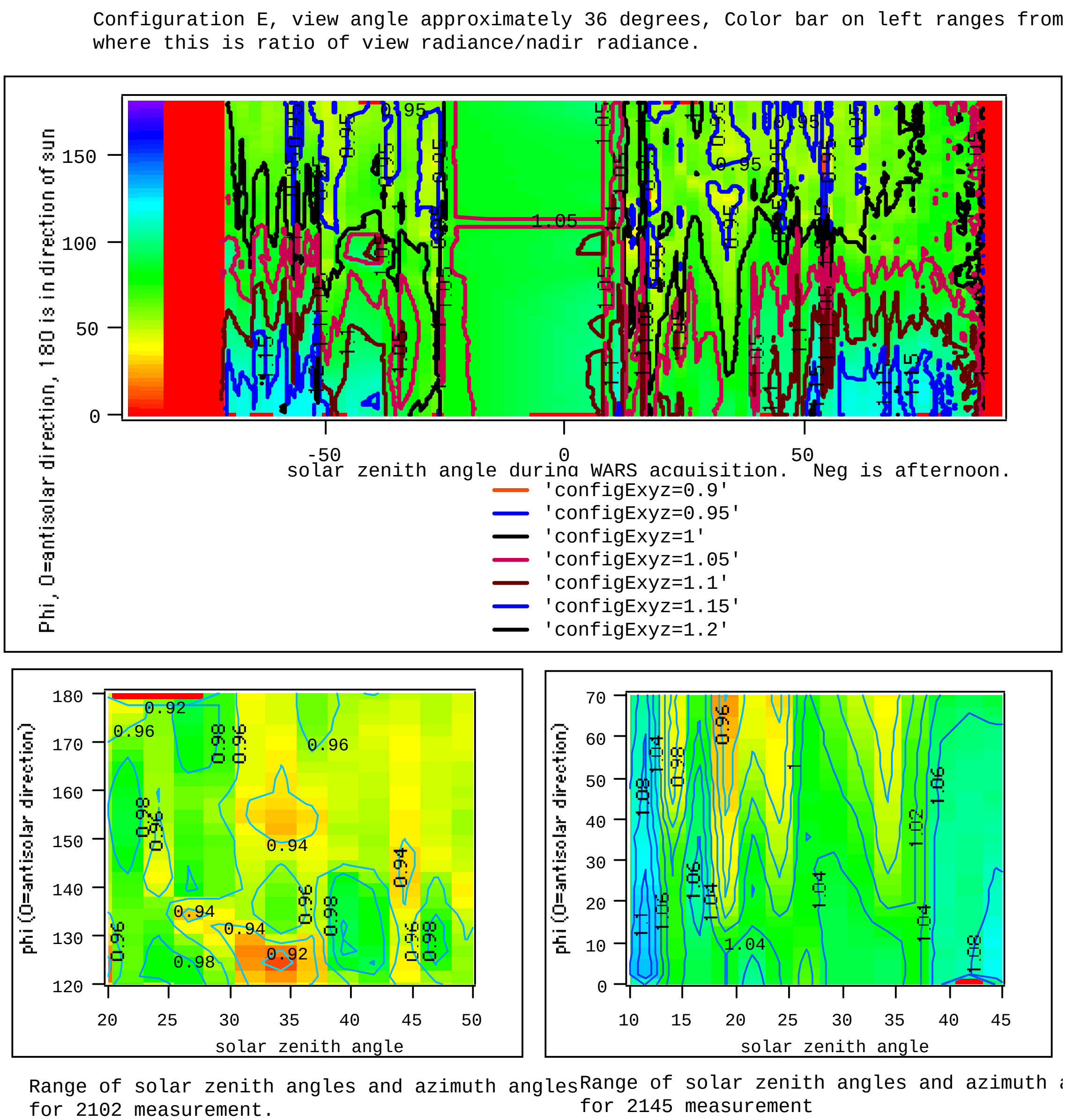


Figure 4: Radiance (Viewing)/Radiance(Nadir) at the MOBY site for configuration "E" (Viewing zenith angle ~ 37 deg). Lower panels provide the 2102 and 2145 overpasses separately.

Anticipated Future Actions:

We will continue to investigate modeling the BRDF effects and work towards a truly validated model. We are also going to continue to work with our RADS data set, to develop better tables for the correction of the BRDF effect at the MOBY site.

In addition, we have designed the new upwelling radiance distribution camera system (NuRADS). The system we have been using, RADS-II, was designed to measure the whole (up and downwelling) radiance distribution for a different application. As such it is much bigger/heavier than we require for the MODIS application. The size is an important consideration because we have found instrument self-shadow to be a significant problem in our measurements, particularly in the green and red portion of the spectrum. The smaller sized system will also be lighter, thus easier to deploy and float at the surface. The combination of lighter and smaller will also make the instrument shadow much smaller and allow us to improve the data quality. As there have been significant improvements in the CCD sensor technology, the data will also be less noisy and therefore more accurate. We anticipate having the first tests of the instrument taking place in the fall. Our current goal, which depends on vendor delivery, is to have the instrument ready for a late September/early October cruise with Dennis Clark.

4. Participate in MODIS Initialization/Validation Campaigns

This task refers to our participation in actual Terra/MODIS validation/initialization exercises.

Task Progress:

During the last six months we reduced the data from the shortened MODIS initialization cruise (MOCE-7). On this cruise there were seven in-water radiance distribution stations, and six sets of sky measurements. In addition we have reduced data from MOCE-6. We also participated in MOCE-8, during March and on a short "buoy swap" cruise (to get high solar zenith angle BRDF measurements) during early June.

We continued to maintain our CIMEL station in the Dry Tortugas during this period. It was returned only recently (late December) and was put back into operation during this period. This station will be used to help validate the MODIS derived aerosol optical depth (AOD) and aid in investigating the calibration of the near infrared (NIR) spectral bands of MODIS.

We also participated, in a limited manner, in ACE-Asia during this period. Basically we supplied a graduate student to run a micro-pulse lidar (with his travel support coming from another project) during the ACE-Asia cruise field work. One of the critical aspects of atmospheric correction is how to deal with vertical structure with absorbing aerosols. Previous field work, during INDOEX and Aerosols99, gave us an idea of vertical structure of aerosols over the Atlantic and Indian Ocean, including regions of Saharan Dust as well as pollution events from the Indian sub-continent. ACE-Asia gave us vertical profiles of Asian Dust over the Pacific. We are currently collaborating on reducing this data and contrasting this data set with our Atlantic data.

Anticipated future efforts:

We will continue our analysis of the MOCE-6, 7, and 8 data. We will participate in the next MODIS ship campaign when it occurs. We will make measurements of the sky radiance distribution (large-angle and aureole), the in-water radiance distribution, AOD, and whitecap radiance during this cruise.

5. Complete Analysis of SeaWiFS Validation Campaign Data

Task Progress:

We have completed analysis of our measurements during the Aerosols99 and INDOEX campaigns, and submitted several papers for publication (See CY-2000 Publications). In addition, we have completed the reduction of the MOCE-5 BRDF data.

Anticipated future efforts:

We will continue our effort to model the MOCE-5 BRDF data as a function of the chlorophyll concentration.

Additional Developments

With the help of D.K. Clark and R.E. Evans, a *Data Quality Summary* was prepared for the Terra/MODIS Normalized Water-leaving Radiance product. It is attached as **Appendix II**.

RETRIEVAL OF DETACHED COCCOLITH/CALCITE CONCENTRATION

This last half year of work has focussed on several areas: 1) publication of a Deep-Sea Research manuscript on coccolithophore distributions from the Indian Ocean, 2) publication of a manuscript on a new 3-band coccolithophore algorithm, 3) preparation for a large-scale manipulative experiment for testing the MODIS suspended calcite algorithm, 4) doing a pixel by pixel comparison of MODIS-derived particulate inorganic carbon and ship derived values taken from a Gulf of Maine bloom which formed during the summer of 2000 and 5) Presentation of MODIS validation results at the Miami MODIS-Oceans meeting.

Algorithm Evaluation/Improvement

Task Progress:

Our second manuscript on Arabian Sea results is now in galley form, and will be published in an upcoming issue of Deep Sea Research I (Balch et al., 2001). The abstract was given in a previous Semi-Annual report. The observation that calcium carbonate accounted for 10-40% of the total optical backscattering, is particularly significant in oceanic optics, as the particles responsible for the observed backscattering in the sea are still not well defined. The manuscript revision involved a significant error analysis for our underway technique to measure suspended particulate inorganic carbon.

A manuscript concerning a new three-band algorithm for retrieval of coccolith calcium carbonate from MODIS imagery appeared in Geophysical Research Letters during this reporting period (Gordon et al., 2001). This algorithm utilizes only red and near infrared bands and does *not* require knowledge of the chlorophyll concentration, which is very difficult to estimate remotely in coccolithophore blooms. The new coccolithophore calcite algorithm has been added into the MODIS processing code (Figure 2 is an example of this processing.).

Validation of MODIS Algorithms and Products

Task Progress:

As this is a new product and Terra was only launched in December 1999, there are relatively few data sets available for validation, particularly for the coccolith and suspended calcite products. This is because coccolith concentration (or particulate inorganic carbon, calcium carbonate) is not frequently measured at sea, while chlorophyll concentration is.

Regional Validation of PIC

In conjunction with NASA SIMBIOS activities, much of our validation estimates comes from the Gulf of Maine, the site of frequent blooms of coccolithophores, and readily accessible from our laboratory. Initial estimates of accuracy of MODIS PIC have been made based on comparison to these shipboard measurements. We also made some measurements in a Bering Sea coccolithophore bloom and performed an experiment we called “Chalk-Ex”.

A small bloom of coccolithophores occurred in the Gulf of Maine during summer 2000, which was sampled on several occasions. In this feature, we made atomic absorption measurements of suspended PIC and microscope enumeration of coccoliths and plated coccolithophores. We report the former here. The results are provided in Figure 5. For the days were the ship was on the west side of the MODIS swath (most accurate radiance retrievals), we report that the overall accuracy in the PIC determination was 0.2-3 ug l^{-1} (or in terms of coccolith concentration, 1 -10 × 10^9coccoliths m^{-3}; Fig. 5). In particular, see results for day 172 (year 2000) in which sea-truth measurements were made for one overpass. However, if one pools all the calibration data made over various days (and hence incorporating the different atmospheric effects, then the accuracy degrades to ~3ug PIC l^{-1}, or 15 × 10^9 coccoliths m^{-3}, 25% better than the theoretical accuracy of 20 × 10^9 coccoliths m^{-3}.

A significant bloom of coccolithophores occurred in the Bering Sea in the fall of 1997 (15 September image). We enumerated coccolith and coccolithophore concentration from water samples collected by a NOAA research ship within the feature (56° 56.24'N x 170° 19.66'W; Samples by Dr. J. Napp; no PIC measurements were available). The MODIS sensor had not yet been launched, so we applied the two-band coccolith algorithm to a SeaWiFS image. The coccolith concentration at this station, in the top 12m of the water column, was 3.6 × 10^{11} coccoliths m^{-3}, and the SeaWiFS-derived estimate was 3.0 × 10^{11} coccoliths m^{-3}, a relative error of 17%. By converting the coccolith concentration to PIC concentration, the Bering Sea results could be included in the validation results shown in Fig. 5.

In order to validate a high concentration bloom with MODIS, we made a small calcite patch in August of 2000 using 25 tons of Cretaceous coccolith chalk. Our first large-scale "Chalk-Ex" experiment was designed to sea-truth the MODIS coccolith algorithm at slightly lower concentrations than found in a bloom, but still high enough to be easily visible to MODIS. The chalk that we used was ground so that it all passed a 10 µm sieve, with 50% of the particles had diameter <1.9 µm. The chalk was ~98% pure.

On 6 August 2000, weather forecasts provided us the clear-sky window that we needed, and beginning 0400h, we diluted 25 cubic yards (~25 metric tons) of Cretaceous coccolith chalk with surface sea water, and adding it to the wake of the steaming vessel in order to further mix it as the ship steamed in an outward concentric spiral. We had a Satlantic SAS radiometer mounted on the bow of the R/V Cape Hatteras, as well as underway measurements of surface inherent optical properties (spectral absorption, attenuation, and backscattering), chlorophyll fluorescence, temperature, salinity, and particle size. at 39.8°N by 67.8°W (water depth ~2000m) which made a patch of a few square kilometers. The MODIS overpass was scheduled for mid-day of 8/6/00. Unfortunately, the MODIS satellite sensor began having unexpected data formatting problems some11h before we began diluting the chalk, and the instrument was turned off a few hours before our overpass! This was a most unfortunate stroke of bad luck, especially given that every other part of the experiment, including the weather, had gone perfectly. All was not lost, however, as SeaWiFS did see the patch, and we were able to do a vicarious check of the $CaCO_3$ algorithm performance (but regrettably, SeaWiFS does not have the sensitivity of MODIS). We occupied the patch for ~1.5d as the chalk sank, mapping its distribution (horizontally and vertically). By the end of 1.5d, we were having trouble locating the chalk as it was being mixed downwards from increasing winds and sea-state. Cloudy conditions prevailed for the next 10d, so we never had any subsequent satellite images to examine, but all indications are that the chalk sank out of surface waters, towards the underlying chalk sediments of the Continental Slope. Ship-derived backscattering data were converted to PIC concentrations using the backscattering cross-section of the chalk (measured in the laboratory). These data are included in the validation results of Fig. 5.

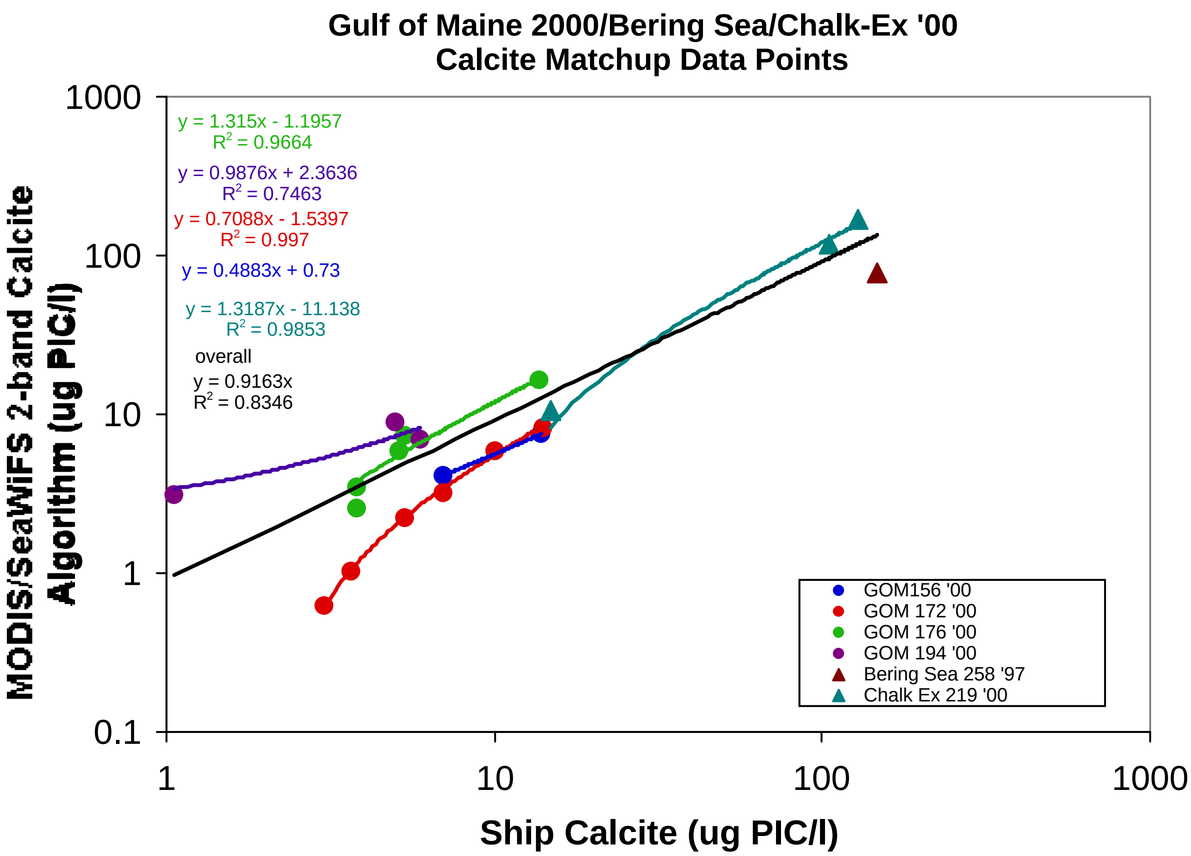


Figure 5. MODIS 2-band suspended PIC values versus ship-derived PIC values. Results taken from Gulf of Maine, 2000, when ship was on west side of MODIS swath. Statistical results: Day 156 (only two data points, no statistics available); Day 172-SE of derived PIC = ±0.18µgPIC l^{-1}; Day 176-SE of derived PIC = ±1.17µgPIC l^{-1}; Day 194-SE of derived PIC = ±2.10µgPIC l^{-1}; All data combined-SE of derived PIC = ±2.85µgPIC l^{-1}. Also shown for comparison are data from a Bering Sea coccolithophore bloom (day 258 of 1997) and the Chalk-Ex calcite patch (August '00). The Bering Sea data, shipboard PIC concentrations were based on coccolith counts converted to PIC, (using a conversion factor of 0.2 pg PIC $coccolith^{-1}$), and satellite PIC estimates based on SeaWiFS data. For the Chalk-Ex data, backscattering was measured, and converted to PIC concentrations using laboratory-derived results on the backscattering cross-section of $CaCO_3$.

Validation of global PIC and coccolithophore pigment data

For the 36km global data, there is no comparable sea-truth data available at this time, thus we compare the statistics of the global values with statistics of regional field surveys or global models (Fig. 6). Two global estimates of surface PIC can be made based on the work of Milliman (Milliman, 1993; Milliman et al., 1999). The former reference provides an estimate of the annual global sinking flux of PIC (in g m^{-2} y^{-1}) and this requires an estimate of the average sinking velocity of particles in order to derive standing stock (=flux/sinking velocity). Here we arbitrarily assume a sinking rate of 3m d^{-1} but we fully realize the limitations of this calculation. Also given on Fig. 6 are regional, direct, estimates of PIC standing stock from cruise work done in the Arabian Sea and Equatorial Pacific for comparison. These estimates are not subject to any sinking rate assumptions.

Globally, the coccolith pigment product is well correlated to the MODIS pigment product (MODIS Ocean Products 15; Coccolith Pigment = exp(-0.1214*(MODIS pigment$^{0.93}$); r^2=0.89). The data are well centered on the 1:1 line (Fig. 7). Regionally, within the Gulf of Maine, however, the correlation is best at high pigment concentrations; at low concentrations, coccolithophore pigment concentration is systematically less than the MODIS pigment value (Coccolith Pigment = exp(-0.188*(MODIS pigment$^{1.125}$); r^2=0.91; Fig. 8). The ratio of MODIS pigment/Coccolithophore pigment was plotted against the MODIS PIC (Fig. 9) in order to see how PIC concentrations affected the ratio of the ratio of the two pigment products. The results suggest that as PIC concentrations approach 5µg l^{-1}, the mean ratio approaches 1, and indeed could become <1 at high PIC levels. Given that we expect most of the satellite-derived blooms of coccolithophores to be *E. huxleyi*, we also would expect the band-ratio algorithms to <u>underestimate</u> the pigment concentration for suspensions of these small coccoliths. Thus, we suggest using the MODIS pigment product for PIC values up to 5µg PIC l^{-1}, above which, the coccolithophore pigment values should be used. Given the accuracy of the algorithm, the threshold value of 5µg PIC l^{-1} is also reasonable.

Citations

Balch, W.M., Drapeau, D., Fritz, J., Bowler, B. and Nolan, J., 2001. Optical backscatering in the Arabian Sea-continuous underway measurements of particulate inorganic and organic carbon. Deep Sea Research I In press.

Balch, W.M., Drapeau, D. and Fritz, J., 2000. Monsoonal forcing ofcalcification in the Arabian Sea. Deep-Sea Research II 47, 1301-1337.

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Gordon, H.R., Boynton, G.C., Balch, W.M., Groom, S.B., Harbour, D.S. and Smyth, T.J., 2001. Retrieval of coccolithophore calcite concentration from SeaWiFS imagery. Geochemical Research Letters 28(8).

Milliman, J., 1993. Production and accumulation of calcium carbonate in the ocean: Budget of a nonsteady state. Global Biogeochemical Cycles 7, 927-957.

Milliman, J., Troy, P.J., Balch, W., Adams, A.K., Li, Y.-H. and MacKenzie, F.T., 1999. Biologically-mediated dissolution of calcium carbonate above the chemical lysocline? Deep-Sea Research 46, 1653-1669.

- **Other independent PIC estimates <u>(mgC m^{-3})</u>**
- Global Average (Milliman, 1993) **1.23**
- Global Average (Milliman et al., 1999) **1.80**
- Eq. Pacific 140W; 12N to 12S (Balch and Kilpatrick, 1996) **~3.0**
- Arabian Sea Avg (Balch et al., 2000) **2.0**

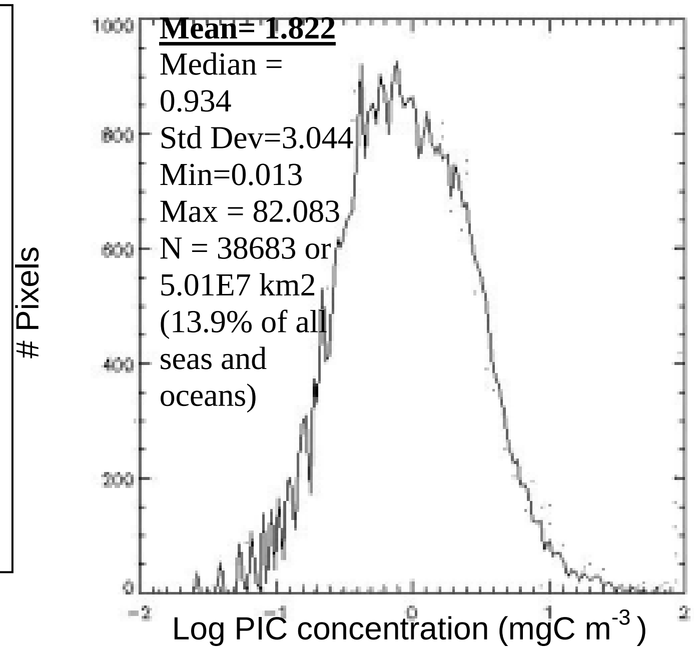

Figure 6. Global MODIS PIC measurements from day 102, 2000 (36km data, calibrated using Gulf of Maine ferry data). Average concentrations from other models or field campaigns also cited.

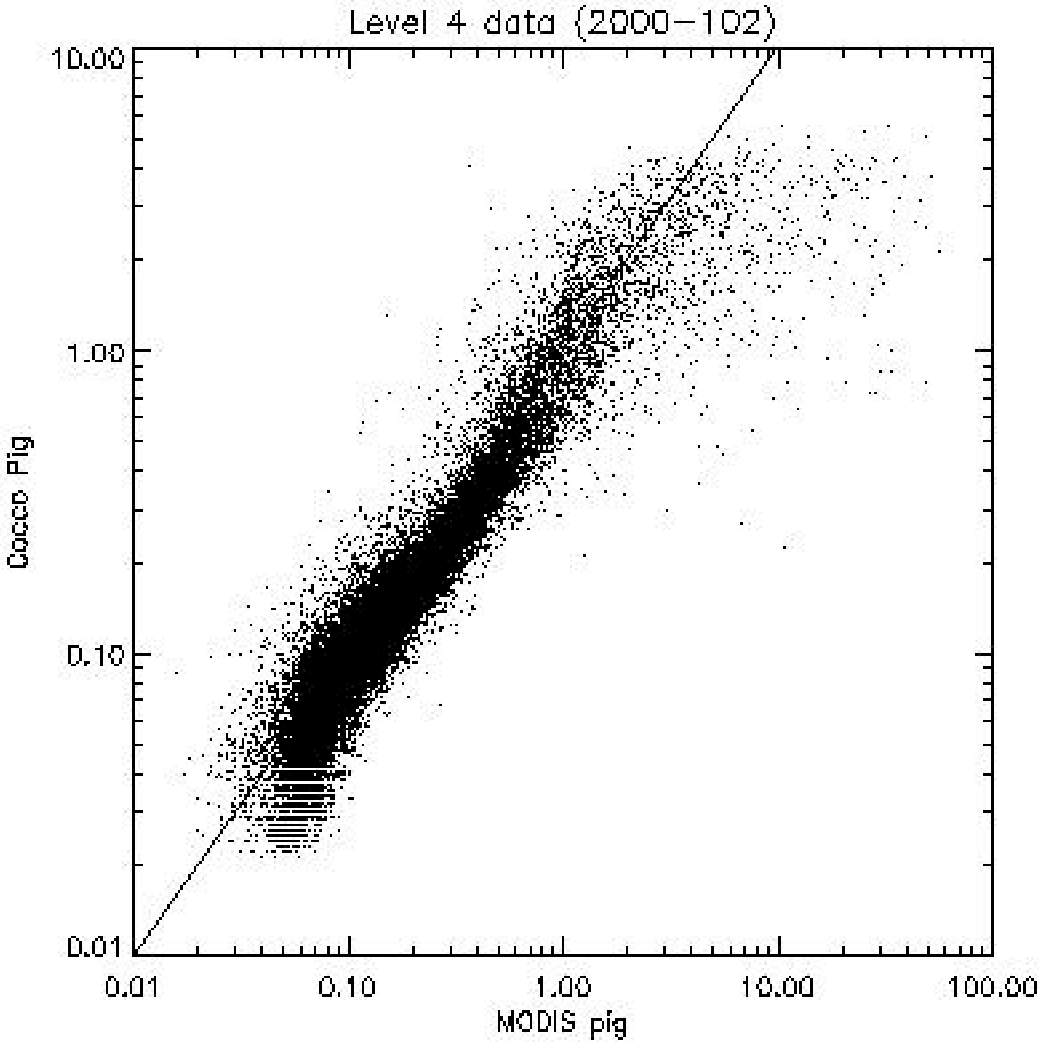

Figure 7. Plot of coccolithophore pigment vs. MODIS pigment on day 102, year 2000. 1:1 line shown for reference.

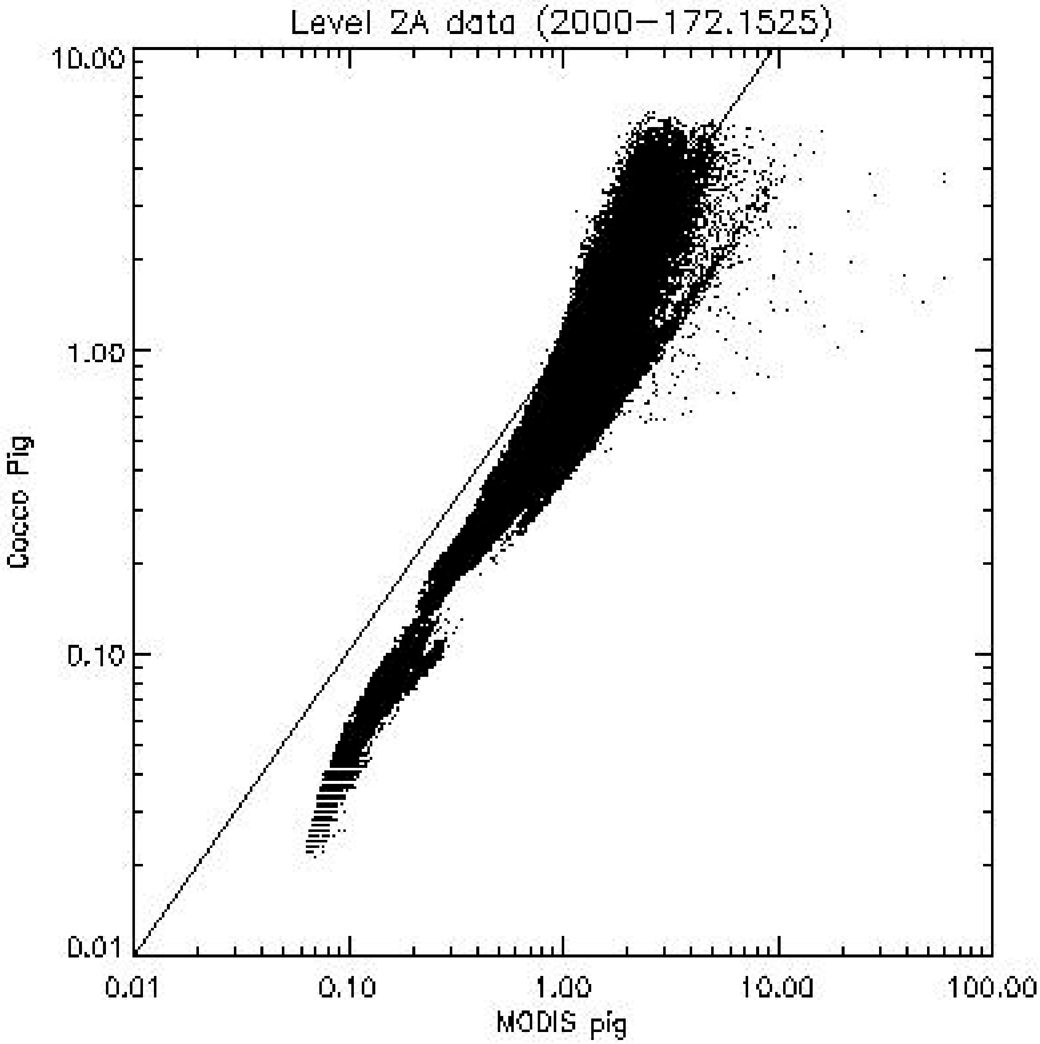

Figure 8. Plot of coccolithophore pigment versus MODIS pigment for Gulf of Maine. A systematic bias is evident at low MODIS pigment concentrations, but with considerably less data scatter than global, 36km data of Fig. 7. 1:1 line shown for reference.

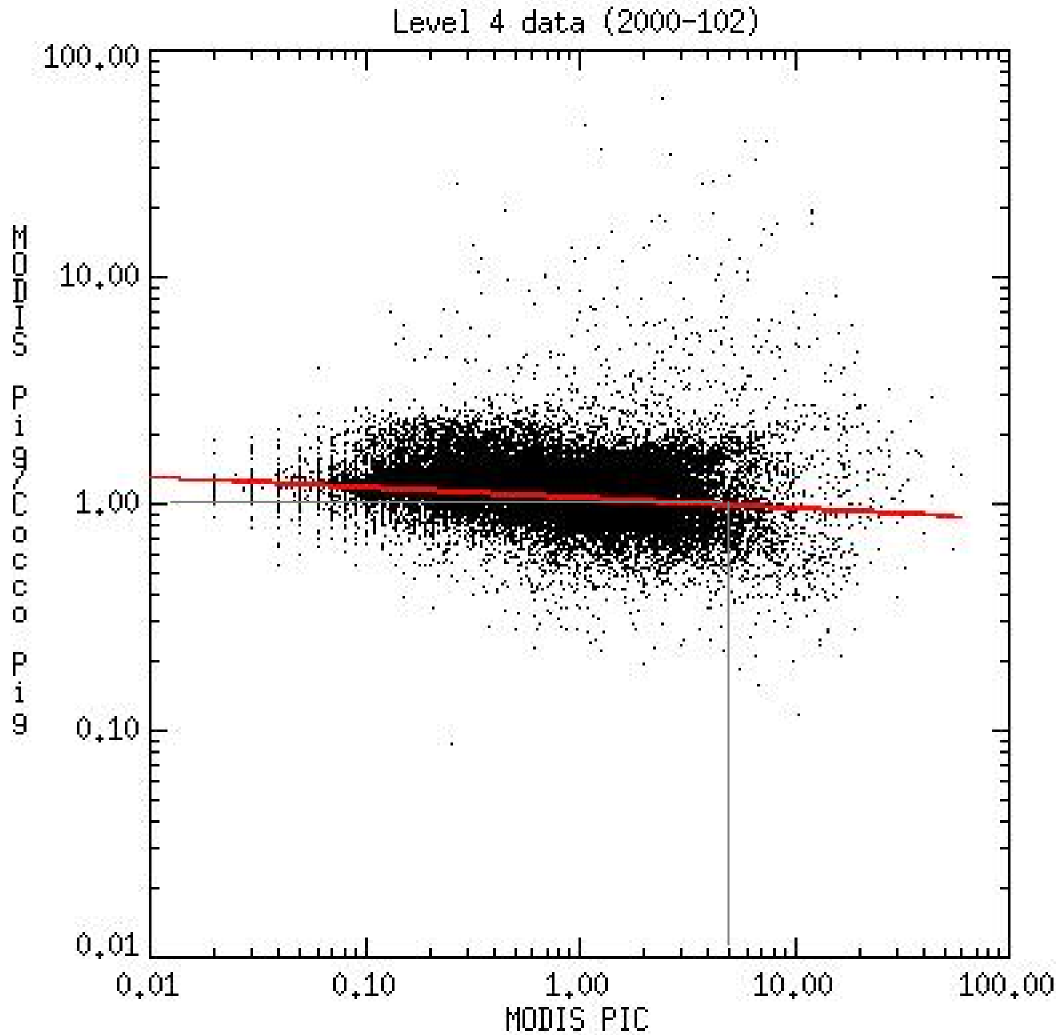

Figure 9. Plot of ratio of MODIS pigment/Coccolith pigment versus derived PIC concentration. Grey lines show the intersection of the trend line with a pigment ratio of 1 at PIC concentration of 5µg PIC l^{-1}.

Additional Developments

A *Data Quality Summary* was prepared for the Terra/MODIS Normalized Water-leaving Radiance product. It is attached as **Appendix III**.

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APPENDIX I

NASA/GSFC Contract No. NAS5-31363

OCEAN OBSERVATIONS WITH EOS/MODIS
Algorithm Development and Post Launch Studies

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Plans for FY 01

Preamble

This document describes plans for Fiscal Year 2001 regarding two MODIS Ocean-related algorithms.

A. Retrieval of the Normalized Water-Leaving Radiance (Atmospheric Correction).

B. Retrieval of the Detached Coccolith/Calcite Concentration

Fiscal Year 2001 will be heavily focused on the evaluation and validation of MODIS-derived products. However, as we already know (from theoretical studies and from SeaWiFS) that there are certain situations in which the algorithms are unable to perform properly or that there are items that have not been included in the initial implementation, a portion of our effort will be directed toward algorithm improvement. Thus, we break our effort into two broad components for each algorithm:

- Algorithm Improvement/Enhancement;

- Validation of MODIS Algorithms and Products.

These components will overlap in some instances.

RETREIVAL OF NORMALIZED WATER-LEAVING RADIANCE (ATMOSPHERIC CORRECTION)

Algorithm Evaluation/Improvement

1. *Evaluation/Tuning of Algorithm Performance*

Now that MODIS imagery has become available the process of evaluation of the MODIS performance is underway. Examination of the imagery shows several major challenges that must be dealt with before the imagery can be usefully employed for ocean studies. Among these difficulties are the fact that

- the imagery is striped suggesting that the individual detectors in each band have different sensitivities,
- that the severity of the striping appears to depend on the scan angle, and
- that there is excessive sun glint in the imagery in the tropics.

We have been working with R. Evans and the RSMAS group to alleviate these problems. This collaboration will continue. Once the principal radiometric challanges are overcome, we will use the MOBY and MOCE-6 data to initialize the overall radiometric calibration. After this initialization procedure, the imagery will be examined on a regular basis to ensure that the algorithms and the instrument are operating properly. Specifically, the sensor-algorithms should provide the expected “clear water radiances” [Gordon and Clark, “Clear water radiances for atmospheric correction of coastal zone color scanner imagery,” *Applied Optics,* **20**, 4175-4180, 1981] in the blue-green region of the spectrum, and should retrieve water-leaving radiances that agree with measurements at the MOBY site [Clark *et al.,* “Validation of Atmospheric Correction over the Oceans,” *Jour. Geophys. Res.*, **102D**, 17209-17217, 1997]. Any deviation from expectation or measurement must be reconciled. Deviations could be due to time dependence of the sensor calibration coefficients (i.e., instability in the sensor’s radiometric response), improper initialization, improper correction for the sensor’s polarization sensitivity, etc. Such analysis of necessity involves a statistical study of the derived water-leaving radiances with sufficient observations to unravel possible effects due to viewing angle, solar zenith angle, and other factors that could influence the retrievals. In addition, the performance of the atmospheric correction algorithm will be carefully studied. For example, does the algorithm choose candidate aerosol models that do not vary significantly from pixel to pixel? Such variation could indicate poor performance of the sensor in the NIR. Do the models that are chosen suggest that $\varepsilon(749,869)$ is undergoing a systematic variation with time? Such a variation would indicate that the radiometric response of the sensor is varying in time.

These studies will enable the algorithms to be tuned to the sensor and, in the event of an expected degradation in the sensor response, provide the necessary corrections to the response.

2*. Implement the Initial Algorithm Enhancements*

Several algorithm enhancements were planned for implementation into the processing stream in the immediate post-lanch era. Among those implemented since launch are

1. the addition of wind-induced surface roughness effects in the computation of the Rayleigh-scattering contribution to the top-of-atmosphere radiance, and
2. our correction of the MODIS residual polarization sensitivity [Gordon, Du, and Zhang, "Atmospheric correction of ocean color sensors: analysis of the effects of residual instrument polarization sensitivity," *Applied Optics*, **36**, 6938-6948] using MCST/SBRS-supplied MODIS polarization sensitivity characterization data.

As mentioned in Section 1, examination of MODIS imagery $\pm$ 20° – 30° from the solar equator reveals significant contamination due to sun glitter, even outside what would normally be considered to be the "glitter pattern." This high glint contribution is particularly troublesome at the MOBY site, which is used to monitor the performance and calibration of MODIS. Thus to fully utilize the MOBY site, and to extend the usefulness of MODIS imagery in these areas, we need to remove as much of the sun glint contribution as possible. At present the glitter pattern is masked using computations described in our ATBD. This mask needs to be refined into a validated scheme for removing sun glint. This will be a major focus of our enhancement effort.

3. Study Future Enhancements

The principal focus of enhancing the basic algorithms are absorbing aerosols. We consider correcting for absorbing aerosols to be the most important of the unsolved atmospheric correction issues because it has such a significant impact in many geographical areas. Algorithms to effect such correction are under intense development now. Among the possibilities we are studying are the spectral matching algorithm (SMA) [Gordon, Du, and Zhang, "Remote sensing ocean color and aerosol properties: resolving the issue of aerosol absorption," *Applied Optics*, **36**, 8670-8684 (1997)], the spectral optimization algorithm SOA [Chomko and Gordon, "Atmospheric correction of ocean color imagery: Use of the Junge power-law aerosol size distribution with variable refractive index to handle aerosol absorption," *Applied Optics* , **37**, 5560-5572 (1998)], and application of a model of Saharan dust transported over the ocean by the winds that is currently in the testing phase (Moulin *et al.*, in preparation).

The SMA is now being studied extensively because it can be added to the present MODIS algorithm with minor impact, as it uses the same look-up-tables (LUTs) as the existing algorithm. Another attractive feature is that it is completely compatible with our present plans for dealing with wind-blown desert dust. We plan to implement this algorithm in phases. In the first phase, the algorithm will be used to provide a flag that signals the presence of absorbing aerosols. In the second phase, the SMA will actually perform the atmospheric correction and retrieve the ocean products. In the third phase, it will be applied to wind-blown dust. Our goal is to implement all three phases during FY00. A question that needs to be resolved is whether or not the SMA, which employs a semi-analytic model of ocean color [Gordon *et al.*, "A Semi-Analytic Radiance Model of Ocean Color," *Jour. Geophys. Res.*, **93D**, 10909-10924, 1988], is compatible with more sophisticated ocean color models, e.g., Lee *et al.* ["Method to derive ocean absorption coefficients from remote sensing reflectance," *Applied Optics*, **35**, 453—462, 1996] or Garver and Seigel ["Inherent optical property inversion of ocean color spectra and its biogeochemical interpretation: 1 time series from the Sargasso Sea," *Geophys. Res.*, **102C**, 18607—18625, 1997].

The SOA is attractive in that it does not require detailed aerosol models to effect atmospheric correction and it has been successfully operated off the U.S. East Coast using the Garver and Seigel [1997] model for the ocean's reflectance. Unfortunately, its efficacy in dealing with wind-blown desert dust, which displays absorption that varies strongly with wavelength, is unclear. The performance of this algorithm will be studied in parallel with the SMA development.

There are two additional enhancements that are now in the research phase: (1) developing an accurate model of the subsurface upwelling radiance distribution as a function of view angle, sun angle, and pigment concentration, and (2) evaluating the performance of the SMA and SOA algorithms in the presence of high concentrations of colored dissolved organic matter (CDOM). The study of these will continue during FY 2000.

Most validation measurements of upwelled spectral radiance (BRDF) in the water are made viewing in the nadir direction. In contrast, ocean color sensors are usually non-nadir viewing. Thus, an important question is how does one validate the sensor performance when the quantity being measured differs from the quantity being sensed? Obviously, one must either correct the validation measurement to the correct viewing angle of the sensor, or correct the sensor observation to what it would be if the view were nadir. Either strategy requires a model of the subsurface radiance distribution. We are using measurements made near the MOBY site to develop such a model. We started using the model of Morel and Gentili ["Diffuse reflectance of oceanic waters. II. Bidirectional aspects," *Applied Optics*, **32**, 6864—6879 (1993)]; however, that model did not agree well with the experimental results. We are now trying to understand the source of the disagreement by examining processes left out of the computation of the radiance distribution, such as instrument self-shadowing and polarization. Once a model of the BRDF is available, we will use it to correct the diffuse transmittance for BRDF effects as described by Yang and Gordon ["Remote sensing of ocean color: Assessment of the water-leaving radiance bidirectional effects on the atmospheric diffuse transmittance," *Applied Optics*, **36**, 7887-7897 (1997)].

Initial work with MODIS imagery shows a pronounced asymmetry in the normalized water-leaving radiance in the visible across the scan (higher on the east). This is exactly what might be expected from water BRDF affects. Thus the BRDF will be given more attention than we felt was justified prior to acquiring the initial MODIS imagery.

The SMA and the SOA identify the presence of absorbing aerosols by using the full spectrum of radiance at the top of the atmosphere (TOA). Typically, absorbing aerosols cause a depression of the TOA radiance in the blue portion of the spectrum. Unfortunately, CDOM in the water leads to a depression in the blue. We are examining the interference of these two effects. Strong interference could limit the usefulness of ocean color sensors in coastal waters where CDOM is high and absorbing aerosols (from urban pollution) are likely to be present.

Validation of MODIS Algorithms and Products

Our participation in validation and initialization exercises requires that an array of instrumentation be maintained and fully operational at all times. Furthermore, data analysis skills need to be maintained as well. Personnel for such maintenance are included in our cost estimates.

4. Participate in MODIS Validation Campaigns

Present plans developed by D. Clark are to have a short validation field campaign in December 2000, followed by a major campaign in the spring of 2001. We will participate in these campaigns by providing several data sets: (1) we shall use our whitecap radiometer [K.D. Moore, K.J. Voss, and H.R. Gordon, "Spectral reflectance of whitecaps: Instrumentation, calibration, and performance in coastal waters," *Jour. Atmos. Ocean. Tech*., **15**, 496-509 (1998)] to measure the augmented reflectance of the water due to the presence of whitecaps; (2) we shall use our radiance distribution camera system (RADS) to measure the BRDF of the subsurface reflectance; (3) we shall employ our micro pulse lidar (MPL) to measure the vertical distribution of the aerosol (of critical importance when absorbing aerosols are present); (4) we shall use our solar aureole cameras and all-sky radiance camera (SkyRADS) to measure the sky radiance distribution to provide the aerosol scattering phase function; and (5) we will measure the aerosol optical depth (AOD). All measurements will be carried out at the station locations with the exception of the MPL which will operate continuously during the campaign. This data will be combined with the data from MOBY to fine tune the sensor and algorithms.

In addition, we will continue to operate our CIMEL station in the Dry Tortugas as part of the Aeronet Network [Holben, *et al*., "AERONET--A federated instrument network and data archive for aerosol characterization," *Remote Sensing of Environment*, **66**. 1-16].

Data from this site will be used to validate MODIS-derived AOD and possibly provide a means to examine the calibration of the near infrared (NIR) spectral bands.

5. Complete Analysis of SeaWiFS Validation Campaign (MOCE-5) Data

We will complete our analysis of the MOCE-5 data acquired in the fall of 1999 simultaneously with SeaWiFS imagery. This data set will serve as a validation platform of the MODIS atmospheric correction algorithm, and a test bed for the more advanced algorithms described in Section 3.

Retrieval of the Detached Coccolith/Calcite Concentration

Algorithm Evaluation/Improvement

1. Evaluation/Tuning of Algorithm Performance

Evaluation of the coccolith/calcite concentration has focused on two sets of observations: a) a coccolithophore bloom which occurred in the Gulf of Maine during the summer of 2000, and b) a large-scale manipulation experiment performed in August, in which 25 tons of coccolith chalk was disseminated into a patch (initial size = $3km^2$). As with the retrieval of normalized water-leaving radiance (above), the coccolith algorithm suffers from the striping and sun glint issues. The Gulf of Maine coccolithophore bloom of 2000 formed in June, and extended well into July. We first observed it during our NASA SIMBIOS cruises aboard the M/S Scotia Prince ferry. During these trips, the acid-labile backscattering increased significantly (to ~50% of the total backscattering). MODIS imagery from this bloom (Fig. 1) showed remarkable detail, and a first look at the acid-labile backscattering values (and assumed calcite-specific backscattering coefficients of the coccoliths) revealed that the algorithm-derived calcite concentrations were reasonable. The true test, however, will await final processing of our coccolith count samples, and suspended calcite analyses (being done by Scripps Analytical Facility on their inductively-coupled atomic absorption spectrometer). These will then be directly compared to the MODIS imagery.

The second part of the algorithm tuning work involved “Chalk-Ex”, a large-scale manipulation experiment in which finely ground coccolith chalk was spread into a patch. The ship work was done aboard the R/*V Cape Hatteras* from 4-10 August, 2000. Twenty five cubic yards of the chalk particles (median size = 2µm--the same size as coccoliths) were mixed with seawater, and dispersed into the wake of the research vessel, as it steamed in widening circles. The weather was excellent for the dispersal, with almost completely clear skies, and low winds. The patch was finished late morning on 6 August 2000, and was ~3km in diameter.

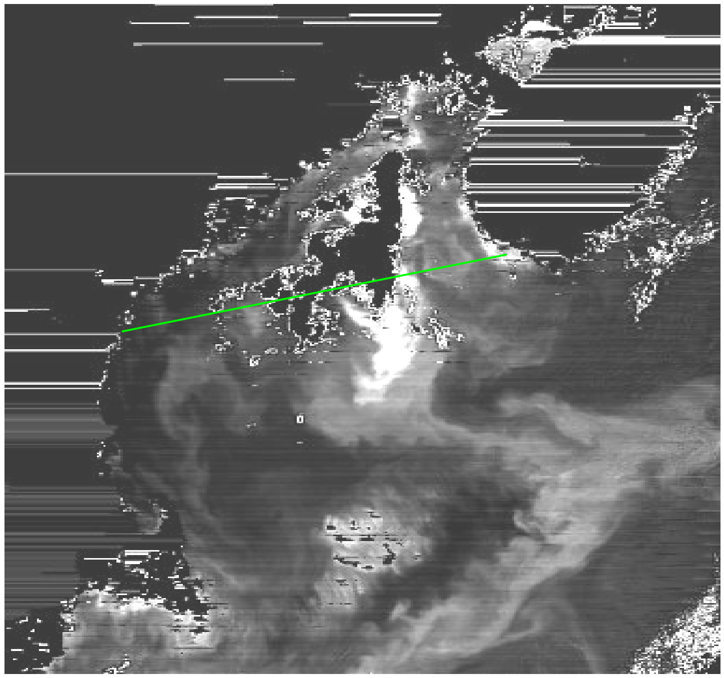

Figure 1- MODIS image of PIC concentration in Gulf of Maine from June 20, 2000. Note advection of coccoliths around northern flank of Georges Bank, with fine-scale eddy structure along the frontal boundary. Scale- White = 3×10^{-3} moles PIC m^{-3} ; light grey =2×10^{-3} moles PIC m^{-3}; dark grey = 0.75×10^{-3} moles PIC m^{-3}; black = 0-0.1 x 10^{-3} moles PIC m^{-3}. Ferry track is shown with green line.

Unfortunately for Chalk-Ex, there was an unexpected formatting problem aboard MODIS 10h before chalk deployment was to begin (~1800 EDT 5 August). The MODIS operations team discovered that the formatter circuitry was resetting itself (~ 330 resets were observed). There was a mixture of valid and invalid data packets observed for some time afterwhich no valid data packets were sent (6:21 PM EDT (22:21 Zulu)). At approximately 11:30 EDT (August 6, 2000 03:30 Zulu; ~1 hour before the first valid MODIS overpass) MODIS was placed in low power mode with the mirror stopped and survival heaters turned on. The instrument was not turned on again until several days following the mishap, thus, no MODIS imagery was collected of the chalk patch. Fortunately, the chalk patch was observed with SeaWiFS and analyses of the derived backscattering values are being done at this time.

2. Implement the Initial Algorithm Enhancements

The initial coccolith algorithm has been implemented with MODIS data. Gordon et al (1988) first described the scheme to derive coccolith concentrations from estimates of blue and green water-leaving radiance. The technique essentially uses a ratio algorithm (Gordon and Morel, 1983) to provide a first guess of chlorophyll concentration. Next, for each unique water-leaving radiance and chlorophyll level, a look-up table is consulted (derived from the specific scattering coefficient of calcite coccoliths and chlorophyll, as well as the specific absorption of chlorophyll) which provides an estimate of the $CaCO_3$ concentration. The process is iterated several times until stable chlorophyll and $CaCO_3$ concentration are achieved. This approach has been implemented after MODIS launch and global maps of suspended CaCO3 concentration are now available.

A new three-band algorithm for deriving suspended CaCO3 concentration has been submitted to *Geophysical Research Letters* for publication:

H. R. Gordon, G. C. Boynton, **W. M. Balch**, S. B. Groom, D. S. Harbour , and T. J. Smyth. Retrieval of Coccolithophore Calcite Concentration from SeaWiFS Imagery. *Geophysical Research Letters* (Submitted)

This paper examines blooms of the coccolithophorid *E. huxleyi*, observed in SeaWiFS imagery, with a new algorithm for the retrieval of detached coccolith concentration. The algorithm uses only bands in the red and near infrared (NIR) bands to minimize the influence of the chlorophyll and dissolved organic absorption. We used published experimental determinations of the calcite specific backscattering and its spectral dependence, and assumed that the absorption coefficient of the medium was that of pure water, to estimate the marine contribution to the SeaWiFS radiance. The aerosol (and Rayleigh-aerosol interaction) contribution to the radiance was modeled as an exponential function of wavelength. These allow derivation of the coccolith concentration on a pixel-by-pixel basis from SeaWiFS or MODIS imagery. Application to a July 30, 1999 SeaWiFS image of a bloom south of Plymouth, England indicates that the SeaWiFS estimates are in good agreement with surface measurements of coccolith concentration.

3. Study Future Enhancements

It is anticipated that, provided future algorithm performance is adequately validated, the three-band algorithm will be implemented for use with MODIS data rather than the two band approach (since it is not affected by chlorophyll and dissolved organic matter).

4. Participate in MODIS Validation Campaigns

We plan to continue MODIS-validation work in ’01. At this time, we are planning two 13 ton Chalk-Ex deployments in the summer of 2001. One will be in blue water, SE of Georges Bank. The other patch will be created in a more productive part of the Gulf of Maine (yet to be determined). MODIS will pay for 3d of this cruise, while the Navy will cover the other 11d. A second cruise is planned for November 2001, in which two more 13 ton patches will be deployed in the same locations as during the first cruise. Ship time for the second cruise will be provided completely by the Office of Naval Research. We also will monitor ocean color imagery for Gulf of Maine Blooms. In the event a Gulf of

Maine feature is observed, we will endeavor to sample it. Our ferry program is currently under review to the NASA SeaWiFS program. If funded, we will collect more coccolithophore data from the ferry during twelve cruises in 2001. These data will be used in MODIS validation.

APPENDIX II

MODIS
Terra Normalized water-leaving radiance
Data Quality Summary

MODIS
Terra Normalized water-leaving radiance
Data Quality Summary

Investigation: MODIS

Data Product: Normalized water-leaving radiance (MOD18)

Data Set: Terra

Data Set Version:

Nature of the product

The water-leaving radiance (L_w) is the radiance exiting the sea surface, i.e., solar irradiance backscattered into the atmosphere from beneath the sea surface. The *Normalized* water-leaving radiance (nL_w) is L_w normalized in a manner that removes most of the effects of variations of the solar zenith angle (Gordon and Clark, 1981). This radiance carries information regarding the concentration of marine biota, etc. MODIS provides the top-of-atmosphere radiance data (L_t) that allows estimation of (nL_w) in seven spectral bands (Bands 8 – 14) centered at wavelengths 412, 443, 490, 531, 551, 667, and 678 nm. For typical marine atmospheres and oligotrophic waters (the brightest in the blue), nL_w composes approximately 10% of L_t in the first three bands (412-490 nm), 4% of L_t in the green bands (531 and 551), and ~ 0.4% of L_t in the two red bands. The rest of the radiance is backscattered from the atmosphere and the sea surface. The water-leaving radiance is extracted from L_t through a process referred to as atmospheric correction. Clearly, atmospheric correction is particularly challenging in the green and red portions of the spectrum. In addition, the MODIS calibration requirements are very exacting, e.g., a 1% error in calibration in the blue, green and red spectral regions is equivalent to an approximately 10%, 25%, and 250% in nL_w error, respectively.

The procedure for atmospheric correction is detailed in the (MOD18) ATBD available at http://modarch.gsfc.nasa.gov/MODIS/ATBD/atbd_ mod17.pdf It uses the fact that nL_w is negligible in the near infrared (NIR) bands at 749 and 869 nm (Bands 15 and 16). Thus these bands are used to estimate the atmospheric contribution.

Data Accuracies

The MODIS atmospheric correction algorithm is virtually identical to that used in SeaWiFS processing. Actually the SeaWiFS and MODIS algorithms are the result of a research effort focussed on development of algorithms for MODIS, e.g., see Gordon and Wang (1994) and Gordon (1997). The validation of the SeaWiFS nL_w product is discussed in detail in Hooker and McClain (2000). An updated description of the validation results based on the third reprocessing of the SeaWiFS data set is available at (http://seawifs.gsfc.nasa.gov/SEAWIFS/TECH_ REPORTS/PLVol10.tex_ typeset.pdf). This report indicates that for the bands at 443 – 555 nm the ratio between of nL_w derived from SeaWiFS to that measured in situ (SeaWiFS:In situ) varied from 0.95 to 1.10 with a standard deviation of ~ 0.25. At 412 nm the ratio was 0.85. The comparison data generally cluster around the 1:1 line; however, at 412 nm at lower values of nL_w the SeaWiFS values tend to be lower than the in situ values. It is important to note that the error in atmospheric correction does not depend on the water properties (as long as nL_w is negligible in the NIR), so as nL_w decreases the *relative* error in nL_w increases.

At the present time (June 2001) detailed nL_w validation data are available only for the MOBY calibration site, so detailed comparisons can only be made for that location. In addition a switch to the “B-side” MODIS electronics restricts the comparison to the time period after October 2000. The results of the comparisons (made by Dennis Clark at NOAA/NESDIS) suggest that for 443 – 551 nm, MODIS and MOBY nL_w’s agree to within ~ 20%. At 412 nm the errors are much larger, reaching as much as 60%. There are significant variations in the retrieved nL_w’s with scan angle (east-west asymmetry, east higher than west) particularly at 412 (±50 %) and 443 nm (10-15%). At the other wavelengths the cross-scan variation is ~10-20%, but in the opposite direction (west higher). These variations can result from incomplete instrument polarization sensitivity correction, variation of the scan mirror reflectance with angle of incidence, etc.

Cautions When Using Data

The MODIS-retrieved nL_w’s are expected to improve with time. For the data accuracies described above, corrections to address several known problems will not be included in the processing until Version 3 of the MODIS ocean suite is released. For example, there is a clear variation in the sensitivity of the individual detectors in each MODIS spectral band (recall MODIS scans ten lines simultaneously with ten detectors for each spectral bands), and this has not been removed in this analysis. The variation of the sensor’s response with scan angle only includes pre-launch corrections, both with respect to mirror side and cross-scan correction. Both of these effects lead to noticeable banding in the nL_w fields. The corrections for the measured MODIS polarization sensitivity are being assessed. The polarization sensitivity is a strong function of the scan angle, so separating polarization and sensor response-versus-scan-angle effects will be particularly difficult.

Expected Revisions

The revisions in the processing code will mainly reflect improvements in the on-orbit characterization of MODIS. In particular, as more validation data become available, they will provide better understanding of the MODIS response-versus-scan-angle effects, detector-to-detector sensitivity variation, and the MODIS polarization-sensitivity correction. As this understanding leads to improvement of the processing, this document will be updated to reflect the expected data accuracies.

Quality Assurances

There are four levels of quality for the nL_w's. These are based on the values of certain flags related to atmospheric correction (http://modis-ocean.gsfc.nasa.gov/qa/). There are two kinds of flags – Common flags and Product Specific flags. Most of the Product flags are for diagnostic purposes, others reflect some failure of the processing.

In the common flag, bits are set as follows:

Bit 1 – Pixel not processed
Bit 2 – Atmospheric correction failed
Bit 3 – Satellite zenith angle > 55 Deg.
Bit 4 – Solar zenith angle > 70 Deg.
Bit 5 – Shallow water
Bit 6 – Sun glint (predicted reflectance > threshold) or Cloud
Bit 7 – Invalid or missing ancillary data
Bit 8 – Land

In the product specific flag that includes nL_w, flag bits are set as follows:

Bit 1 – Contribution from molecular scattering could not be computed.
Bit 2 – $nL_w(551)$ too low (< Threshold)
Bit 3 – Bright water – Coccolithophores detected (Brown and Yoder [1994] test)
Bit 4 – (Not related to nL_w)
Bit 5 – Aerosol contribution too large (AOD at 865 nm > Threshold)
Bit 6 – (Not related to nL_w)
Bit 7 – (Not related to nL_w)
Bit 8 – Absorbing aerosol (not implemented)
Bit 9 – Cloud (Albedo > Threshold)
Bit 10 – One or more bands missing.
Bit 11 – Any $nL_w < 0$. (Bands 8-14)
Bit 12 – Any invalid L_t value (e.g., saturated)
Bit 13 – Not used
Bit 14 – Aerosol correction failed.
Bit 15 – $\varepsilon(749,869)$ out of range.
Bit 16 – Aerosol contribution $(L_t - L_r) < 0$ in Bands 15 and 16

The quality levels range from 0—3 according to the setting of various flags above. Quality Level 0 indicates no known problems, Quality Level 3 indicates that the data are unusable. The Quality Levels are related to the Common and Product flags as follows:

Quality Level 0: No Common or Product flag bits set.
Quality Level 1: Common flag bit 3 (Satellite Zenith Angle > 45 Deg.) set
Quality Level 2: Common flag bit 6 (Sun Glint above threshold) set.
Quality Level 3: Common flag bit 2 (Failed Atmospheric Correction) or bit 8 (Land) set, or Product flag bits 10, 11, 12 (Impossible nL_w) set.

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APPENDIX III

MODIS
Terra Coccolith Products
Data Quality Summary

MODIS
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Data Quality Summary
William M. Balch and Howard R. Gordon

Investigation: MODIS

Data Product: Coccolith Products (MOD25)

Data Set: Terra

Data Set Version:

Nature of the products

There are three individual products related to coccolithophores: coccolith pigment concentration (C, MODIS Ocean Parameter #20), coccolith concentration (C_{cc}, MODIS Ocean Parameter #21), and suspended calcium carbonate concentration (PIC, MODIS Ocean Parameter #22). All three products are based on normalized water-leaving radiance (nL_w) at 443nm (MODIS Band 9/MODIS Ocean parameter 2) and 551 nm (MODIS Band12/MODIS Ocean parameter 5). The accuracy of the coccolithophore products is subject to the quality flags for the above radiance bands. The three products will be presented together, as they are highly inter-related.

The detailed theoretical basis of the Coccolith/Suspended Calcite Algorithm can be found at the MODIS site http://modarch.gsfc.nasa.gov/MODIS/ATBD/atbd_ mod23.pdf Briefly, variations in the coccolithophore calcite concentration influence the nL_w's at 443 and 551 nm in significantly different manners, depending on the concentration of phytoplankton pigments. The algorithm uses a two-parameter model for nL_w (Gordon et al., 1988) and solves for the particulate backscattering and pigment concentrations given nL_w(443) and nL_w(551). The calcite-specific backscattering coefficient $(b_b)^*_{PIC}$ is then used to estimate the detached coccolith concentration and the calcite concentration.

Predicted Data Accuracy

Since the two-band PIC algorithm uses absolute values of the water-leaving radiances, it is more susceptible to errors in atmospheric correction than the usual ocean color algorithms that employ radiance ratios. Thus, atmospheric correction can be an important source of error over and above the inherent error in the algorithm due to natural variability. In addition errors in sensor calibration can also cause errors in the recovered water-leaving radiance. (See MODIS Normalized Water-leaving Radiance Algorithm Theoretical Basis Document, by H.R. Gordon, for a discussion, with numerical examples, of atmospheric correction errors and the influence of sensor calibration errors on nL_w. The site is http://modarch.gsfc.nasa.gov/MODIS/ATBD/atbd_ mod17.pdf). We estimate that the error due to atmospheric correction will be small at $C_{cc} < 5 \times 10^9$ coccoliths m^{-3} for low pigment concentrations (C) and 10×10^9 to 15×10^9 coccoliths m^{-3} for C of 2 mg m^{-3}. Another potential source of error is the fact that the atmospheric correction algorithm assumes that $nL_w = 0$ for $\lambda = 765$ and 865 nm, i.e., in the near infrared (NIR). For sufficiently high coccolith concentrations this will be violated, which will degrade the atmospheric correction and therefore the retrieval of nL_w in the blue and green, introducing more uncertainty in C_{cc}. However, thus far our field and laboratory studies suggest that the largest potential error is natural variability of the $(b_b)_{PIC}$ - C_{cc} relationship (Balch et al., 1999).

Validation Study Results

As this is a new product and Terra was only launched in December 1999, there are relatively few data sets available for validation, particularly for the coccolith and suspended calcite products. This is because coccolith concentration (or particulate inorganic carbon, calcium carbonate) is not frequently measured at sea, while the chlorophyll concentration is. In conjunction with the NASA SIMBIOS activities, much of our validation estimates comes from the Gulf of Maine, the site of frequent blooms of coccolithophores, and readily accessible from our laboratory. We also made some measurements in a Bering Sea coccolithophore bloom.

Initial estimates of accuracy have been made based on comparison to shipboard measurements. A significant bloom of coccolithophores occurred in the Bering Sea in the fall of 1997 (15 September) We enumerated coccolith and coccolithophore concentration from water samples collected by a NOAA research ship within the feature (56^o 56.24'N $\times$ 170^o 19.66'W; Samples by Dr. J. Napp; no PIC measurements were available). The MODIS sensor had not yet been launched, so we applied the two-band coccolith algorithm to a SeaWiFS image. The coccolith concentration at this station, in the top 12 m of the water column, was 3.6×10^{11} coccoliths m^{-3}, and the SeaWiFS-derived estimate was 3.0×10^{11} coccoliths m^{-3}.

A small bloom of coccolithophores occurred in the Gulf of Maine during summer 2000, which was sampled on several occasions. In this feature, we made atomic absorption measurements of suspended PIC and microscope enumeration of coccoliths and plated coccolithophores. We report the former here. For the days where the ship was on the west side of the MODIS swath (most accurate radiance retrievals), we report that the overall accuracy in the PIC determination was 0.2-3 mg PIC m^{-3}. (or in terms of coccolith concentration, 1 - 10×10^9coccoliths m^{-3}). However, if one pools all the calibration data made over various days (and hence incorporating the different atmospheric effects, then the accuracy degrades to ~3 mg PIC m^{-3}, or 15×10^9 coccoliths m^{-3}.

For the 36 km global data, there are no comparable sea-truth data available at this time, thus we compared the statistics of the global values with statistics of regional field surveys or global models. Good agreement was found between the models, surveys, and the MODIS-derived global mean PIC (all within ~ ± 1 mg PIC m^{-3}).

Globally, the coccolith pigment product is well correlated to the MODIS pigment product (MODIS Ocean Products 15). Regionally, within the Gulf of Maine, however, the correlation is best at high pigment concentrations; at low concentrations, coccolithophore pigment concentration is systematically less than the MODIS pigment value. Given that we expect most of the satellite-derived blooms of coccolithophores to be *E. huxleyi*, we also would expect the band-ratio algorithms to underestimate the pigment concentration for suspensions of these small coccoliths (Balch et al., 1989). Thus, we suggest using the MODIS pigment product for PIC values up to 5 mg PIC m^{-3}, above which, the coccolithophore pigment values should be used.

Data Flags

For the discussion of product flags, we first require that the common flags for level 0 and 1 products are all zero (acceptable) in order to process any of the coccolith products. The product quality level for the level 2, coccoliths, PIC concentration and coccolith pigment directly depends on the quality of the input radiance data. Therefore, these products will be assigned the minimum quality level of the input data (normalized water-leaving radiance products at 443nm and 551nm). For coccolith/PIC products, if PIC concentration is ≤ 0 or > 1000 mg PIC m^{-3}, then the product quality level for the coccolith/PIC products and coccolithophore pigment concentration will be assigned a quality level of 3 (worst). We suggest using the coccolith pigment product (product #20) rather than the MODIS pigment product (product #15), if PIC concentration > 5 mg PIC m^{-3}. Otherwise, the MODIS pigment should be used in preference to the coccolith pigment product (assuming that the quality level of the former is at least as good as the latter).

Cautions When Using Data

The coccolithophore data products should be treated as "preliminary", until more shipboard validation work can be done, and accuracy checked. In addition, the normalized water-leaving radiances that are used in the estimations are also "preliminary" and expected to improve significantly.

From the validation work done so far, if validation data are available on the same day as the MODIS measurements, the accuracy can be expected to be from 0.2 - 2 mg PIC m^{-3}. If no validation data are available, then one can assume a best-case accuracy of ± 3 mg PIC m^{-3}. Moreover, until all BRDF problems are resolved, we do not recommend using these MODIS coccolithophore data products unless they are from the western third of the MODIS swath. We also caution using these data from shallow ocean regions, particularly near carbonate banks (e.g. Grand Bahamas), where bottom reflectance will appear as a high-reflectance coccolithophore bloom (presumably such pixels would be flagged due to their shallowness). Moreover, near river mouths and in shallow waters, resuspended sediments (of non-calcite origin) may appear as high suspended calcite concentrations. Only use these data if the waters are sufficiently deep to not have such bottom resuspension or direct river impact. Beware that MODIS-derived coccolith concentrations assume that the coccoliths are from the prymnesiophyte, *E. huxleyi*. If this is not true, then inaccuracies will increase. Even when using the data in units of mg PIC m^{-3}, they nevertheless assume a constant backscattering cross-section for *E. huxleyi* , which is known to vary with the size of the calcite particle (Balch et al., 1999; Balch et al., 1996).

More information about the algorithm and inputs can be found in:

Esaias, W., et al., 1998, Overview of MODIS Capabilities for Ocean Science Observations, IEEE Transactions on Geoscience and Remote Sensing, vol. 36, no. 4, July 1998, pp. 1250-1265.

Planned Algorithm Improvements

As the normalized water-leaving radiances used in the estimations improve, a concomitant improvement in PIC is to be expected. Additionally, a three-band algorithm has been recently described for determining suspended calcite concentration (Gordon et al. 2001). This algorithm has the added advantage that chlorophyll does not interfere with the acquisition of the PIC. Validation checks are ongoing before the algorithm will be fully implemented within the MODIS data stream.

Referencing Data in Journal Articles

Results derived from this algorithm should cite the paper of Gordon et al. (1988) for the original discussion, and (Balch et al., 1999; Balch et al., 1996) for field data on the backscattering cross-section of calcite.

Citations

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