MODIS
Terra Chlorophyll_a Pigment Concentrations (Case 2 Waters)
Data Quality Summary

Last updated: February 15, 2003

Investigation:	MODIS
Data Product:	Chlorophyll_a Pigment Concentrations (Case 2 Waters; MOD21)
Data Set:	Terra
Data Set Version:	Collection 4 version 4.2 reprocessed
Dates:	November 1, 2000 through March 2002
Status:	Validated

Nature of the Product

Chlorophyll-*a* concentration is the most widely used product derived from ocean color remote sensing data. The first such measurements were made by the Coastal Zone Color Scanner (CZCS) operating between 1978 and 1986, and were termed chlorophyll-like pigment concentration. The CZCS pigment concentration was believed to be more closely related to the sum of chlorophyll *a* plus phaeophytin *a*, a degradation product of chlorophyll *a*, than to chlorophyll *a* alone. It was believed that phaeophytin *a* could not be distinguished from chlorophyll *a* given the spectral resolution of the CZCS. With improved spectral and radiometric resolution, the Sea-viewing Wide Field-of-View (SeaWiFS) sensor began producing global maps of chlorophyll-*a* concentration in September 1997.

Chlorophyll_a pigment concentrations for Case 2 waters (Chlor_a_3; MOD21) are defined as values retrieved in the presence of absorption by colored dissolved organic matter (CDOM). This separation is achieved by using the spectral differences between absorption curves for phytoplankton, $a_{ph}(\lambda)$, and absorption curves for CDOM, a.k.a. gelbstoff, $a_g(\lambda)$. In reality, $a_g(\lambda)$ also includes absorption due to particulate detritus, which has a similar spectral shape. Together they are termed the Dissolved Organic Matter Absorption product, having one parameter: dissolved organic matter absorption at 400nm (absorp_coef_gelb, parameter 30). The strategy for achieving this separation is discussed by Carder et al. [1999] and in the updated version of the algorithm theoretical basis document ATBD-19 found at *http://modis.gsfc.nasa.gov/data/atbd/atbd_mod19.pdf* .

Without this separation relatively accurate chlorophyll concentrations can be obtained for tropical-subtropical waters where CDOM, detritus, and other optically active substances co-vary with chlorophyll *a* concentrations. Accuracy decreases, however, in CDOM-rich environments such as coastal zones with terrestrial runoff. Differences in the CDOM-to-chlorophyll ratio occur even in open-ocean waters, as the ratio is higher in the river-rich northern hemisphere than in the southern hemisphere.

Chlor_a_3 also differs from other approaches to retrieving chlorophyll concentrations in that the spectrum of chlorophyll-specific phytoplankton absorption coefficients, $a^*_{ph}(\lambda)$, is adjusted dynamically using sea-surface temperature, SST (MOD-28) [Carder et al. 1999; ATBD-19]. Since satellite algorithms implicitly determine pigment concentration through the absorbed light by pigments in the ocean, and $a^*_{ph}(440)$ can vary by more than a factor of 10 between nutrient-poor, photon-rich subtropical gyres and nutrient-rich, photon-poor upwelling or high-latitude waters, a means to express these dynamics was developed. Comparing SST to the nitrate-depletion temperature, NDT [Kamykowski, 1987], as an indicator of nutrient availability and light history provides a means of evaluating whether upwelling or convective overturn has replenished the surface waters with nutrients from below the surface mixed layer, changing the species and pigment composition of the phytoplankton ensemble observed. High light increases temperature, photo-protective pigments, and decreases cell size and pigment concentration per cell (pigment packaging), increasing $a^*_{ph}(\lambda)$. The SST-NDT difference provides a space-based cue for changing the pigment-packaging parameters used in describing $a^*_{ph}(\lambda)$ more accurately.

Data Accuracies

The inherent accuracy of the Chlor_a_3 algorithm for various field locations has been addressed by Carder et al. (1999) and by ATBD-19. In summary, for open-ocean tropical-subtropical and summer temperate regions, linear accuracy to within ~24% (278 points) of measured chlorophyll values was observed, while for an eastern-boundary upwelling region, the accuracy was about 28% (326 points) [*Carder et al.,* 1999]. Allowing SST-NDT to be used to classify which pigment-packaging parameters are required, provided accuracies to within 31% (13 points) for an upwelling zone transitioning to a temperate spring region in the Southern California Bight. For northern high-latitude waters the accuracy of the Chlor_a_3 algorithm performance was 48.5% (75 points), while for the Southern Ocean it dropped to 66% (971 points over 10 years)[ATBD-19]. Northern high-latitude chlorophyll-specific absorption coefficients can be very species-specific for ice-melt regions with large blooms compared to coefficients from adjacent deeply mixed waters [*Stuart et al.,* 2000]. High variability has similarly been observed in the Southern Ocean [*Brody et al.,* 1992].

Assigning an accuracy of ~10% to the chlorophyll *a* measurements results in algorithm accuracies of 22%, 26%, 30%, 47%, and 65%, respectively for the regions mentioned above. Ryther (1969) estimated that 55.8% of the ocean area between 50^o N and 50^o S is oligotrophic (chla < 0.1 mg m^{-3}), 41.8% is mesotrophic (0.1 < chla < 1.0 mg m^{-3}), and 2.4% is eutrophic (chla > 1.0 mg m^{-3}). Roughly 10% of the ocean surface is found south of 50^o S. Because solar zenith angles are limited to less than 70^o, for data to be considered of the highest quality level (0), only southern latitudes lower than 50^o S are mapped by Terra data of Quality Level 0 in December, for example. Renormalization to 110%, then, provides roughly 50.7% of the ocean that is oligotrophic with an accuracy of about 22%, some 38% is mesotrophic with an accuracy between 26 and 30%, and 11.3% is eutrophic and/or Southern Ocean data with an accuracy of about 66%. This provides a global algorithm accuracy estimate for December of 0.507*0.22 + 0.38*0.30 + 0.113*0.66 = ±0.30. A similar accuracy for June (±0.28) can be generated by replacing 0.66 by 0.47. So, a best-case accuracy for Chlor_a_3 of 28% to 30% can be expected for MODIS Terra given a well-calibrated sensor, good atmospheric corrections, and appropriate nitrate-depletion temperatures and sea-surface temperatures. Note also that algorithm performance for each of these regions was found to be (ATBD-19) essentially bias-free, suggesting that little error in globally integrated chlorophyll *a* values will result, and that chlorophyll-based primary production models should not be appreciably biased using Chlor_a_3 values.

Field and satellite (SeaWiFS) comparisons were made by an independent group (Smyth et al. 2002) of the semi-analytical Chlor_a_3 algorithm ($R^2 = 0.871$) against several other algorithms including the OC4v4 SeaWiFS algorithm ($R^2 = 0.652$) for a match-up area west of the Iberian Peninsula. They state that "overall the Carder approach would be the model of choice in the determination of chlorophyll *a* from satellite sensor measurements of remote-sensing reflectance, as it combines a physical approach with good performance in terms of slope, standard error and R^2."

The accuracy of retrievals of Terra Chlor_a_3 is dependent upon the accuracy of the water-leaving radiance values of Terra, the accuracies of daytime SST and NDT values, field values of chlorophyll *a*, and the inherent accuracy of the algorithm. The SST values are validated (http://modis-ocean.gsfc.nasa.gov/qa/dataqualsum/sst_qualsum.V4.pdf) at Stage 1 to within about ±0.25^o C, and the normalized water-leaving radiance values (http://modis-ocean.gsfc.nasa.gov/qa/dataqualsum/nLw_qualsum.V4.pdf) are validated at Stage 1 to within about 10%, especially for the period 1 November 2000 through 19 March 2002.

An independent validation study by Watson Gregg and Nancy McCabe (W. Gregg, NASA GSFC, personal communication) of MODIS Terra chlorophyll products Chlor_MODIS, Chlor_a_2, and Chlor_a_3 and SeaWIFS OC4v4 data using NOAA's National Ocean Data Center and NASA's SeaBASS data bases for data from MODIS launch until December 2002. Note that while this includes periods before November 2000 and after March 2002 when the MODIS normalized water-leaving radiance values have been of than for the validation period lower quality or have not been recalibrated vicariously, it is clear that the chlorophyll products are in general are equal or superior to those of SeaWiFS. Chlor_a_2 global performance for Level 3 daily 4.6 km data collected within 24 hours of field collections was virtually identical to that of SeaWiFS ($r^2 = 0.757$, n = 1642, slope = 0.84, bias = -0.01), Chlor_a_3 global performance was superior to the others ($r^2 = 0.784$, n = 1282, slope = 0.911, bias = 0.04). The chlorophyll biases of –0.01 and 0.04 at 1 mg m^3 for the log-log data presentations were only off by 1% and 4%, respectively. Not only was the correlation better of Chlor_a_3 data about the best-fit line, the slope of the best-fit line was much closer to 1:1. Considering only data from within the radiance-validation period is expected to further improve these results.

For Terra retrievals of Chlor_a_3 collected within the radiance validation window and within 6 hours of field data, a match-up data base was prepared by the MODIS DAAC and the SeaWiFS SIMBIOS Project using Terra Collection 4 Version 4.2 reprocessed data collected between 1 January 2001 and 30 June 2001. Match-ups (http://seabass.gsfc.nasa.gov/matchup_results.html) were made with field data collected synoptically within 3 hours of Terra overpasses within a 5 km box (SeaWiFS Postlaunch Technical Report Series Volume 10, Chapter 7). The match-ups provided by SIMBIOS (http://seabass.gsfc.nasa.gov/RESULTS/MODIS/MODIS_chl_matchups.gif) included 1 Southern Ocean point, 4 equatorial Pacific points, 8 California Current points (2 within 50 pixels of the swath edge), and 7 Florida shelf points. The field chlorophyll data were averaged over the first 25 meters by SIMBIOS for the comparisons.

The initial match-ups produced root-mean-square errors (RMSE) for log-transformed data (n=20) of 0.199 or 1/5 of a log unit (Fig. 1a), a better result with MODIS Terra from space than the best-fit regression curve (RMSE=0.222; n=2804) of the SeaWiFS OC4v4 algorithm using field radiometry from ships (O'Reilly et al. 2000). On closer inspection it was found that if one more appropriately used, throughout the analyses, chlorophyll *a* data averaged within just the top 10 meters, and averaged 5x5 Terra pixels around the field location for the 2 swath-edge pixels, the RMS error was reduced to 0.176 (Fig. 1b; Carder et al. accepted).

Swath edges are regions where banding or striping is greatest for the 412 and 443 nm bands of Terra for Collection 4, and structured latitudinal variance is repeated every 20 pixels. Unless this striping is minimized by latitudinal averaging, structured variations from about 0.35 to 0.90 mg m^{-3} can occur compared to an average value of 0.60 mg m^{-3}. Much of the striping problem will be alleviated as a result of the next reprocessing.

The nitrate-depletion temperature is less relevant for continental shelves where nutrients are provided by terrigenous runoff and shelf-break upwelling in addition to seasonal convective overturn. For shelves that are shallower than the permanent pycnocline (usually also the nutricline), seasonal convective overturn is less relevant, and NDT is not conceptually linked in any way with terrigenous runoff. To evaluate the accuracy of data excluding continental-shelf waters, the West Florida Shelf stations were first omitted from the comparison, resulting in an RMS value of 0.107 for 13 points, with a bias less than 0.003 and a slope of 0.99 (Fig. 1c). This is equivalent to a linear error (RMS_{lin}) of 10^{RMS}-1, or 28%.

If the NDT value for the West Florida Shelf is reduced from its present value of about 22^o C to 19.5^o C, in order to be more indicative of the temperature of up-welled Subtropical Underwater found at times on the edge of the shelf break, the error including these shelf points is reduced significantly. RMS error including the WFS points becomes 0.098 (n=20), with a bias of 0.004, a slope of 0.986, and a linearized error RMS_{lin} = 25.3% (n=20) (Fig. 1d). Most of the retrievals to date are well within the project accuracy goal of 35% for Chlor_a_3, at least if shelves and scene edges are avoided. Adjusting the NDTs to values appropriate to specific continental shelf regions significantly improves algorithm performance.

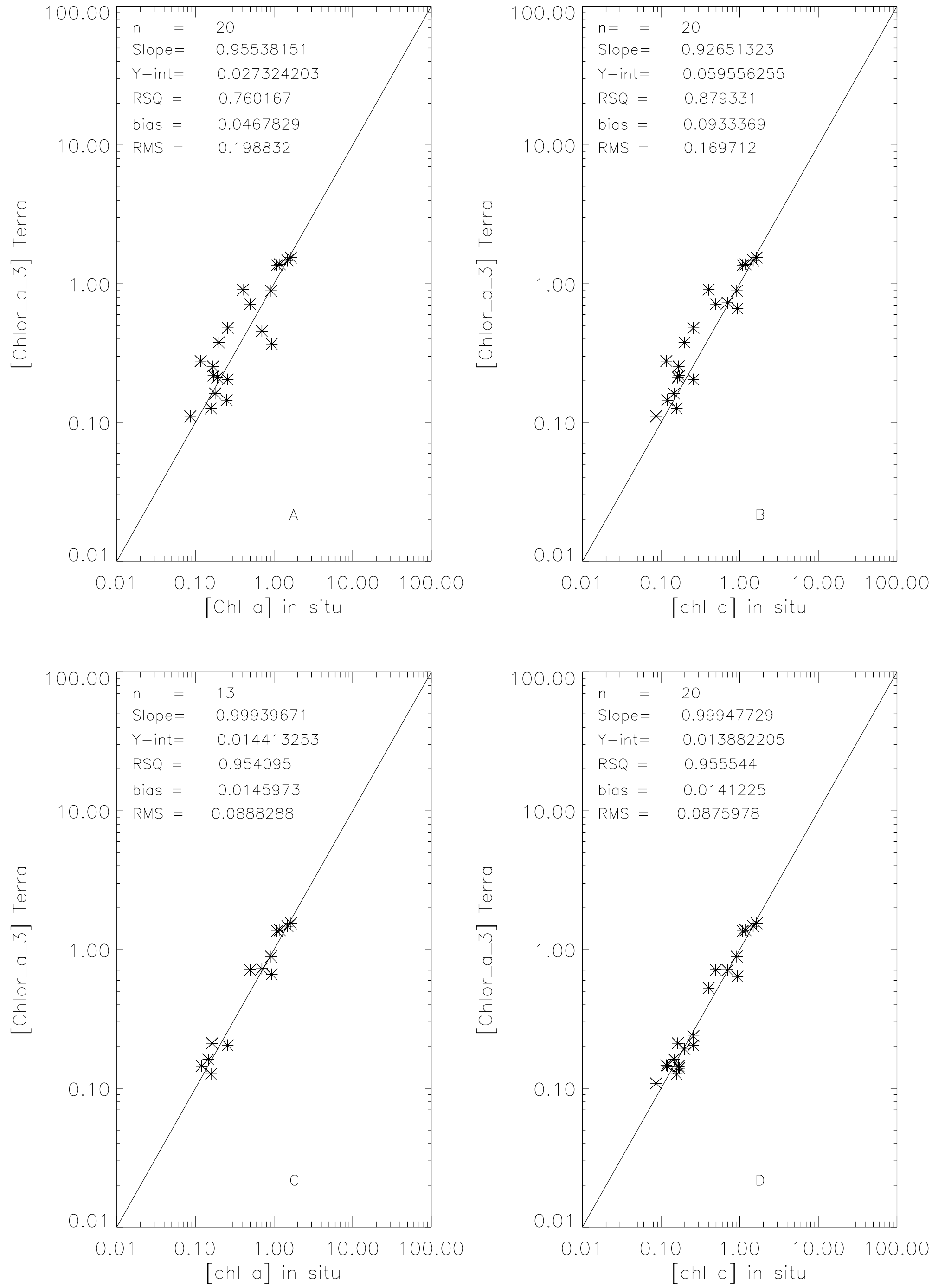

Figure 1. Results from independent SeaWiFS SIMBIOS evaluation of MODIS match-up data for chlorophyll *a* concentrations at global sites:

- **a)** Chlor_a_3 compared to 0 – 25m field measurements;
- **b)** Chlor_a_3 match-ups using top-layer (0 – 10m), *in situ* chlorophyll *a* concentrations, 5x5 pixel averages for scene-edge data (14 March 2001);
- **c)** Same including no Florida-shelf data (13 points); and
- **d)** Same including Florida shelf data (20 points) using NDT = 19.5^{o} C.

Under all conditions tested to date, Chlor_a_3 data have been validated (Stage 1). Validated (Stage 1) means that comparisons with surface data at a limited number of locations (e.g. 20 global) and times (January-June 2001) have been carried out successfully, leading to an estimate of the uncertainty in the validated quantity (see http://modis-ocean.gsfc.nasa.gov/datamaturity.html for a description of the validation stages). Product accuracy using ship data has been investigated at a large number field locations, and the results have been reported in the refereed literature (Carder et al. 1999; Smyth et al. 2002), and recent results have been posted on the web at the following site: http://modis.gsfc.nasa.gov/data/atbd/atbd_mod19.pdf . Furthermore, global accuracies for MODIS Terra Chlor_a_3 data have been assessed by an independent group (SeaWiFS SIMBIOS Project), for a number of sites and times, which are representative of global conditions. The accuracies reported for most areas observed by Terra are similar to those observed using ship observations (e.g. <35% for the eastern boundary Pacific Ocean and equatorial Pacific), suggesting that regional accuracy estimates with ship-based radiometry appear to be faithfully reproduced using Terra data of quality level 0.

While the period for which match-up data were available at the time of this QA update runs only from January to June 2001, the data quality are expected to hold for reprocessed data from Collection 4 from 1 November 2000 to 1 March 2002, the period of performance with validated normalized water-leaving radiances. Scene-edge striping of Bands 8 and 9, which most strongly affects Chlor_a_3 data from Terra, is expected to be reduced significantly after the next reprocessing.

Cautions When Using Data

Only data of Quality Level 0 were used in the data match-up comparisons (Carder et al. accepted), meaning that screening has been employed for sun glint, shallow water (<30 m), and extreme-angle pixels. More relaxed conditions for data of Quality Levels 0 and 1 were employed by Gregg and McCabe. Definitions of Quality Levels can be found at http://modis-ocean.gsfc.nasa.gov/qa/L2QLflags.V4.html. In addition to the exceptions listed above, the user should be cautioned regarding use of Collection 4 data at the scene edges where obvious striping is occurring. Avoiding the 100 pixels or so along each swath edge reduces this effect somewhat, but the degree of the problem varies from scene to scene as a result in part of unresolved polarization effects in Collection 4 data (see http://modis-ocean.gsfc.nasa.gov/qual.html/dataqualsum/nLw_qualsum.V4.pdf).

Anticipated Revisions

Recent improvements in Terra calibration knowledge based upon MODIS Aqua performance and calibration history regarding polarization effects suggest that the striping problem of Terra for Bands 8 and 9 can be significantly reduced and will be much less apparent for Aqua and for Terra after the next reprocessing (R. Evans, personal communication). This should significantly improve scene-edge and near-sun-glint accuracy of Chlor_a_3 retrievals. Evaluating regional data will permit revisions of the effective nitrate-depletion temperature values for unique regions such as demonstrated by Carder et al. accepted) for the west Florida shelf.

Riverine nutrients do not respond to the NDT approach, which depends upon the temperature-nutrient relationship near the top of the permanent nutricline from whence up-welled and convectively over-turned waters originate. Continental shelves that are shallower than the nutricline and which have alternative nutrient sources are not expected to respond to the NDT approach without minor adjustments. The adjustments include changing the NDT value such as was done successfully for West Florida Shelf data (compare Fig. 1b and 1d). Evaluation of other shelves will be made as more field data become available.

A second change that will help accuracies for extended river plumes is the fact that reduced photo-protective pigments are typically found when CDOM-rich water is present. CDOM absorbs much of the damaging ultraviolet irradiance that must be blocked by photo-protective pigments were the CDOM not present. This effect reduces parameter values for chlorophyll-specific absorption coefficients, especially during the summer months. Tests are being made using Gulf of Mexico data to prepare an adjustment based upon the CDOM:pigment absorption coefficients at 443 nm.

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