#### **Product:** Chlorophyll-*a* OC3M Algorithm (Chlor\_oc3m) **Units:** mg m<sup>-3</sup> **Product Description:**

The Case 2 chlorophyll-*a* algorithm is based on a semi-analytical, bio-optical model of remote-sensing reflectance,  $Rrs(\lambda)$ , where  $Rrs(\lambda)$  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  $Rrs(\lambda)$  model has two free variables, the absorption coefficient due to phytoplankton at 675 nm,  $a\phi(675)$ , and the absorption coefficient due to colored dissolved organic matter (CDOM) or gelbstoff at 400 nm, ag(400). The Rrs model has several parameters that are fixed or can be specified based on the region and season of the MODIS scene. These control the spectral shapes of the optical constituents of the model. Rrs ( $\lambda$ i) values from the MODIS data processing system are placed into the model, the model is inverted, and  $a\phi(675)$ , ag(400), and chlorophyll-a are computed.

The algorithm also outputs both the total absorption coefficients,  $a(\lambda i)$ , and permits calculation of the phytoplankton absorption coefficients,  $a\phi(\lambda i)$ , based on  $a\phi(675)$  retrievals. These are used in the calculation of the radiation absorbed by phytoplankton for use in the calculation of chlorophyll fluorescence efficiencies.

Algorithm development is initially focused on tropical, subtropical, and summer temperate environments, and the model is parameterized for three different bio-optical domains: (1) high ratios of photo-protective pigments to chlorophyll and low self-shading, which for brevity we designate A-unpackaged; (2) low ratios and high self-shading, which we designate A-packaged; and (3) a transitional or global-average type. These domains can be identified from space by comparing sea-surface temperature to nitrogen-depletion temperatures 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 (Carder et al. 1999). Algorithm errors are reduced from 41% for an empirical algorithm to 20% using the semianalytical approach for global MODIS data (Carder et al. 2003).

Introduction from Algorithm Theoretical Basis Document 19: MODIS Ocean Science Team (http://modis.gsfc.nasa.gov/data/atbd/atbd\_mod19.pdf).

## **Product:** Chlorophyll-*a* Generalized Inherent Optical Properties (chl\_giop) **Units:** mg m<sup>-3</sup> **Product Description:**

In 2008, NASA proposed to provide the datasets, processing framework, and international forum within which a new generation of global IOP products could be developed and evaluated. The theoretical basis of GIOP is as published by NASA: Remote-sensing reflectance  $(R_{rs}(\lambda); sr^{-1})$  are related to absorption  $(a(\lambda); m^{-1})$  and scattering coefficients via the following equation:

$$R_{rs} = G \frac{b_b}{a + b_b},\tag{1}$$

where  $b_b(m^{-1})$  is the total backscattering coefficient and all terms are spectral.  $G(sr^{-1})$  varies with illumination conditions, sea surface properties, and the shape of the marine volume scattering function. The absorption coefficient can be expanded as the sum of all absorbing components, and each component can be further expressed as the product of its concentrationspecific absorption spectrum (eigenvector;  $a^*$ ) and its concentration (eigenvalue; A):

$$A = a_w + A_{dg}a^*_{dg} + A_{\phi}a^*_{\phi} \tag{2}$$

Where the subscripts w, dg, and  $\phi$  indicate contributions by water, dissolved organic matter (gelbstoff) + non-algal particles (detritus), and phytoplankton, respectively. The dg combination cannot currently be decomposed into its two components using remote-sensing methods. Total backscattering can be expanded to the following:

$$b_b = b_{bw} + B_{bp} b_{bp}^*, b_b = b_{bw} + B_{bp} b_{bp}^*$$
(3)

where the subscripts bw and bp indicate contributions by water and particles, respectively. Both  $a_w$  and  $b_{bw}$  are known. Using  $R_{rs}$  as input, eigenvalues for absorption and scattering (A and B) can be estimated via linear or nonlinear least-squares inversion of Eq. (1) (see http://oceancolor.gsfc.nasa.gov/WIKI/GIOP.html).

## **Product:** Chlorophyll-*a* Garver-Siegel-Maritorena bio-optical model (chl\_gsm01) **Units:** mg m<sup>-3</sup> **Product Description:**

The GSM algorithm considers that Chl, colored dissolved and detrital organic materials (CDOM), and particulate abundances each independently affect ocean color and these properties are retrieved simultaneously from a water-leaving radiance spectrum (Maritorena et al. 2002; Siegel et al. 2002, 2005).

**Product:** Fluorescence Line Height (flh) **Units:** mW cm<sup>-2</sup>µm<sup>-1</sup> sr<sup>-1</sup> **Product Description:** 

# From Algorithm Theoretical Basis Document 20: Chlorophyll Fluorescence (Abbott & Letelier, 1999)

[http://modis.gsfc.nasa.gov/data/atbd/atbd\_mod22.pdf].

- Fluorescence Line Height Algorithm
  - The FLH algorithm is a relative measure of the amount of radiance leaving the sea surface, which is presumably a result of chlorophyll fluorescence.
  - By constructing a baseline using bands on either side of the fluorescence band, we can estimate the deviation from the amount of radiance expected for pure water from the radiance that results from chlorophyll fluorescence.
  - The increase in radiance (centered at 683 nm for chlorophyll) has been noted for decades in measurements of the light field in the ocean. This signal is generally weak, even in regions of high chlorophyll concentration.
  - To measure fluorescence, the signal-to-noise ratio (SNR) was increased for the fluorescence band and the adjacent "baseline" bands at 665.1 nm (band 13) and 746.3 nm (band 15). The fluorescence measurement itself is made at 676.7 nm (band 14) as a compromise between measuring the fluorescence peak (683 nm) and the presence of an oxygen absorption band at 687 nm.
  - Chlorophyll fluorescence will increase the amount of water-leaving radiance at 683 nm that would be expected for chlorophyll-free water.
  - The amount of this increase will depend on several factors, including the specific absorption of chlorophyll, fluorescence quantum efficiency, the amount of incident sunlight, and various atmospheric effects. Wavelengths need to be selected by how much they minimize the atmospheric effects.
  - The main component of the algorithm is the estimation of the increased radiance caused by fluorescence. By defining a baseline underneath the expected fluorescence peak, one can estimate the relative contributions to the upwelled radiance field by chlorophyll fluorescence.
- Chlorophyll Fluorescence Efficiency

- FLH will form the basis of chlorophyll fluorescence efficiency.
- The primary use of fluorescence has been the estimation of chlorophyll concentration.
- Most fluorescence studies collect occasional calibration samples where the pigment would be extracted from the phytoplankton, and chlorophyll would be measured using spectrophotometric methods. Using these calibration samples, the ratio of chlorophyll to in-vivo fluorescence was assumed to be constant. However, the literature is filled with studies that document the numerous processes that can change the relationship between chlorophyll and in-vivo fluorescence on a wide range of time and space scales. These processes included species changes, nutrient concentrations, and incident radiation. Overall, these processes are related to the physiological state of the phytoplankton.
- The resulting ratio provides an estimate of the efficiency of the conversion of absorbed solar radiation into fluorescence by phytoplankton.
- This product is converted into radiance units.

Product: Sea-Surface Temperature (sst) Units: °C Product Description:

From Algorithm Theoretical Basis Document: MODIS Infrared Sea Surface Temperature Algorithm (Brown et al. 1999) [http://oceancolor.gsfc.nasa.gov/DOCS/atbd\_mod25.pdf].

- Sea-surface temperature is calculated using satellite infrared retrievals of ocean temperature. It is corrected for atmospheric absorption using a combination of MODIS mid- and far-infrared bands.
- The quality-assessment SST output products are vectors composed of the estimated SST value, input calibrated radiances, and derived brightness temperatures for each band, flags that quantify the cloud screening results and scan coordinate information, latitude, longitude, and time.

The long-wave SST algorithm makes use of MODIS bands 31 and 32 at 11 and 12  $\mu$ m. The brightness temperatures are derived from the observed radiances by inversion (in linear space) of the radiance versus blackbody temperature relationship. These relationships were pre-computed for the spectral response of each MODIS channel, and the tables were then stored in HDF files to be loaded at run-time. In MODIS sst, the radiance versus blackbody temperature relationship was computed at run-time. The nonlinear SST algorithm was tuned for two different regimes based on brightness temperature difference. The algorithm for computing long-wave SST (sst) from observed brightness temperatures is shown below.

$$\begin{split} &d_{BT} <= 0.5\\ &sst = a00 + a01*BT11 + a02*d_{BT}*b_{sst} + a03*d_{BT}*(1.0/mu-1.0)\\ &d_{BT} >= 0.9\\ &sst = a10 + a11*BT11 + a12*d_{BT}*b_{sst} + a13*d_{BT}*(1.0/mu-1.0)\\ &0.5 < dBt < 0.9\\ &sst_{lo} = a00 + a01*BT11 + a02*d_{BT}*b_{sst} + a03*d_{BT}*(1.0/mu-1.0)\\ &sst_{hi} = a10 + a11*BT11 + a12*d_{BT}*b_{sst} + a13*d_{BT}*(1.0/mu-1.0)\\ &sst_{hi} = a10 + a11*BT11 + a12*d_{BT}*b_{sst} + a13*d_{BT}*(1.0/mu-1.0)\\ &sst_{hi} = sst_{lo} + (d_{BT}-0.5)/(0.9-0.5)*(sst_{hi}-sst_{lo}) \end{split}$$

where:  $d_{BT} = BT11 - BT12$  BT11 = brightness temperature at 11 um, in °C BT12 = brightness temperature at 12 um, in °C  $b_{sst} =$  baseline SST mu = cosine of sensor zenith angle

The coefficients a00, a01, a02, and a03 and a10, a11, a12, and a13 are derived and continuously verified by RSMAS [Rosenstiel School of Marine and Atmospheric Science (RSMAS) at the University of Miami] based on match-ups between the satellite retrievals of brightness temperature and field measurements of sea surface temperature. As currently implemented, these coefficients can be time-dependent. The coefficients are provided to msl12 through external files, which are in a columnated ascii format of "sensor start-date end-date ai0 ai1 ai2 ai3", with each pair of lines corresponding to low and high dBT difference cases, respectively

**Product:** Measured (Observed) Back Scatter GIOP (Measured\_Bksctr\_giop) [Intermediate Product]

Units: m<sup>-1</sup>

**Product Description:** This product is the default GIOP particulate back scatter product for the 547 nm wavelength produced during processing within SeaDAS.

## **Product:** Calculated Back Scatter GIOP (Calculated\_Bksctr\_giop) [Intermediate Product] **Units:** no units

## **Product Description:**

The calculated back scatter was derived from the early work by Morel (1988). Morel noted that particle scattering has been shown to vary approximately with  $\lambda^{-1}$  (Morel, 1988; 1973). Algal cells exhibit very low particulate backscatter values (Bricaud et al., 1983), as is fully supported by theory (Bricaud and Morel, 1986). The particulate backscatter relationship is numerically expressed as:

$$\tilde{b}_b b = 0.30C^{0.62} \left[ 2.10^{-3} + 2.10^{-2} \left( \frac{1}{2} - \frac{1}{4} \log C \right) \right]$$

Where:  $\tilde{b}_b b$  represents particulate backscattering, C indicates chlorophyll-a concentration.

Morel (1988) rationale for this model is to obtain a progressive change from an oligotrophic environment where detritus are relatively more abundant (detrital particles, characterized by  $\tilde{b}_b = 2\%$  and a  $\lambda^{-1}$  scattering dependency) to eutrophic environments where algal cells are the predominant particles, with low  $\tilde{b}_b(0.2\%)$  and practically no spectral dependency.

**Product:** Chlorophyll Subtraction Product (chl\_phb2) [Intermediate Product] **Units:** <0 = No Toxic Bloom Present; >0 = Potential Toxic Bloom Present **Product Description:** 

The difference measured between the observed backscatter and calculated backscatter from the generalized inherent optical properties provides an indication of the probability of toxic algal bloom occurrences. A drop in remote sensing reflectance  $R_{rs}(\lambda)$  was noticed in Chl-a rich waters that have high concentrations of *K. brevis* when compared to areas with lower *K. brevis* concentrations and was attributed to a drop in particulate backscatter ( $b_{bp}(\lambda)$ ) rather than changes in absorption (Morel, 1988; Carvalho et al. 2010; 2011). This product is ultimately utilized as an intermediate product to develop the Karenia Brevis product for condition one.

**Product:** Karenia Brevis (Karenia\_Brevis) [Final Product] **Units:** mg m<sup>-3</sup> **Product Description:** 

A drop in remote sensing reflectance  $R_{rs}(\lambda)$  was noticed in Chl-*a* rich waters that have high concentrations of *K*. *brevis* when compared to areas with lower *K*. *brevis* concentrations and

was attributed to a drop in particulate backscatter  $(b_{bp}(\lambda))$  rather than changes in absorption (Morel, 1988; Carvalho et al. 2010; 2011). Given these observations, a method was developed (Morel, 1988; Carvalho et al., 2011) to detect *K*. *brevis* blooms based on two conditions:

(1) Measured particulate backscatter ( $b_{bp}(\lambda)$ ) at 551 nm ( $b_{bpSAT}(\lambda)$ ) < particulate backscatter calculated at  $\lambda = 550$  nm ( $b_{pbMorel}$ ) (Morel 1988), and

(2) Chl-a concentration >  $1.5 \text{ mg/m}^3$ .