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Band ratio to band difference for Chl of oceanic waters: broke a self-imposed no-touch zone

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Abstract:

There are many empirical algorithms developed for the remote sensing of chlorophyll-a concentration (Chl) from ocean color measurements, with the blue-green band-ratio type of algorithms dominating these practices. During the phase of algorithm development, which is data-driven, generally the errors of remote sensing reflectance (R_{rs}) from satellites are ignored until Hu et al. (2012) developed a band-difference type algorithm where R_{rs} at the blue, green, and red bands were used as the input, where the errors in R_{rs} were kept in mind. This band-difference algorithm generated significantly better Chl image products for oceanic waters from satellite ocean color measurements, which contributed greatly to satellite ocean color remote sensing and influenced the way of thinking in algorithm development.

1. Band ratio to band difference for chlorophyll concentration in the ocean: a 30-year self-imposed no-touch zone

As stated in the IOCCG Report #2, “A primary goal of ocean-colour remote sensing is to produce synoptic fields of chlorophyll pigment ...” (IOCCG 1999). To achieve this, a robust algorithm for the estimation of chlorophyll-a concentration (Chl) from ocean color data is one of the key components of any processing system. Traditionally, this has been achieved through blue/green band-ratio algorithms (Hu and Campbell 2014; O’Reilly et al. 1998), because, at least conceptually, the ratio would decrease with increasing Chl. About 10 years ago, Hu et al. (2012) introduced a new concept in algorithm design, which used a 3-band difference to estimate Chl in relatively clear waters. The algorithm base of Hu et al. (2012) is the difference of remote sensing reflectance (R_{rs}) at the blue, green, and red bands, rather than the base of “standard” algorithms adopted by NASA and ESA for many decades, which is the blue-green ratio of R_{rs} . Because of the improved performance in data product accuracy and cross-sensor consistency, subsequently, NASA, NOAA, and ESA adopted a mixed algorithm to process satellite ocean color data for the generation of global Chl, with the band-difference algorithm for waters with $\text{Chl} < \sim 0.2 \text{ mg/m}^3$ (more than 70% of the global ocean), band-ratio algorithm for waters with $\text{Chl} > \sim 0.3 \text{ mg/m}^3$, and an empirical bridge for waters with Chl between ~ 0.2 and $\sim 0.3 \text{ mg/m}^3$.

The development of algorithms for the estimation of Chl from ocean color measurements is a key aspect of research in ocean optics and ocean color remote sensing, which could be dated back to the 1970s, where nearly all algorithms took an approach based on the blue-green ratio of water color, represented either by R_{rs} or the water-leaving radiance. Why did it take many decades to reach this new level, and thinking, on the processing of satellite ocean color images? Note that 30 years earlier, before Hu et al. (2012), Viollier et al. (1978; 1980) developed empirical Chl algorithms based on the difference of water-leaving radiance at two bands (which is equivalent to the difference of R_{rs} at two bands).

One likely reason for this hiatus is the analyses presented in the book authored by Gordon and Morel (1983), which used a model of reflectance to demonstrate the variables related to the reflectance difference of “Case 2” waters. Gordon and Morel (1983) stated that the model “... would be a good approximation to some Case 2 waters,” which “... can be used to demonstrate the dangers associated with the use of such an algorithm”, i.e., band-difference type of algorithms will inherently not perform well for such waters. This statement was somehow interpreted by the community that the band difference algorithm is not a good option for all waters, thus no longer evaluated or practiced until Hu et al. (2012), resulting in a 30-year hiatus or no-touch zone. However, Gordon and Morel’s analyses are about a “danger” in “Case 2” waters for such band-difference algorithms; they did not evaluate the situations of oceanic waters, and they did not state that there is such a “danger” for oceanic waters where Chl is low. It is rather that nearly all practitioners in ocean-color-algorithm development insensitively, and incorrectly, extended the interpretation to such waters, where the practitioners were not careful or rigorous enough in extending results from one environment to another. As presented in Hu et al. (2012) and below, for oceanic waters where Chl is low, actually there is no such “danger”.

2. The essence of blue-green-red difference of R_{rs}

The band difference algorithm for Chl proposed by Hu et al. (2012) can be written as

$$BD_{Rrs} = R_{rs}(\lambda_G) - \left[R_{rs}(\lambda_B) + \frac{\lambda_G - \lambda_B}{\lambda_R - \lambda_B} (R_{rs}(\lambda_R) - R_{rs}(\lambda_B)) \right] \quad (1a)$$

$$Chl = f(BD_{Rrs}) \quad (1b)$$

where BD_{Rrs} is the difference of R_{rs} at the blue (λ_B), green (λ_G) and red (λ_R) bands. R_{rs} is in general a function of water's inherent optical properties (Gordon et al. 1988), and to the first order it can be expressed as

$$R_{rs} = G \frac{b_b}{a + b_b} \quad (2)$$

Here, b_b and a are the backscattering and absorption coefficients, respectively, with G (sr^{-1}) a model coefficient. For b_b , commonly it is divided into two terms

$$b_b = b_{bw} + b_{bp} \quad (3)$$

with subscripts “w, p” representing pure (sea)water and particles. For BD_{Rrs} , based on Eq. 2, considering $a \gg b_b$ and ignoring $b_b(\lambda_R)/a(\lambda_R)$ for low Chl waters, there is

$$BD_{Rrs} \approx G \frac{(a(\lambda_B)b_{bw}(\lambda_G) - \beta a(\lambda_G)b_{bw}(\lambda_B)) + (a(\lambda_B)b_{bp}(\lambda_G) - \beta a(\lambda_G)b_{bp}(\lambda_B))}{a(\lambda_B)a(\lambda_G)} \quad (4a)$$

$$= -G \frac{\Delta_{\text{water}} + \Delta_{\text{particle}}}{a(\lambda_B)a(\lambda_G)} \quad (4b)$$

Here β is $(\lambda_R - \lambda_G)/(\lambda_R - \lambda_B)$. Δ_{water} and Δ_{particle} represent the contributions to BD_{Rrs} related to the backscattering coefficient of pure seawater and particles, respectively. As demonstrated in Hu et al. (2012), for waters with Chl less than about 0.2 mg/m^3 (more than 70% of the global ocean), with $\lambda_B = 443 \text{ nm}$, $\lambda_G = 555 \text{ nm}$ and $\lambda_R = 670 \text{ nm}$, $|\Delta_{\text{water}}|$ is significantly greater than $|\Delta_{\text{particle}}|$ (see Fig. 1), thus BD_{Rrs} can be approximated as

$$BD_{Rrs} \approx -G \frac{a(\lambda_B)b_{bw}(\lambda_G) - \beta a(\lambda_G)b_{bw}(\lambda_B)}{a(\lambda_B)a(\lambda_G)} \quad (5)$$

Further, considering $a(\lambda_G)$ is nearly a constant for oceanic waters, the variation of BD_{Rrs} is thus mainly driven by $a(\lambda_B)$. Because Chl is a major contributor to $a(\lambda_B)$, thus a change of BD_{Rrs} represents a change of Chl, and BD_{Rrs} can be used as an index to infer Chl as showing by Eq. 1b.

This scheme, however, as presented in Gordon and Morel (1983), will not work for waters with high loads of particles (waters with high Chl), where $|\Delta_{\text{water}}|$ could be significantly less than $|\Delta_{\text{particle}}|$ (see Fig. 1). For such waters, the variation of BD_{Rrs} is driven by both b_{bp} and $a(\lambda_B)$, consequently large uncertainties will be resulted in the estimated Chl if BD_{Rrs} is used as the input, which is the “danger” warned in Gordon and Morel (1983).

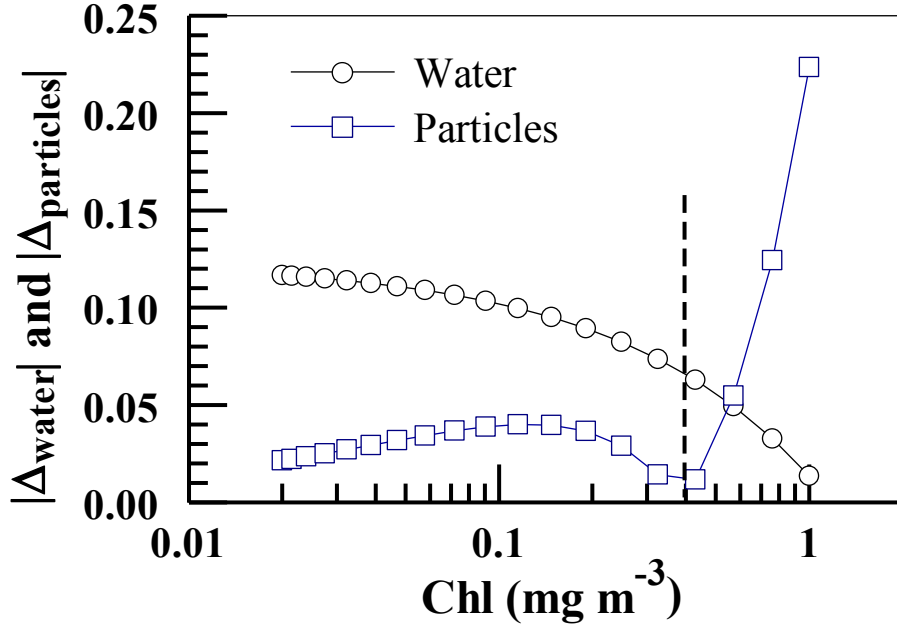


Fig. 1. Contrast between Δ_{water} and Δ_{particle} for different Chl. To show their relative significance, the absolute values (x 1000) are shown here. (From Hu et al. 2012).

More importantly, the uniqueness of the blue-green-red BD_{Rrs} of Hu et al. (2012) is that it is nearly immune to residual errors in R_{rs} . Due to reasons from sensor's calibration to atmospheric correction, R_{rs} from satellite measurements always contains some residual errors (represented as δ), which generally can be considered as a linear function of wavelength (Hu et al. 2013), thus satellite remote sensing reflectance (R_{rs}^{Sat}) could be expressed as

$$R_{rs}^{Sat}(\lambda) = R_{rs}(\lambda) + \delta(\lambda) = R_{rs}(\lambda) + y\lambda + x \quad (6)$$

with x and y empirical parameters to model the wavelength dependence of δ . Through simple algebra, it can be shown that the blue-green-red band difference of $R_{rs}^{Sat}(\lambda)$ equals to the blue-green-red band difference of R_{rs} , i.e.,

$$BD(R_{rs}^{Sat}) = BD_{Rrs} \quad (7)$$

This feature is very important for processing ocean color images, i.e., $BD(R_{rs}^{Sat})$ is simply driven by bio-optics, not affected by δ when the residual error is a linear function of wavelength. Even for the value of y slightly changes for different ranges of wavelength (Chen et al. 2016), Hu et al. (2012) showed that uncertainties in the retrieved Chl due to the variation of y are still $< 2\%$, indicating the algorithm's strong tolerance to input R_{rs} errors.

Such a feature is not available if simply taking a difference of R_{rs}^{Sat} between two bands, as the slope term in Eq. 6 could not be cancelled out, and this slope could vary for different pixels in the

same satellite image. This limitation is likely another reason that the band-difference approach was not continued in those decades.

Further, when Chl is calculated from R_{rs}^{Sat} with a band-ratio algorithm, it becomes

$$Chl = f \left(\frac{R_{rs}(\lambda_B) + \delta(\lambda_B)}{R_{rs}(\lambda_G) + \delta(\lambda_G)} \right) \quad (8)$$

where the residual error ($\delta(\lambda)$) could not be cancelled out. Especially, when $R_{rs}(\lambda_G)$ is small (for most oceanic waters), $\delta(\lambda_G)$ could significantly impact this ratio, which then results in noisy and speckled images (see Fig. 2). Comparing Eq. 7 with Eq. 8, it shows the fundamental reason why the blue-green-red difference is superior to the blue-green ratio for processing satellite ocean color images of oceanic waters.

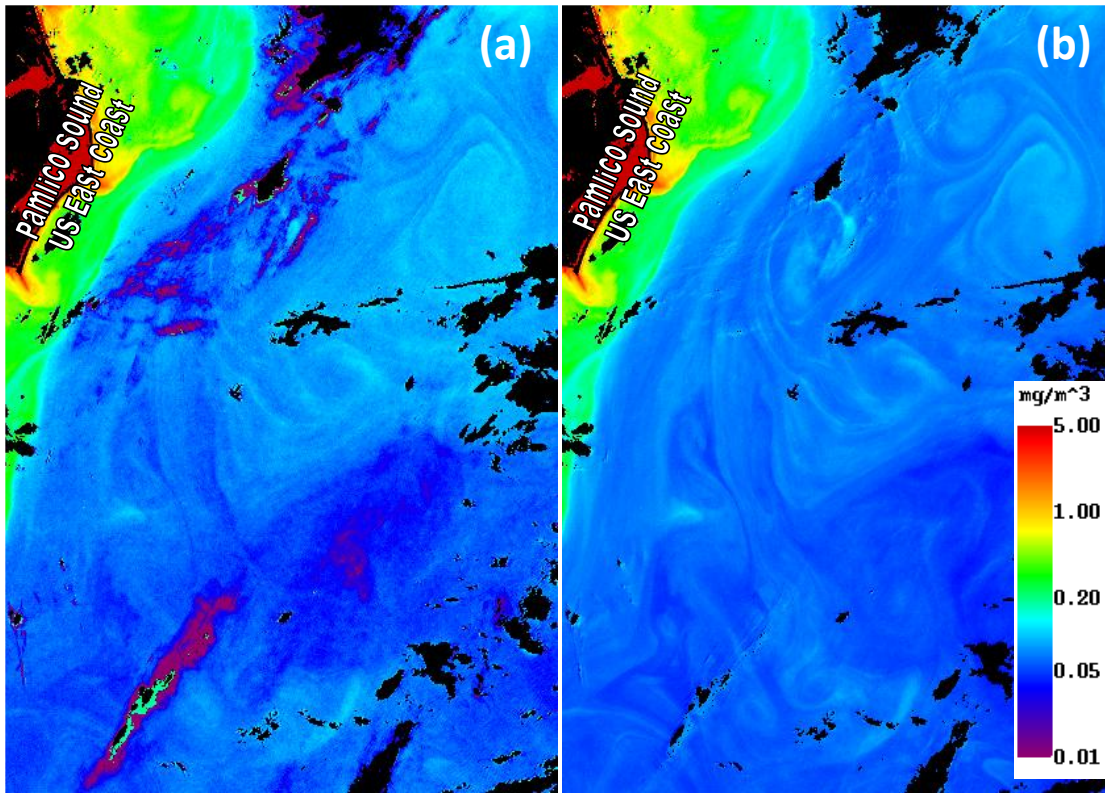


Fig. 2. Contrast of Chl image product obtained from band ratio (a) and band difference (b) algorithms. Note that some eddy features are clearly revealed in the band-difference image but absent in the band-ratio image due to noise and residual errors in atmospheric correction and other corrections. (From Hu et al. 2012).

However, no matter if it is band ratio or band difference of R_{rs} , it is necessary to keep in mind that the variation of $a(\lambda_B)$ is not simply driven by Chl alone, as $a(\lambda_B)$ in general is

$$a(\lambda_B) = a_w(\lambda_B) + a_{ph}^*(\lambda_B)Chl + a_{dg}(\lambda_B) \quad (9)$$

Here, a_w is the absorption coefficient of pure seawater, with a_{dg} the contributions from detritus and gelbstoff. a_{ph}^* is the Chl-specific absorption coefficient, which is defined as the ratio of phytoplankton absorption coefficient (a_{ph}) to Chl. Thus, to accurately infer Chl from BD_{Rrs} , it is either required that a_{ph}^* and a_{dg} co-vary with Chl, or these two properties are determined separately. In short, the uncertainties introduced by the variations of $a_{ph}^*(\lambda_B)$ and a_{dg} in the estimated Chl could not be avoided regardless of using band ratio or band difference of R_{rs} . Understanding and estimating the spatial and temporal changes of $a_{ph}^*(\lambda_B)$ of global ocean is still one of the biggest challenges in ocean color remote sensing.

3. A few extensions

3.1 Band difference for the remote sensing of other bio-optical variables

The concept of band difference is not new but has been used to estimate fluorescence line height (FLH, Abbott and Letelier 1999) and maximum chlorophyll index (MCI, Gower et al. 2005) from satellite measurements. Likewise, a three-band difference floating algae index (FAI) algorithm has been designed to detect and quantify floating algae (Hu 2009), with several alternative forms developed for different purposes (Xing and Hu 2016). The algorithm concept has also been applied to the red-green-blue bands using satellite-derived Rayleigh-corrected reflectance data (Rrc), which showed success in deriving relative ocean color patterns even if Rrc contains contributions from sun glint and aerosols (Hu 2011).

In view of the tolerance to atmospheric correction errors of the band-difference algorithm, the concept has also been extended to other bio-optical variables, including particulate inorganic carbon (PIC, Mitchell et al. 2017) and particulate organic carbon (POC, Le et al. 2018). In these efforts, the same 3-band difference concept has been used, but the three bands were selected to optimize the algorithm performance (e.g., 547-667-748 nm for PIC and 488-547-667 nm for POC). Improvements in both accuracy and cross-sensor consistency over the earlier empirical algorithms (mostly based on band ratios) have been demonstrated. The success of band difference might also be attributed to the fact that this approach effectively exploits both absorption and backscattering properties in the algorithm design, whereas the band-ratio algorithms focus mainly on the absorption properties.

3.2 Correction of the residual error

Clearly, the residual error in R_{rs} is a significant source of uncertainty, resulting in a non-smooth image product from satellite ocean color remote sensing. While BD_{Rrs} cleverly solved this issue for the estimation of Chl, PIC, POC and other properties separately and empirically, it is also of great interest to correct $\delta(\lambda)$ in R_{rs}^{Sat} , where the resulted R_{rs} can then be applied in semi-analytical algorithms for the inversion of inherent optical properties and other variables. For this objective, Chen et al. (2016) developed an algebraic system based on Eq. 6 to solve the residual error pixel-

by-pixel. While much smoother image products of R_{rs} were presented in Chen et al. (2016), more practice and evaluations are deserved.

4. Concluding remarks

Developing a remote sensing algorithm is an on-going process, where better and more robust algorithms will emerge with the pass of time. However, the blue-green-red band-difference algorithm developed by Hu et al. (2012) **completely** changed the way of thinking in developing ocean color algorithms for the estimation of Chl and other bio-optical variables, especially its unique approach in handling residual errors in R_{rs} . The hiatus, or no-touch, of practicing band difference for Chl estimation, on the other hand, highlights a common and implicit “danger” of automatically extending results from one scenario to another, thus hinder the progresses in science and technology.

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