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## Estimating oceanic primary productivity from ocean color remote sensing: A strategic assessment

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### ABSTRACT

It has long been realized that approaches using satellite ocean-color remote sensing are the only feasible means to quantify primary productivity (PP) adequately for the global ocean. Through decades of dedicated efforts and with the help of various satellite ocean-color missions, great progresses have been achieved in obtaining global PP as well as its spatial and temporal variations. However, there still exist wide differences between satellite estimations and *in situ* measurements, as well as large discrepancies among results from different models. The reasons for these large differences are many, which include uncertainties in measurements, errors in satellite-derived products, and limitations in the modeling approaches. Unlike previous round-robin reports on PP modeling where the performance of specific models was evaluated and compared, here we try to provide a candid overview of three primary modeling strategies and the nature of present satellite ocean-color products. We further highlight aspects where efforts should be focused in the coming years, with the overarching goal of reducing the gaps between satellite modeling and *in situ* measurements.

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### 1. Introduction

Photosynthesis is a process that occurs on the illuminated Earth. In a complex light-dependent process, photosynthesis transfers absorbed photon energy to organic compounds (Falkowski and Raven, 2007). Since this process ultimately leads to the conversion of inorganic carbon to organic carbon, photosynthesis not only plays an important role in the global carbon cycle, but also provides the food to support all the heterotrophs. In the ocean, phytoplankton are the primary photosynthesizers, supporting the ocean's food web. As realized ~50 years ago (Goldman, 1965), because of the vast expanse of the oceans, detailed information about the temporal and spatial variation of oceanic photosynthesis is essential for studying and understanding air–sea CO<sub>2</sub> exchange, carbon fixation, and vertical export – the so called “biological pump” (Antoine et al., 1996; Behrenfeld et al., 2002; Bosc et al., 2004; Dunne et al., 2005; Falkowski et al., 2003; Nevison et al., 2012; Platt and Sathyendranath, 1988; Sathyendranath et al., 1995).

The production of organic carbon during photosynthesis is defined as primary productivity (PP, or net primary productivity, NPP; Cullen, 2001; Marra, 2002; Platt and Sathyendranath, 1993). In the ocean, PP provides a measure of inorganic carbon fixed by phytoplankton per

unit of water volume per unit of time. Integration of this rate over desired basins and for a given period of time (*e.g.*, a year) provides a measure of carbon transformation for that area for that time period. It has been – and remains – an elusive goal for researchers in biological oceanography to obtain accurate and consistent estimates of PP for the global oceans. Beside limitations in measurement technology (Cullen, 2001; Marra, 2002; Platt and Sathyendranath, 1993), the major limitation is the extreme under sampling of the oceans (Perry, 1986), where the spatial and temporal variations in water properties (including optical, chemical, and biological, *etc.*) cannot be easily scaled-up from a few measurements made at limited space–time grids.

To overcome such spatial–temporal limitations, it has long been recognized that the repetitive measurement by satellite sensors provides the only possible and feasible means for the estimation of PP on basin and global scales (Eppley et al., 1985; Falkowski, 1998; Perry, 1986; Platt, 1986), *i.e.*, to obtain estimates at large scales by linking discrete *in situ* measurements with the synoptic and repetitive satellite observations. The linkage for this scaling-up, as discussed in detail in later sections, is centered on information on phytoplankton (either a biological property such as chlorophyll concentration or an optical property such as phytoplankton absorption coefficient). This is based on the fact that phytoplankton not only plays a key role in photosynthesis, but also alters the appearance of ocean (water) color. Therefore, when a relationship between PP and phytoplankton is developed, the estimation of basin-scale PP becomes possible when the information of

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phytoplankton can be derived from the measurement of ocean color by a satellite sensor. Because of this necessity, the estimation of the global phytoplankton (and then oceanic PP) is a central goal of all ocean-color satellite missions (IOCCG, 1998; McClain, 2009), which include the Sea-Viewing Wide Field-of-View Sensor (SeaWiFS) and the MODerate-resolution Imaging Spectroradiometer (MODIS) supported by NASA, and the Medium Resolution Imaging Spectrometer (MERIS) supported by ESA. In addition, new and advanced ocean color satellites are on the horizon, including the Pre-Aerosol Cloud and Ecosystems (PACE, NASA) mission and the Ocean and Land Colour Instrument (OLCI, ESA). At the same time, in order to properly scale-up the limited field measurements with satellite data, various models have been developed (e.g., Antoine and Morel, 1996; Arrigo et al., 2008; Balch et al., 1989b; Behrenfeld, 1998; Dierssen et al., 2000; Ishizaka, 1998; Kahru et al., 2009; Longhurst et al., 1995; Ondrusek et al., 2001; Sathyendranath and Platt, 1995; Sathyendranath et al., 1989; Sathyendranath et al., 1991) and estimates of global oceanic PP have been achieved (Antoine et al., 1996; Behrenfeld et al., 2002; Longhurst et al., 1995; Platt and Sathyendranath, 1988).

After decades of practice, however, the estimates based on satellite remote sensing are far from satisfactory. For instance, results from the Joint Global Ocean Flux Study (JGOFS) (Ducklow, 2003) have found that, in four of eight oceanic provinces (Longhurst et al., 1995) where data are available for  $PP_{\text{basin-year}}$  (basin-scale, annual, depth-integrated primary production) from both *in situ* measurements and from the measurements of the Coastal Zone Color Scanner (CZCS), the satellite estimates were a factor of two or three smaller than the measured values. In only two out of the eight provinces were the CZCS  $PP_{\text{basin-year}}$  within 20% of the measured values. If the comparison is made on local-daily instead of basin-year scales regarding the spatial and time ranges, the disagreement could be much larger between measured and ocean color-derived  $PP_{\text{eu}}$  (daily depth-integrated primary production) as shown in some studies (e.g., Balch et al., 1989a; Behrenfeld and Falkowski, 1997b; Quay et al., 2012), although better results were presented in Platt and Sathyendranath (1988) and Kyewalyanga et al. (1997).

The discrepancies between modeled and measured PP, and among modeled PP, were also highlighted in a series of round-robin experiments (Campbell et al., 2002; Carr et al., 2006; Friedrichs et al., 2009). Even with measured chlorophyll concentration as an input, Campbell et al. (2002) found that PP estimates from the best-performing algorithms were generally within a factor of 2 of measured PP; while Carr et al. (2006) found that global average PP varied by a factor of 2 between models when input parameters (chlorophyll concentration and solar radiation) were derived from SeaWiFS. For a dataset consisting of ~1000 *in situ* measurements in the tropical Pacific, Friedrichs et al. (2009) found that all models underestimated the observed variance of PP, and no models successfully captured a broad-scale shift from low biomass-normalized productivity in the 1980s to a higher biomass-normalized productivity in the 1990s.

Such inconsistent results undermine the confidence of using primary production estimated from satellite ocean color to study the “biological pump” in the oceans, and suggest that there is difficult work ahead in designing the strategy and system for estimating primary production based on remotely sensed data. Here we try to provide a candid overview of the strategies in estimating PP from ocean color remote sensing, discuss the status of “standard” satellite ocean-color products, and highlight areas where efforts should be focused on for improving the estimation of PP from satellite ocean color remote sensing.

## 2. Principles of ocean color remote sensing

It has been known for centuries that the change of water (ocean) color reflects change of constituents in the water column. To be able to quantitatively, and mechanistically, estimate the constituent concentrations, models have been developed to link ocean color with desired

constituents. In ocean color remote sensing, “ocean color” is commonly described with the spectrum of remote-sensing reflectance ( $R_{rs}(\lambda)$ ,  $sr^{-1}$ ), which is defined as the ratio of water-leaving radiance to downwelling irradiance just above the surface. “Water-leaving radiance” represents photons originating from absorption and scattering processes below the surface and emitting into space, which excludes photons going to space due to sea-surface reflectance, a process having no information of in-water constituents.

Based on the radiative transfer theory,  $R_{rs}$  can be expressed as (Gordon et al., 1988; Sathyendranath and Platt, 1997; Zaneveld, 1995)

$$R_{rs} \approx 0.53 \left( g_0 + g_1 \frac{b_b}{a + b_b} \right) \frac{b_b}{a + b_b}. \quad (1)$$

Here  $a$  and  $b_b$  are the total absorption and backscattering coefficients, respectively, and wavelength dependence is omitted for brevity.  $g_0$  and  $g_1$  are model coefficients, which are spectrally independent, although slightly varying with sun-sensor angular geometry (Albert and Mobley, 2003; Lee et al., 2011a; Morel and Gentili, 1993).

$a$  and  $b_b$  are bulk inherent optical properties (IOPs) (Preisendorfer and Mobley, 1984), which are sums of the contributions of various constituents (Stramski et al., 2001), with the primary components as water molecules, suspended particulates and dissolved materials (also termed as “gelbstoff”, etc.). Practically, the bulk IOPs are generally described as

$$\begin{aligned} a &= a_w + a_{ph} + a_{dg}; \\ b_b &= b_{bw} + b_{bp}, \end{aligned} \quad (2)$$

with subscripts “w, ph, dg, p” representing water, algae pigments, the combination of detritus and gelbstoff, and particles, respectively. Values of  $a_w$  and  $b_{bw}$  have been measured or derived from laboratory or field measurements (Morel, 1974; Pope and Fry, 1997; Smith and Baker, 1981), and are considered global constants (vary slightly with temperature and salinity) (Pegau et al., 1997; Sullivan et al., 2006).  $a_{ph}$ ,  $a_{dg}$  and  $b_{bp}$ , on the other hand, vary spatially and temporally, and are considered as volatile properties.

For studies in ocean biology and biogeochemistry, traditionally the focus of ocean color remote sensing is on the concentration of chlorophyll, thus the component IOPs are commonly expressed as

$$\begin{aligned} a &= a_w + a_{ph}^* \times Chl + G_{Chl} \times a_{ph}^* \times Chl, \\ b_b &= b_{bw} + b_{bp}^* \times Chl. \end{aligned} \quad (3)$$

Here  $a_{ph}^*$  and  $b_{bp}^*$  are the chlorophyll-specific (or concentration of chlorophyll normalized) absorption and chlorophyll-specific backscattering coefficients ( $m^2/mg$ ), respectively, with  $Chl$  the concentration of chlorophyll ( $mg/m^3$ ).  $G_{Chl}$  is the ratio (at a specific wavelength, such as 440 nm) of  $a_{dg}$  to  $a_{ph}$ .

Therefore, if values of  $a_{ph}^*$ ,  $b_{bp}^*$  and  $G_{Chl}$  are known, or if they co-vary with  $Chl$ , Eq. (1) is a function of one variable:  $Chl$ , which can then be solved from known  $R_{rs}$ . Because particle backscattering coefficient ( $b_{bp}$ ) could not be accurately modeled with  $Chl$  alone (see Stramski et al., 2001),  $b_{bp}^*$  encompasses a wide range of variations for a given  $Chl$  (Babin et al., 2003; Loisel and Morel, 1998). To minimize the impact of this variation on the retrieval of  $Chl$  from  $R_{rs}$ , usually the band ratio of  $R_{rs}$  (either blue to green, or red to green; Le et al., 2013) is used as input, with a general form as (Gordon and Morel, 1983; O'Reilly et al., 1998)

$$Chl = f_1(R_{rs}(\lambda_i)/R_{rs}(\lambda_j)). \quad (4)$$

Here  $f_1$  stands for function number 1. Following Eqs. (2–3), in essence the above ratio algorithm includes (assuming the impact of parameter  $b_{bp}^*$  is minimized through the  $R_{rs}$  ratio), implicitly, variables other than the ratio of  $R_{rs}$  (Carder et al., 1999; Gordon et al., 1988; Sathyendranath and Platt, 1989; Sathyendranath et al., 1994)

$$Chl = f_1(a_{ph}^*, G_{Chl}, R_{rs}(\lambda_i)/R_{rs}(\lambda_j)). \quad (5)$$

This simplified, but general, conceptual relationship clearly indicates the fundamental dependence of *Chl* retrieval on the values of  $a_{ph}^*$  and  $G_{Chl}$ .

On the other hand, if the focus on the retrieval is IOPs, the ratio of  $R_{rs}$  is

$$R_{rs}(\lambda_i)/R_{rs}(\lambda_j) = f_2 \left( \frac{b_{bw}(\lambda_i) + b_{bp}(\lambda_i) a_w(\lambda_j) + a_{ph}(\lambda_j) + a_{dg}(\lambda_j)}{b_{bw}(\lambda_j) + b_{bp}(\lambda_j) a_w(\lambda_i) + a_{ph}(\lambda_i) + a_{dg}(\lambda_i)} \right), \quad (6)$$

where the concentration-normalized parameters are not involved, thus lower uncertainty in retrieving IOPs is expected (Lee et al., 1998), at least in theory.

### 3. Basics of primary productivity modeling

As defined earlier, primary productivity quantifies fixed carbon from photosynthesis, which represents a transfer of absorbed photon energy to organic carbon (note: we recognize that not all reductants produced from absorbed photon energy are used in reduction of  $CO_2$ , but rather in the reduction of nitrate and other compounds). Because chlorophyll-a pigment is critical for the photosynthesis process, a generalized conceptual model for this quantification has commonly been written as (Bannister, 1974; Behrenfeld and Falkowski, 1997a; Eppley et al., 1985; Platt and Sathyendranath, 1988; Ryther, 1956)

$$PP = \phi \times a_{ph}^* \times Chl \times E, \quad (7)$$

with  $E$  for available photon energy (representing photosynthetic available radiation, PAR, 400–700 nm, quanta/m<sup>2</sup>). The product of  $a_{ph}^*$ ,  $Chl$ , and  $E$  is the absorbed photon energy by phytoplankton.  $\phi$  (the photosynthetic quantum yield) represents the efficiency factor for the conversion of the absorbed photon energy to organic carbon (essentially, the energy stored in organic carbon; Morel, 1978). The product of  $\phi$  and  $a_{ph}^*$  (represented by  $\varphi$  in the following equation) is commonly termed as biomass-normalized (or chlorophyll-normalized) photosynthesis rate, and Eq. (7) is also commonly written as (Behrenfeld and Falkowski, 1997a):

$$PP = \varphi \times Chl \times E. \quad (8)$$

Because light penetrates deep below the sea surface and changes spectrally with depth, impact from both depth and wavelength must also be included. A generalized wavelength-resolved model for the quantification of primary production can be expressed as (Behrenfeld and Falkowski, 1997a; Sathyendranath and Platt, 1988)

$$PP(z) = \int \varphi(z) \times Chl(z) \times E(\lambda, z) d\lambda, \quad (9)$$

with  $PP(z)$  representing the primary production at depth  $z$ , and the integration of  $PP(z)$  over depth provides a measure of the photosynthesis of the whole water column. Based on the radiative transfer equation, the propagation of light in the water column can be expressed as

$$E(\lambda, z) = E(\lambda, 0) e^{-K(\lambda) \times z}, \quad (10)$$

with  $E(\lambda, 0)$  for spectral light energy just below the surface and  $K(\lambda)$  the spectral diffuse attenuation coefficient (m<sup>-1</sup>) for  $E(\lambda)$ . Because this system has  $Chl$  as the core input ( $K(\lambda)$  can be modeled from  $Chl$  for Case-1 waters (Morel, 1988; Morel and Maritorena, 2001)), this scheme is termed as the  $Chl$ -based approach (Behrenfeld et al., 2005).

The implication of Eqs. (9) and (10) is quite clear; the desired quantities for modeling  $PP(z)$  are three variables:  $E$ ,  $Chl$ , and  $\varphi$ . Studies have shown that both  $E$  and  $Chl$  can be either measured easily *in situ* or estimated from remotely sensed ocean color. If variable  $\varphi$  can be

characterized and parameterized, products of  $E$  and  $Chl$  thus provide the linkage to scale-up discrete *in situ* PP measurements to basin-scale PP estimations. To meet this demand, models for the estimation of  $E(0)$  have been developed in the past decades (Frouin et al., 1989; Frouin et al., 2003; Gregg and Carder, 1990; Journée and Bertrand, 2010; Van Laake and Sanchez-Azofeifa, 2005). There have been enormous efforts to develop algorithms for the retrieval of  $Chl$  from ocean color measurements (e.g., Bukata et al., 1981; Carder et al., 1999; Dall'Olmo and Gitelson, 2005; Devred et al., 2005; Doerffer and Fisher, 1994; Gordon and Morel, 1983; Hu et al., 2012b; Le et al., 2013; Mitchell and Holm-Hansen, 1990; Morel et al., 2006; O'Reilly et al., 1998; Sathyendranath et al., 2005). Additionally, field studies have focused on characterization and parameterization of the variable  $\varphi$  (e.g., Cullen, 1990; Cullen et al., 1992; Marra and Barber, 2005; Platt et al., 1980). Many different forms and models for the  $Chl$ -normalized photosynthesis rate have been reported (Falkowski and Raven, 2007; Sakshaug et al., 1997), but Platt (1986) and Sathyendranath and Platt (1995) have found that most of those equations yield similar results for water-column integrals of primary production.

### 4. Discussion of applying current ocean-color products with the $Chl$ -based approach

Based on Eqs. (9) and (10), the estimation of basin-scale primary production requires inputs of  $\varphi$ ,  $E(0)$ ,  $Chl$  and  $K$ . And, because of this demand, there have been thousands of concurrent measurements of PP,  $E$ , and  $Chl$  in the past decades (Behrenfeld and Falkowski, 1997b; Platt et al., 1991). Variation of  $\varphi$  depends on phytoplankton physiology, its value cannot be directly provided from ocean color remote sensing, but has to be estimated and modeled based on laboratory and/or field measurements.  $E(0)$  can be determined with information on sun position and atmospheric properties.  $Chl$  and  $K$ , however, are bio-optical properties that are derived from the measurement of ocean color, empirically or semi-analytically. These features frame the basic logic why  $E(0)$ ,  $Chl$  and  $K$  (but limited to  $K_d(490)$  at present) are standard products of all satellite ocean color missions (e.g., <http://oceancolor.gsfc.nasa.gov/cgi/13?per=DAY>). However, as discussed in details below, these standard ocean-color products are not straightforwardly applicable for a PP model like Eq. (9) for such estimations.

#### 4.1. Standard product of $Chl$

$Chl$  is a key input for PP modeling (see Eqs. (7–10)), hence an accurate  $Chl$  retrieval from satellite ocean color remote sensing is critical for the estimation of global PP (Behrenfeld and Falkowski, 1997a, b). Due to its importance, tremendous efforts have been focused on the development of algorithms for the derivation of  $Chl$  from ocean color data dating back to the CZCS era (Bukata et al., 1981; Doerffer and Fisher, 1994; Gordon and Morel, 1983; Gordon et al., 1983). Presently, as discussed earlier, the standard satellite  $Chl$  product is still derived from the band ratio of  $R_{rs}$ , with a general form as Eq. (4). However, as depicted by Eq. (5), to get  $Chl$  from the  $R_{rs}$  band-ratio, not only the  $G_{Chl}$  value has to be specified (or has to co-vary with  $Chl$ ), the value of  $a_{ph}^*$  need also be known (or co-vary with  $Chl$ ). In the empirical algorithm for the standard  $Chl$  product (O'Reilly et al., 1998), the values (or variations) of  $G_{Chl}$  and  $a_{ph}^*$  are not specified, but embedded implicitly in the algorithm coefficients. In other words, such values or variations are implicitly treated as universally stable constants or dependances. On the other hand, numerous field studies (Babin et al., 1993; Bricaud and Morel, 1986; Bricaud et al., 1981; Bricaud et al., 1995; Carder et al., 1986; Carder et al., 1989; Carder et al., 1991; Carder et al., 1999; Carder et al., 2004; Cleveland, 1995; Del Castillo et al., 2000; Kirk, 1994; Lutz et al., 1996; Mitchell and Kiefer, 1988; Morel and Bricaud, 1981; Sathyendranath et al., 1987; Sosik and Mitchell, 1995; Stuart et al., 1998) have pointed out that both  $G_{Chl}$  and  $a_{ph}^*$  are not constants even for oceanic waters, and there are no fixed values for either  $G_{Chl}$

or  $a_{ph}^*$  for a given *Chl*. As a result, the empirical algorithms developed from such globally and seasonally inclusive datasets tend to produce regional biases, which further obscure the spatial and temporal characteristics of *Chl* in the global oceans (Brown et al., 2008; Szeto et al., 2011).

This might not be too surprising because the spectral variation of  $b_b$  is mild compared to the spectral variation of  $a$ , so a change of the  $R_{rs}$  ratio indicates mostly a change of the absorption coefficient. Therefore, the so-called *Chl* product is indeed an index of this bulk absorption coefficient (comparing Eq. (4) with Eq. (6)) and can be written as

$$Chl = f_2(a). \quad (11)$$

This fundamental relationship indicates that the standard *Chl* product does not match the desired chlorophyll-a required in a *Chl*-based PP model (e.g., Eq. (8)), where the model was developed based on “real” chlorophyll-a – a biological property, not the total absorption coefficient – an optical property. This mismatch helps explain a conclusion in Saba et al. (2011) that “ocean color models did not accurately estimate the magnitude of the trends of NPP over multidecadal time periods, and were even more challenged over shorter time periods, especially when the models used satellite-derived *Chl*-a”.

#### 4.2. Uncertainties of $\varphi$

Prior studies (Balch et al., 1992; Behrenfeld and Falkowski, 1997b) have pointed out that even with *in situ* measured *Chl*, PP can only be quantified with an accuracy of at best 50–60%. This is because whenever PP is modeled with *Chl* as a scaling parameter (see Eq. (8)), it automatically requires the specification of  $\varphi$  or a similar *Chl*-normalized photosynthetic parameter (such as biomass-normalized growth rate). More specifically, the biomass- (or chlorophyll-) normalized photosynthesis parameter is (Behrenfeld and Falkowski, 1997a; Cullen, 1990)

$$\varphi = \phi \times a_{ph}^*. \quad (12)$$

The quantum yield of photosynthesis ( $\phi$ ) and  $a_{ph}^*$  are, in principle, two independent properties, and both vary spatially and temporally. This nature helps explain why a PP model may not perform well even with measured *Chl* as input. As discussed earlier, due to variations in pigment composition and the “package effect” (Bidigare et al., 1990; Bricaud et al., 1988; Hoepffner and Sathyendranath, 1991),  $a_{ph}^*$  can vary over a factor of 4 or more for the same *Chl* value (Bricaud et al., 1995). This indicates that the biomass-normalized photosynthesis rate will fundamentally vary significantly for a given *Chl* (Platt et al., 2008). Consequently, without knowing the  $a_{ph}^*$  value associated with the development of the PP model, a mismatch in the  $a_{ph}^*$  will result in different  $\varphi$  (assuming  $\phi$  values are the same), and then different PP even if *Chl* and  $E$  values are the same. This natural variability, at least partially, explains a conclusion of Behrenfeld and Falkowski (1997b) that “significant improvements in estimating oceanic primary production will not be forthcoming without considerable advance in our ability to predict temporal and spatial variability in  $P_{opt}^B$ .” Note that  $P_{opt}^B$  is similar to  $\varphi$  as a biomass-normalized parameter (Falkowski, 1998). The same conclusions can also be found from other modeling studies (Morel et al., 1996; Sosik, 1996). It is quite a challenge to reach this goal from remote sensing though, because there is no reliable method as yet to accurately estimate the spatial and temporal variation of  $P_{opt}^B$  from satellite measurements.

#### 4.3. Light-related products

Photosynthesis needs light, and it might be envisioned that the combination of  $E(0)$  and  $K_d(490)$  products can somehow provide the necessary input of solar radiation at depth. However, a few caveats prevent a direct application of these standard ocean color products for the estimation of  $E(z)$ . These include the following:

- 1) The algorithm used for the generation of  $K_d(490)$  was developed in a similar fashion as for the retrieval of *Chl*, i.e., by pulling together global datasets to produce the best empirical relationship between the desired product and  $R_{rs}$  band-ratio. Although the  $R_{rs}$ -ratio does reflect optical properties (see Eq. (6)), the practice overlooked, or ignored, a fundamental feature that  $K_d$  is an apparent optical property (AOP) (Preisendorfer, 1976). Unlike *Chl*,  $K_d$  can differ by more than 40% between the sun at zenith and the sun just above the horizon (Gordon, 1989; Kirk, 1984; Sathyendranath and Platt, 1988). Consequently, the empirically-derived  $K_d(490)$  is best for sun positions matching the mode of the dataset used for the algorithm development (Lee et al., 2013), but will result in large errors for other sun angles, even assuming that the algorithm is perfect.
- 2)  $K_d(490)$  is for light attenuation at one wavelength only, which cannot be applied for the attenuation of photosynthetic available radiation (PAR), a broad-band (usually 400–700 nm) radiometric quantity. A separate attenuation product, called  $K_d(\text{PAR})$ , has also been developed empirically (Morel and Maritorena, 2001; Morel et al., 2007). This  $K_d(\text{PAR})$ , however, in addition to having the same sun-elevation issue as that of  $K_d(490)$ , is only good for the estimation of PAR at depth where  $PAR(z)$  is 1% of  $PAR(0)$  (Morel et al., 2007). This is because  $K_d(\text{PAR})$  varies significantly (a factor of 3 or more) with depth even for vertically well-mixed waters (Lee, 2009; Morel, 1988; Zaneveld et al., 1993). Thus the  $K_d(\text{PAR})$  value for one depth interval cannot be used for the estimation of broad-band radiation at other depths.
- 3)  $E(0)$  is either an instantaneous product or a daily product (Frouin et al., 1989; Frouin et al., 2012).  $K_d(490)$  and  $K_d(\text{PAR})$ , on the other hand, as discussed above, are valid for their own specific sun elevations, and thus cannot be directly applied with the  $E(0)$  product for the estimation of daily  $E(z)$  unless there is a match in solar elevation.

In summary, the present  $E(0)$  and  $K_d$  products of satellite ocean color missions are not directly applicable for an accurate estimation of  $E$  at depth. For easy and straightforward estimation of solar radiation in the upper water column, it is necessary to generate a new set of optical products from ocean color remote sensing.

### 5. Carbon-based algorithm to estimate primary productivity

Another scheme, the “carbon-based approach” (Behrenfeld et al., 2005) has also been developed, where PP can be estimated as

$$PP_{eu} = C \times \mu \times Z_{eu} \times f_3(E), \quad (13)$$

with  $PP_{eu}$  the water-column integrated productivity,  $C$  for phytoplankton carbon,  $\mu$  the growth rate,  $Z_{eu}$  the euphotic-zone depth (practically defined as the depth where the solar radiation is 1% of its surface value), and  $f_3(E)$  a parameter related to light-adjusted physiology (Behrenfeld et al., 2005). In this system,  $C$  is converted from  $b_{bp}$ , and  $\mu$  is described as a function of the ratio of *Chl* to  $C$  (Behrenfeld et al., 2005). Such an approach “removes any dependence on some empirical value for assimilation efficiency, and allows one to distinguish between growth rate, light, and biomass driven changes in chlorophyll” (M. Behrenfeld, personal communication). The derived  $PP_{eu}$ , however, is mostly proportional to *Chl* because the  $C$  component is more or less mathematically canceled out (less so in the later updated version; Westberry et al., 2008).

The model of Arrigo et al. (1998, 2008) could also be put in this category as the estimated  $PP(z)$  is proportional to the product of *Chl* and  $C/\text{Chl}$ , although the net biomass-specific growth rate is modulated with temperature and light. The  $C/\text{Chl}$  ratio, however, is set as a constant (75 or 88.5 g:g), then the  $PP(z)$  estimated from this model is in general also proportional to *Chl*. Therefore, when the standard *Chl* product from ocean color remote sensing is used, the derived primary productivity represents mainly a conversion of the total absorption coefficient (see

Eq. (11)), and large uncertainties will thus remain (Lee et al., 2011b) because the variability associated with the spatial–temporal changes of  $a_{ph}^*$  is not removed. This  $a_{ph}^*$  impact could be reduced if a regional- and temporal-specific *Chl* algorithm is developed and implemented (Arrigo and Sullivan, 1994; Arrigo et al., 1994).

Because of such a complex impact from  $a_{ph}^*$  on the estimation of PP from ocean color remote sensing, large uncertainties in estimated  $PP_{eu}$  result. Siegel et al. (2001) found that “Site-specific and previously published global models of primary production both perform poorly and account for less than 40% of the variance in  $\int PP$ ,” and the series of round robin reports (Campbell et al., 2002; Carr et al., 2006; Friedrichs et al., 2009) also found a large difference in spatial distributions of global primary production from PP models that use *Chl* as a critical input parameter.

There are also efforts to implement phytoplankton class- (or taxon-) specific photosynthesis parameters (Alvain et al., 2006; Claustre et al., 2005; Mouw and Yoder, 2005; Uitz et al., 2010), which may reduce the impact of  $a_{ph}^*$  as different  $a_{ph}^*$  and  $\varphi$  values might be assigned to different class or taxon groups. But we are at an early stage to properly set class- or taxon-specific  $\varphi$  values and to sense phytoplankton class groups accurately from the measurement of ocean color.

## 6. Strategy centered on phytoplankton absorption

Because  $a_{ph}^*$  is a ratio of the phytoplankton absorption coefficient to *Chl*, a mathematical manipulation of the parameters in Eq. (9) results in a generalized model for primary productivity at depth as (Kiefer and Mitchell, 1983)

$$PP(z) = \int \phi(z) \times a_{ph}(z, \lambda) \times E(z, \lambda) d\lambda. \quad (14)$$

In this model, the required phytoplankton-related input is  $a_{ph}$  instead of *Chl*. That means, when  $\phi$  is determined, the parameter needed for scale-up *in situ* PP is  $a_{ph}$  (in addition to  $E$ ) – an optical property, instead of *Chl* – a biological property (Marra et al., 2007). This optical attribute matches that of ocean-color remote-sensing, where the direct derivatives will always be optical properties. In other words, the physiology ( $\phi$ ) and optical actions ( $a_{ph}$ ) associated with photosynthesis are described with two separate parameters in this scheme, whereas they are tangled in both  $\varphi$  and *Chl* in the *Chl*-based approaches. More specifically, there will be no more need to specify the value of  $a_{ph}^*$  in this  $a_{ph}$ -based approach when estimating PP from ocean color remote sensing, thus avoiding one of the biggest uncertainty sources. To implement this strategy for the scale-up of primary production in basin scales, it thus requires information on the following:

- 1) The light at the sea surface:  $E(0)$
- 2) Absorption coefficient of phytoplankton pigments:  $a_{ph}$
- 3) Light attenuation coefficient:  $K$
- 4) Quantum yield:  $\phi$ .

$E(0)$  is independent of the PP models and is a standard product for all ocean color missions. Although there are no standard products of  $a_{ph}$  from satellite ocean-color sensors yet, algorithms (empirical or semi-analytical) to derive  $a_{ph}$  from  $R_{rs}$  have been under development and evaluation in the past decades (e.g., Carder et al., 1991; Carder et al., 1999; Carder et al., 2004; Hoge and Lyon, 1996; IOCCG, 2006; Lee and Carder, 2004; Lee et al., 1998; Lee et al., 2002; Roesler and Perry, 1995; Smyth et al., 2006). Further, semi-analytical models have been developed for the estimation of spectral  $K$  from spectral IOPs (Lee et al., 2005; Lee et al., 2013; Sathyendranath and Platt, 1988). Therefore, the optical components associated with the quantification of photosynthesis, at least the bulk IOPs, can be well retrieved from ocean color measurements. Also, there has been quite a long history (e.g., Bannister and Weidemann, 1984; Bidigare et al., 1987; Carder et al., 1995; Cleveland et al., 1989; Culver and Perry, 1999; Hiscock et al.,

2008; Kiefer and Mitchell, 1983; Kishino et al., 1986; Marra et al., 1992; Marra et al., 2000; Morel, 1978; Smith et al., 1989; Sorensen and Siegel, 2001; Wozniak et al., 2002) in the determination of the quantum yield for photosynthesis ( $\phi$ ). Furthermore, techniques to make routine measurements of optical properties (including  $a_{ph}$ ) have also advanced significantly in the past decades (Allali et al., 1995; Bricaud and Stramski, 1990; Kishino et al., 1985; Mitchell et al., 2002; Roesler, 1998; Zaneveld et al., 1994), thus it is now feasible to use an optical property ( $a_{ph}$ ), instead of a biological property (*Chl*), as the linkage parameter to scale-up discrete *in situ* PP measurements for global scale estimates (Marra et al., 2007). Preliminary results with this scheme (Hirawake et al., 2011; Lee et al., 1996; Lee et al., 2011b) do support that modeling based on Eq. (14) provides promising potentials for basin-scale PP estimation from satellite ocean color remote sensing.

## 7. Focus for future studies

We have discussed three strategies for the estimation of basin-scale primary production from satellite ocean-color remote sensing. The three strategies are separated by their two different foci: two on the concentration of chlorophyll (*Chl*), and one on the absorption by phytoplankton ( $a_{ph}$ ). In ocean-color remote sensing,  $a_{ph}$ , an optical property, can be directly derived from  $R_{rs}$ ; while *Chl* values can only be inferred from  $a_{ph}$  or  $R_{rs}$ . Such general pictures indicate that, at least in theory, estimation of PP centered on  $a_{ph}$  will involve less uncertainty. To implement such a strategy for the estimation of basin-scale PP, it requires community efforts with objectives discussed in the following sections.

### 7.1. Improving measurement and retrieval of $a_{ph}$

Because the accuracy of modeling PP is strongly dependent on the accuracy of remotely derived *Chl* or  $a_{ph}$ , in addition to improving satellite sensor's sensitivity (Hu et al., 2001; Hu et al., 2012a), calibration (Bailey et al., 2008; Eplee et al., 2001; Franz et al., 2007; Gordon, 1998) and atmospheric correction (Antoine and Morel, 1999; Gao et al., 2000; Gordon, 1997; Gordon and Wang, 1994; Wang and Shi, 2007), all strategies require major efforts to improve algorithms for the derivation of these properties from ocean-color data. Though *Chl* and  $a_{ph}$  are two different kinds of properties (one biological and the other optical), they both depend on accurate  $R_{rs}$  for their derivations, no matter if the algorithm is semi-analytical or empirical. The analytical retrieval of  $a_{ph}$  is associated with spectral modeling of  $b_{bp}$  and  $a_{dg}$ , neither of which has a spectrally constant shape for the global waters. In particular, usually  $a_{ph}$  is derived mechanistically from ocean color information at the blue-green bands, and it requires accurate description of the detritus–gelbstoff spectral dependence (Lee et al., 2010; Maritorea and Siegel, 2005). Schemes to improve the modeling of the spectral shapes of both  $b_{bp}$  and  $a_{dg}$  are needed. An effective strategy that divides the global ocean into dynamic-biogeochemical provinces (Ducklow, 2003; IOCCG, 2009; Moore et al., 2001; Platt et al., 1991; Sathyendranath et al., 1995) may improve the description of these spectra and facilitate the derivation processes. To achieve this, it requires adequate support from various agencies to carry out comprehensive field measurements in various regions of the global oceans.

For waters where the contribution of  $a_{dg}$  to the total absorption (at 440 nm) is much higher, say, a factor of 2 or more than that of  $a_{ph}$ , the retrieval of  $a_{ph}$  using the optical information in the blue-green bands runs into difficulties (Lee et al., 2010). It is necessary to develop new algorithms for the retrieval of  $a_{ph}$  for such waters. One scheme for the retrieval of  $a_{ph}$  under such conditions is to use signals of chlorophyll-a fluorescence (e.g., Abbott and Letelier, 1999; Gower et al., 1999; Hoge et al., 2003; Huot et al., 2005; Yentsch and Yentsch, 1979). This will require improved understanding of chlorophyll-a fluorescence efficiency (Behrenfeld et al., 2009; Culver and Perry, 1997; Huot et al., 2005; McKee et al., 2007).

In addition to algorithms to retrieve  $a_{ph}$  from ocean color data,  $a_{ph}$  determined from field measurements still has large uncertainties (Allali et al., 1995; Bricaud and Stramski, 1990; Mitchell et al., 2002; Mueller et al., 2003; Tassan and Ferrari, 1995), and there is no universally accepted standard method for determining phytoplankton pigment absorption.

### 7.2. Improving the estimation of diurnal radiation

It is necessary to note that frequently and variably, the Earth surface is covered by clouds that greatly impact the photosynthesis of the Earth system (Belanger et al., 2013; Graham et al., 2003). A Low Earth Orbit (LEO) sensor normally has about one visit per day for an area of interest. Therefore LEO observations will not be able to capture the diurnal photosynthesis of the upper water column. Such a sampling limitation will not only affect the estimation of daily  $E(0)$  (Frouin et al., 2003), it will also cause errors in the longer-time scale estimates of PP as photosynthesis is not a linear function of  $E(0)$  (Behrenfeld and Falkowski, 1997a; Cullen, 1990; Kiefer and Mitchell, 1983; Sathyendranath and Platt, 1995). In addition, cloud coverage modifies the existence of UV light at the surface and in the water column (Bartlett et al., 1998; Mitchell and Lubin, 2003; Smyth, 2011), and UV light has a profound impact on photosynthesis (e.g., Arrigo and Brown, 1996; Conde et al., 2000; Cullen and Neale, 1994; Gao et al., 2012; Lorenzen, 1979; Mitchell and Lubin, 2003; Smith and Cullen, 1995). It is thus necessary to model the impact of the diurnal variation of UV light on the estimation of PP. In addition, because light history always affects photo-physiology and photosynthesis (Cullen et al., 1992; Falkowski and Raven, 2007; Guasch and Sabater, 2002; Perry, 1986; Platt et al., 1980), there is a clear demand to develop PP models that take into account the diurnal variation of solar radiation and photosynthesis (e.g., Arrigo et al., 1998; Arrigo et al., 2008), where measurements from geostationary platforms will be useful significantly (IOCCG, 2012; Perry, 1986).

### 7.3. Improving the determination of quantum yield ( $\phi$ )

For the photosynthesis parameters, extensive studies (e.g., Balch and Byrne, 1994; Behrenfeld and Falkowski, 1997b; Cullen et al., 1992; Lohrenz et al., 1997, 1999; Platt, 1986; Platt et al., 1980; Sosik, 1996) have been carried out on the variation of  $\varphi$  (or  $\alpha^B$  and  $P_m^B$ , the biomass-normalized initial rate and biomass-normalized maximum photosynthesis), although no robust model yet to describe the variation of these parameters with nutrient, temperature, and light histories. For  $\phi$ , there has been a long history of *in situ* measurements, but it is still far from known how  $\phi$  (in particular the maximum quantum yield,  $\phi_m$ ) varies for different ecosystems. Especially, there is no reliable model yet to describe the spatial and temporal variations of  $\phi$  for the global oceans.

In addition, not all the phytoplankton absorbed photons participate in photosynthesis (Falkowski and Raven, 2007; Perry et al., 1981), so a more appropriate expression of Eq. (14) should be written as

$$PP = \phi \times a_{psp} \times E, \quad (15)$$

with  $a_{psp}$  the absorption coefficient of photosynthetic pigments (note that wavelength and depth are omitted for brevity). It is thus necessary to develop methodologies/algorithms to separate this absorption property from  $a_{ph}$  (e.g., Bidigare et al., 1990; Hoepffner and Sathyendranath, 1993). On the other hand, the measurement of  $a_{ph}$  could be much easier and straightforward than the measurement of  $a_{psp}$  in the field. In such a case, it is important to clearly specify the absorption coefficient ( $a_{ph}$  or  $a_{psp}$ ) used for the derivation of  $\phi$  in the field. In short, we need to know how  $\phi$  varies spatially and temporally, and to know and characterize how  $\phi$  changes with different species (Napoleon et al., 2013; Uitz et al., 2010), depths, and seasons, and if  $\phi$  value can be effectively

estimated from remotely sensible data. All these objectives demand appropriate, and concurrent, measurements of PP and the optical properties.

### 7.4. *In situ* measurement of primary productivity

Because it is the at-sea *in situ* PP that is used as a base for the scale up for basin-scale estimates, it is critical to have accurate *in situ* measurements of primary productivity. The topic of the measurement of PP has been reviewed many times, and recently by Marra (2002, 2009), and the reader is referred to those publications for a more extended analysis. Here, we can categorize the measurement on the basis of the scale of the measurement, and the kind of incubation “container.” Traditionally, the incubation container has been a transparent bottle of some kind or size that isolates a water sample from the environment so that physiological measurements can be made, using isotopes of elements ( $^{13}\text{C}$ ,  $^{14}\text{C}$ ,  $^{18}\text{O}$ ), or the fluxes of the molecules themselves ( $\text{O}_2$ ,  $\text{CO}_2$ ), involved in photosynthesis. Recently, methods have been developed that allow the mixed layer itself to be the “container,” using isotopes of oxygen to estimate PP, and also net community production (e.g., Quay et al., 2012). The advantage of the former method is that the water sample is perfectly isolated, however, the containers are usually very small, and incubation time is short relative to how the ocean is viewed by satellite. There may be deleterious effects from the enclosure of a water sample for any length of time.

The advantage of the latter method is a broader scale, both in depth (the mixed layer) and time (1–2 weeks) that may be more amenable to scaling up to the scale of remote sensing. However, the larger “container” is also more dynamic, and “leaky.” Mixed layer depth can easily change diurnally, and day-by-day, limiting the environments for which the *in situ* isotope methods can be employed. Too, exchanges across the base of a mixed layer cannot be easily measured or estimated. Finally, the depth of the euphotic zone usually extends beyond the mixed layer, and those depths are typically characterized by a chlorophyll-*a* maximum contributing to water column productivity.

A third alternative exists, fluorescence kinetics, in the method of fast repetition rate fluorometry (FRRF), or pulse-amplitude modulated (PAM) fluorescence. These measurements are relatively simple, and do not require incubation. Recent reports suggest that there is a meaningful correlation between FRRF measurements and the photosynthetic assimilation of  $^{14}\text{C}$  (Cheah et al., 2011), thus FRRF measurements could serve as a simple mapping variable for larger-scale distributions of PP. Moreover, since all PP algorithms currently use PP estimates from  $^{14}\text{C}$  assimilation, there would be a means to extend the measurements in space, at least to the extent of shipboard coverage.

Comparisons among these measurement options are rare or non-existent. The mixed layer measurements are usually accomplished without direct comparisons with incubation technologies, and *vice-versa*. If we are to reach the goal of accurate assessments of PP for the global ocean, a research program will be required that incorporates as many different methods to estimate PP in a given environmental setting. Perhaps something analogous to NOAA's MOBY program (see <http://moby.mlml.calstate.edu/>) for validation of PP would be a good start.

### 7.5. Improving the description of the vertical distribution of IOPs

Another important factor for accurate PP estimation is the vertical distribution of the water properties (Platt et al., 1988; Sathyendranath and Platt, 1989). The above discussion has assumed that the water column is well mixed. For natural waters, however, this assumption is not always valid. For stratified waters, vertical variation in water properties needs to be taken into account (Sathyendranath and Platt, 1989). In the current models (Chl-based model) that include the vertical variation, the attenuation coefficient is deduced from the vertical distribution of phytoplankton biomass (Sathyendranath and Platt, 1993), with the

vertical distribution of biomass collected from field surveys (Morel and Berthon, 1989; Platt et al., 1988). Recent field measurements have found that the vertical distribution of the optical properties do not necessarily follow the same phase as that of phytoplankton biomass, mainly because the vertical distribution of gelbstoff can be independent of biomass (Siegel and Michaels, 1996). Since it is the optical properties that determine the vertical propagation of solar radiation, information on the vertical distribution of the optical properties is an important component for improving PP estimation. Data banks that contain (or remote-sensing methods to derive) the vertical distribution of  $a_{ph}$ ,  $a$ , and  $b_b$  are strongly needed. If no such datasets exist for a given region, dynamic models (e.g., Chai et al., 2002) are a useful alternative to generate appropriate vertical profiles of these properties.

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