ESTIMATE OF CHLOROPHYLL CONCENTRATION FROM OCEAN COLOR: UNCERTAINTY ASSOCIATED WITH UNKNOWN BACKSCATTERING

Xiaodong Zhang and Andrei Kirilenko

Department of Earth System Science and Policy, University of North Dakota, zhang@aero.und.edu

ABSTRACT:

It is backscattering of solar radiation by water body that makes ocean color observable from above, either by airplanes or satellites. Given the very low direct contribution to backscattering by phytoplankton cells, it is curious why the retrieval of phytoplankton concentration from remotely observed ocean color is evidently successful. From semi-analytical bio-optical models, a dataset is created of spectral absorption, scattering and backscattering coefficients as a function of chlorophyll concentration. Four scenarios are considered, 1) only molecular and no particle scattering, 2) random particle backscattering uncorrelated with chlorophyll concentration, 3) constrained random particle scattering with known backscattering ratio, and 4) constrained random scattering with random backscattering ratio. Scenario 1 only introduces moderate errors of -20% - 90%. And for scenarios 3 and 4, the errors are largely within 30% and 100%. Scenario 2 introduces the largest errors, with the retrieved chlorophyll concentration virtually uncorrelated with the true values, implying the backscattering must somehow be related to the trophic state. The results of the study suggested These 3 cases confirmed that while it is the absorption by phytoplankton that in large part decides the accuracy of chlorophyll concentration retrieval, for the success of monitoring of global ocean primary productivity we have to improve our knowledge on particle backscattering.

KEY WORDS: backscattering, scattering, absorption, ocean color, chlorophyll

1. INTRODUCTION

Spectral reflectance at the ocean surface, ocean color (R), is governed by, to the first approximation, the ratio of the total backscattering (b_b) to the total absorption (a) coefficients of water body,

$$R(\lambda) = f\frac{b_b(\lambda)}{a(\lambda)}, \qquad (1)$$

where f is a parameter that depends on the illumination condition as well as the optical properties of water (Gordon 1989; Morel and Gentili 1993). Equation 1 is in agreement with in situ measurements for clear open ocean waters (Morel and Prieur 1977; Smith and Baker 1978).

Roughly 95% of world's open ocean and coastal waters belong to the Case 1 water class (Morel and Prieur 1977), where phytoplankton predominately determines the optical properties of the water column. Bio-optical models based on chlorophyll concentrations have been developed empirically. For absorption the model can be summarized as (e.g. Bricaud et al. 1998),

$$a(\lambda) = a_w(\lambda) + a_p(\lambda) + a_{CDOM}(440)\,, \qquad (2.1)$$

$$a_p(\lambda) = A_p(\lambda)[chl]^{E_p(\lambda)}\,, \qquad (2.2)$$

$$a_{CDOM}(\lambda) = a_{CDOM}(440)\exp[-0.014(\lambda - 440)]\,, \qquad (2.3)$$

$$a_{CDOM}(440) = 0.2[(a_w + a_p)(440)]\,, \qquad (2.4)$$

where $a_w(\lambda)$ is the absorption coefficient of pure seawater (Pope and Fry 1997), $a_p(\lambda)$ and $a_{CDOM}(\lambda)$ the absorption coefficients for particulate and dissolved organic matter, respectively, and the values of $A_p(\lambda)$ and $E_p(\lambda)$ can be found in Fig. 4 of Bricaud et al. (1998). Scattering and backscattering models follows (e.g. Loisel and Morel 1998; Morel and Maritorena 2001),

$$b_b(\lambda) = 0.5b_w(\lambda) + b_{bp}(\lambda) \qquad (3.1)$$

$$b_{bp}(\lambda) = b_p(550)\tilde{b}_b(\lambda) \qquad (3.2)$$

$$\tilde{b}_b(\lambda) = 0.002 + 0.01[0.5 - 0.25\log[chl]](\lambda/_{550})^{\nu} \qquad (3.3)$$

$$b_p(550) = 0.416[chl]^{0.766} \qquad (3.4)$$

$$\nu = -1, \quad [chl] < 0.02\,mg\,m^{-3}$$

$$\nu = 0.5(\log[chl] - 0.3), \qquad 0.02 < [chl] < 2\,mg\,m^{-3}$$

$$\nu = 0, \quad [chl] > 2\,mg\,m^{-3} \qquad (3.5)$$

where $b_w(\lambda)$ is spectral the scattering coefficient for pure seawater (Morel 1974), $b_p(\lambda)$ the scattering coefficient for particles and $\tilde{b}_b(\lambda)$ the backscattering ratio for particles.

While phytoplankton and their associated biogenic particles can account for the absorption coefficient observed, it is well known that they only contribute to a small part of the total particulate backscattering (Morel and Ahn 1991; Stramski and Kiefer 1991; Zhang et al.

1998). It has been proposed that the small-sized non-living particles (Stramski et al. 2004) or small-sized bubbles (Zhang et al. 2002) stabilized by organic coating (Johnson and Cooke 1981) could be major sources of particulate backscattering. However, because their concentrations can vary significantly, a complete explanation of the 'missing' backscattering still can not be reached.

Both absorption and scattering processes modify the underwater light field, it is backscattering, though insignificant in magnitude in comparison to absorption, that ultimately determines how much light can be scattered back by a water body and therefore give rise to the color of the ocean. Given the fact that phytoplankton contributes less than 10% of backscattering (Morel and Ahn 1991), it is interesting to ask why estimation of pigments from remote sensing has been so evidently successful.

The object of this study is to investigate the potential error in estimating the chlorophyll concentration from remote sensing associated with the uncertainty of knowledge in backscattering.

2. METHOD

The bio-optical models for estimating chlorophyll concentration from color ratio have been developed using *in situ* data (e.g. O'Reilly et al. 1998). For consistency, we we have created datasets of absorption, scattering and backscattering at wavelengths 490 nm and 555 nm using Eqs. 2 and 3 as function of chlorophyll concentration between 0.01 mg m^{-3} and 10 mg m^{-3}. From this dataset, the chlorophyll concentration can be derived as using Eq. 1,

$$\log[chl] = 0.67 - 5.12\rho + 9.25\rho^2 - 9.65\rho^3 \qquad (4.1)$$

$$\rho = \log\left(\frac{R(490)}{R(555)}\right). \qquad (4.2)$$

The uncertainty in the retrieval of chlorophyll concentration that are due to scattering mainly arises from the variability in total particulate scattering (Eq. 3.2) and insufficient knowledge in backscattering ratio (Eq. 3.4). Here we examined the effect of uncertainty that is due to total scattering only (and assuming Eq. 3.4 is correct).

The correlation coefficient (r^2) for Eq. 3.4 at 550 nm determined using a global dataset of 850 data points is 0.89 (Loisel and Morel 1998); a simulation of Eq. 3.4 is shown in Figure 1, with chlorophyll concentration following a lognormal distribution (Campbell 1995) with mean at 0.20 mg m^{-3} (Fig. 1, O'Reilly et al. 1998).

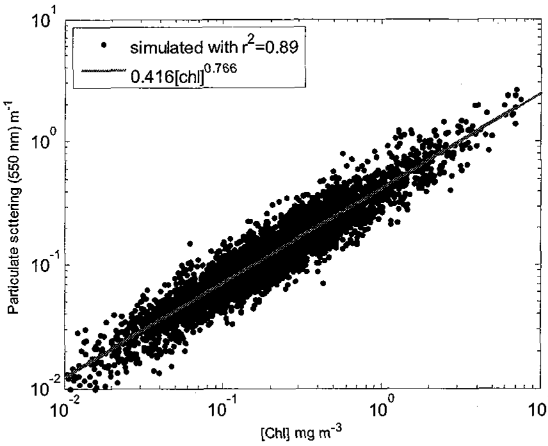

Figure 1. Simulated variation of total particulate scattering at 550 nm as a function of chlorophyll concentration.

Implied in Eqs. 3.3 and 3.4 is that particulate scattering and backscattering will also follow a lognormal distribution as displayed by global chlorophyll concentration. Based on Fig.1 we generated 3 randomly distributed datasets for the particulate backscattering. The first dataset used the mean and standard deviation for the particle backscattering coefficients determined over the entire [Chl] range, which are -2.9851 and 0.3285 at 490 nm, and -2.9710 and 0.3444 at 555 nm, respectively, in the logarithmic domain. The second dataset assumed Eq. 3.3 is valid and variations in the backscattering are entirely due to the variations in the scattering following Fig. 1. Dataset 3 is similar to dataset 2 but assuming the backscattering ratio varies randomly between its low and high boundaries, 0.45% to 1.2%. We added one more case, which represents no particulate scattering and backscattering.

3. RESULTS AND DISCUSSION

3.1 No particulate scattering (Scenario 1)

Scenario 1 is essentially assuming the phytoplankton only absorbs light and its effect on the color of the ocean is reflected by molecular scattering by water itself. The uncertainty under this scenario, expressed in relative error, is shown in Figure 2. The chlorophyll concentration will be underestimated; however, the error is not excessively large (20-90%). Actually in the very clear ocean water, the backscattering by water molecules themselves can contribute as much as 80% to the total backscattering coefficient in the blue spectral region. This explains why the errors are only moderate.(< 50%) at low chlorophyll concentration (< 0.4 mg m^{-3}).

3.2 Entirely random backscattering (scenario 2)

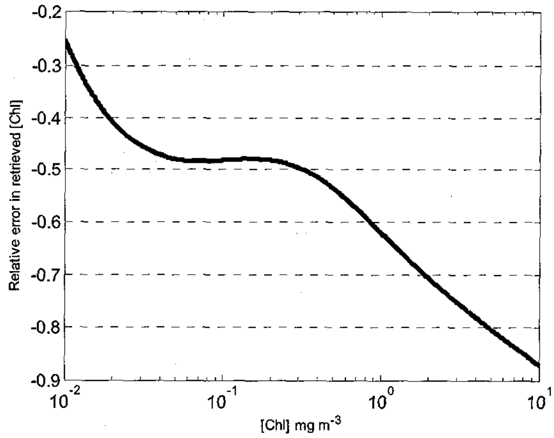

Figure 2 The relative error in the retrieved [chl] using Eq. 4.1 by assuming that there were no particulate backscattering.

Figure 3 shown the result of scenario 2 using dataset 1 which assumed that the backscattering is totally uncorrelated with the chlorophyll concentration.

As can be expected, the retrieved chlorophyll concentrations differ significantly from the input, with errors up to factors of 100. The correlation coefficient between them, r^2, is only 0.13. Given the extremely large errors shown in Fig. 3 and the evidently success of chlorophyll remote sensing in general, we can safely say scenario 2 does not represent a realistic situation. It is interesting to note that errors in neglecting particulate backscattering are much less than errors associated with unknown backscattering

3.3 Scattering co-varying with trophic state (scenario 3)

Figure 4 shows the results of scenario 3 using dataset 2 and assuming that the backscattering ratio is exact and the total particulate scattering varies with chlorophyll concentration, and superimposed over this trend is a natural variability constrained by a correlation coefficient of $r^2 = 0.89$ (Fig. 1).

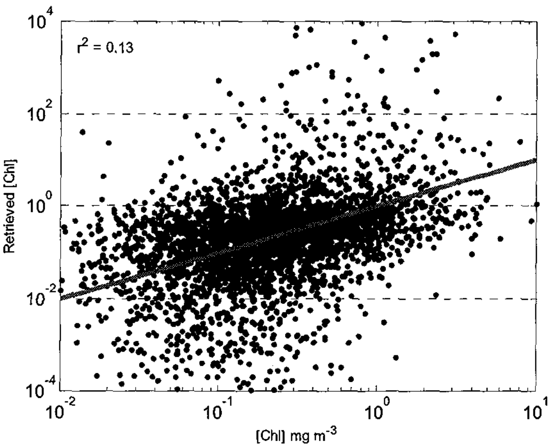

Figure 3 The scatter plot of retrieved [Chl] vs. true [Chl] under scenario 3 with a correlation coefficient $r^2 = 0.13$. The darker line is 1:1 line.

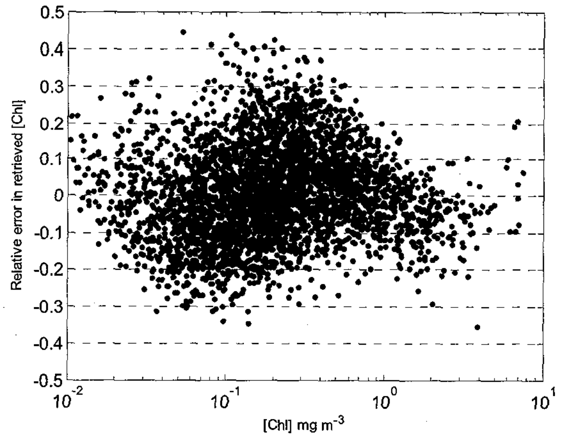

Figure 4 The same as Fig. 2 but assuming scattering changes as a function of [chl] according to Eq. 3.4 with additional random variability.

Surprisingly, errors shown in Fig. 4 are within 30-40% over 3 order of magnitude changes in [Chl]. Recall that the overall error budget for the ocean color remote sensing is 30%, e.g., for SeaWiFS chlorophyll concentration retrieval (Hooker et al. 1992). On the other hand, if all other factors involved in ocean color remote sensing, e.g., atmospheric correction, are perfectly resolved, the phytoplankton concentration can be estimated no better than 30% given the present knowledge of backscattering.

3.4 Constrained random backscattering (scenario 4)

Scenario 4 is similar to scenario 3 but instead of assuming Eq. 3.4 is valid we randomly changed the backscattering ratio within the ranges between 0.45% and 1.2%. It has been argued that the variation in the

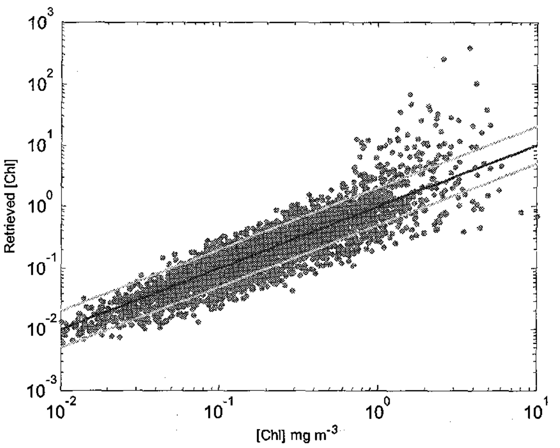

Figure 5 Scatter plot of retrieved [Chl] vs. true [Chl] under scenario 4. The dark line is 1:1 line, on both sides of which are ±100% lines in lighter shade.

backscattering ratio is due to changes in proportions of small particles to phytoplankton (Ulloa et al. 1994)or in dominance of inorganic particles with higher index of refraction (Boss et al. 2004). Figure 5 shows the error in [Chl] retrieved. Majority of errors are well constrained within ±100%, with larger errors can be found at higher chlorophyll concentrations.

4. CONCLUSIONS

Relatively moderate errors shown in Figs. 2 4, and 5 suggested that the absorption by phytoplankton primarily determines the spectral reflectance of the seawater and hence the retrieval of chlorophyll concentration. Due to the instrumentation limit, there have been few field measurements of backscattering (Zhang et al. 2002; Lee and Lewis 2003; Boss et al. 2004). Even in the presence of uncertainties associated with backscattering, the chlorophyll concentration can still be retrieved within ±30-100%. In the meantime, the success operation of ocean color does imply that backscattering correlates to [chl] in some ways. Obviously, to meet the project goal of NASA ocean color missions, i.e., to retrieve [Chl] within 30%, we have to advance our understanding of backscattering and its relationship with biotic community.

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