REMOTE ESTIMATION OF CHLOROPHYLL-A IN COASTAL WATERS USING RED AND NEAR INFRARED SPECTRAL REGIONS

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Introduction

Recent advances in the development of the atmospheric correction models made the retrieval of surface reflectance spectra of coastal waters from the top of atmosphere signals more accurate and inspired the further development of the coastal retrieval algorithms. This includes algorithms which employ the red and NIR bands and which are less sensitive to the absorption of the colored dissolved organic matter (CDOM) and scattering of mineral particles than traditional blue-green ratio algorithms. Simple Red-NIR band ratio algorithms are known for a long time [1,2] and successfully used for the estimation of chlorophyll a [Chl] concentrations from reflectance spectra in coastal and inland waters [3], as [Chl] is above 5 mg/m^3 when peak around 700 nm is becoming pronounced. Generally this peak includes two components: i) elastic one which is due to the local minimum of absorption coefficient as a result of the confluence of the phytoplankton and water absorption spectra, and ii) chlorophyll fluorescence with the maximum near 685 nm [2,4,5]. For [Chl]<5mg/m^3 elastic component is small and the magnitude of the peak and [Chl] are mostly related to the fluorescence signal. For [Chl]>5mg/m^3 both components contribute to the signal with the peak of elastic component and combined reflectance moving to the red with increasing [Chl]. Advanced version of Red-NIR algorithms includes 3 bands instead of 2 [6], which assumes better separation of the phytoplankton absorption related to [Chl] from other absorption and scattering components in the red and NIR part of the spectrum. Both 2 and 3 bands algorithms have been tested in the multiple water environments [3,7,8] but the origins of the uncertainties were difficult to trace because multiple unknown parameters involved were not measured directly in the experiments. Optimization of the band positions was done on the synthetic datasets simulated using semi-analytical model [9], however, sensitivity of the retrievals to the CDOM absorption, concentration of minerals, phytoplankton absorption spectra were not considered. In this work we tested 2 and 3 bands algorithms with the bands available on MODIS and MERIS satellite sensors using comprehensive synthetic datasets of reflectance spectra and inherent optical properties (IOP) related to a wide range of water parameters as well as a new field dataset.

Description of datasets

1000 reflectance spectra with and without chlorophyll fluorescence were simulated using HYDROLIGHT [10] with 1 nm resolution for conditions typical of coastal waters: [Chl] = 1 – 100 mg/m^3, CDOM absorption at 400 nm $a_y(400)$ = 0 – 5 m^{-1}, 5 different specific chlorophyll absorption shapes and concentrations of non-algal particles in the range C_{NAP} = 0 – 1 (500 runs) and C_{NAP} = 1-10 mg/l (500 runs). All details and assumptions used for the simulation of the water parameters are given in [11]. They were based on the findings of many authors for IOP characteristics, and were similar to the assumptions used in the construction of the Lee IOCCG datasets [12]. Solar input was simulated with a cloud-free sky. A set of specific absorptions was taken according to Ciotti et al. [13] as a sum of specific absorptions of microplankton and picoplankton with different weights S_f where S_f = 0.1 – 0.5 according to the expression (1)

$$a^*_{ph}(\lambda) = S_f \cdot a^*_{pico}(\lambda) + (1 - S_f) \cdot a^*_{micro}(\lambda) \qquad (1)$$

These spectra are shown in Fig. 1a. The chlorophyll absorption was considered proportional to [Chl]. These specific absorption shapes do not cover full typical range of the maximum at 675 nm which can be up to 0.03 m^2/mg [7,14], so four other shapes were also considered as shown in Fig. 1b in other 300 runs with the

same range of [Chl] and CDOM absorption and C_{NAP} = 0-1 mg/l. These shapes include standard Case 1 water – (1) [10], Cryptophyta "H" (2), Diatoms (3) and Green algae (4) [15].

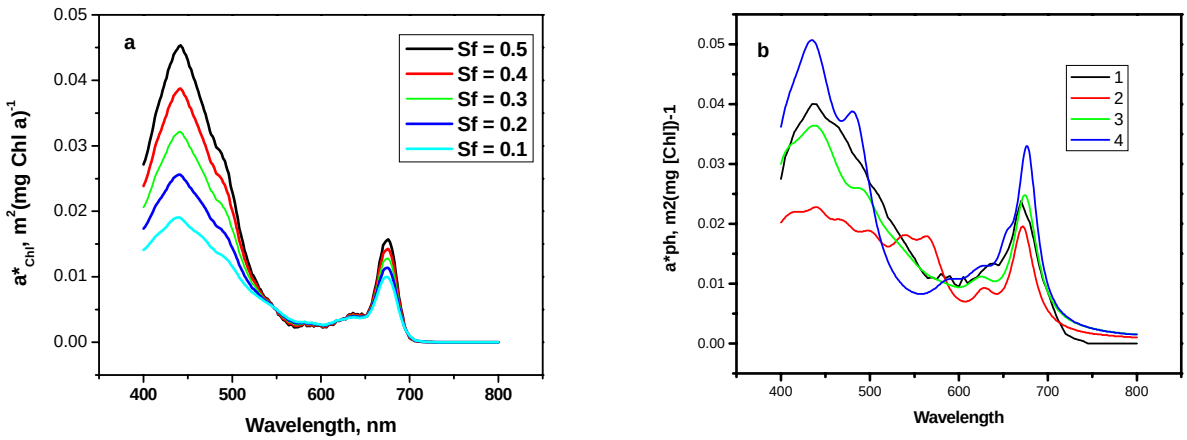

Fig. 1. Specific chlorophyll absorption spectra used in simulations.

Fluorescence quantum yield (together with the reabsorption coefficient) in original simulations was η = 0.5% but the fluorescence contribution was calculated as the difference between the total and elastic reflectances and was assumed to change proportionally to η which permitted to assess the impact of the fluorescence component. All reflectances were simulated for the sun zenith angle θ_i = 30° and nadir viewing.

Field dataset consisted of data collected by the CALMIT group at 85 stations in Fremont State Lakes, NE USA with [Chl] = 2 – 100 mg/m3, $a_y(400)$ = 0.9 – 3 m^{-1} and C_{NAP} below 3mg/l [16].

Comparison of the synthetic and field data

2 band NIR algorithm $R_{rs}(708)/R_{rs}(665)$, which corresponds to MERIS bands was chosen for the comparison between synthetic and field datasets. There was no visible impact of C_{NAP} on [Chl] estimates using field data, so the data for all stations are shown in Fig. 2. Reflectance ratios retrieved from simulated data, as C_{NAP} < 1mg/l and the high a* set (Fig. 1b) was used, matched well the field data for [Chl] < 30-40 mg/m^3. However, relationship was weaker for [Chl] > 40 mg/m^3 (not shown). It is obviously due to the fact that such high a* values are unrealistic for the range of [Chl] concentrations considered in this study. The packaging effect should be taken into account by the gradual change of a* shapes with increasing [Chl] but the closest in our datasets is Sf = 0.5 shape, data points for which lay slightly above the field data with the minimum variability for the whole [Chl] range. Reflectances with this specific absorption shape will be primarily used in the further analysis.

Sensitivity of 2 band algorithms to water parameters

The same 2-band algorithm $R_{rs}(708)/R_{rs}(665)$ was further analyzed using synthetic datasets. The impact of a* through Sf factor is shown in Fig. 3a. For high Sf values the relationship is very close. However, as Sf decreases, the slopes of the relationships increase and relationships between [Chl] and the ratio become much weaker. In Fig. 3a for all Sf values, CDOM range was $0<a_y(400)<5m^{-1}$, though almost no effect of variation of CDOM concentration on the relationships can be noticed. Results of simulations for three values of fluorescence quantum yield η = 0.25, 0.5 and 1.0 are shown in Fig. 3.b. Small differences can be observed only for [Chl] > 60 mg/m^3.

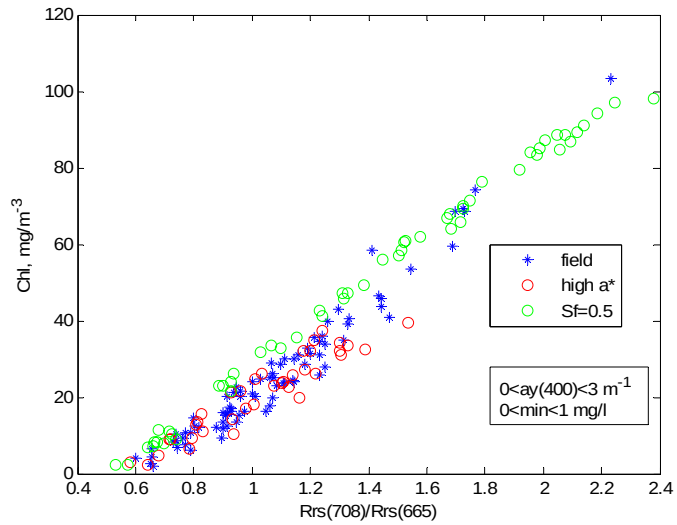

Fig. 2. Chlorophyll-a concentration vs. 2-band Red-NIR algorithm for the synthetic and field data.

The algorithm output is significantly affected by variation in concentrations of mineral particles C_{NAP} is (Fig. 4a). With the increase in C_{NAP} the ratio decreases and the algorithm underestimates [Chl] concentration. This effect can be reduced considerably taking into account that $R_{rs}(665)$ values are quite good proxies for mineral concentrations. By using $R_{rs}(708)(1+25\times R_{rs}(665))/Rrs(665)$ instead of the simple ratio the split between estimates for various C_{NAP} can be significantly reduced (Fig. 4b).

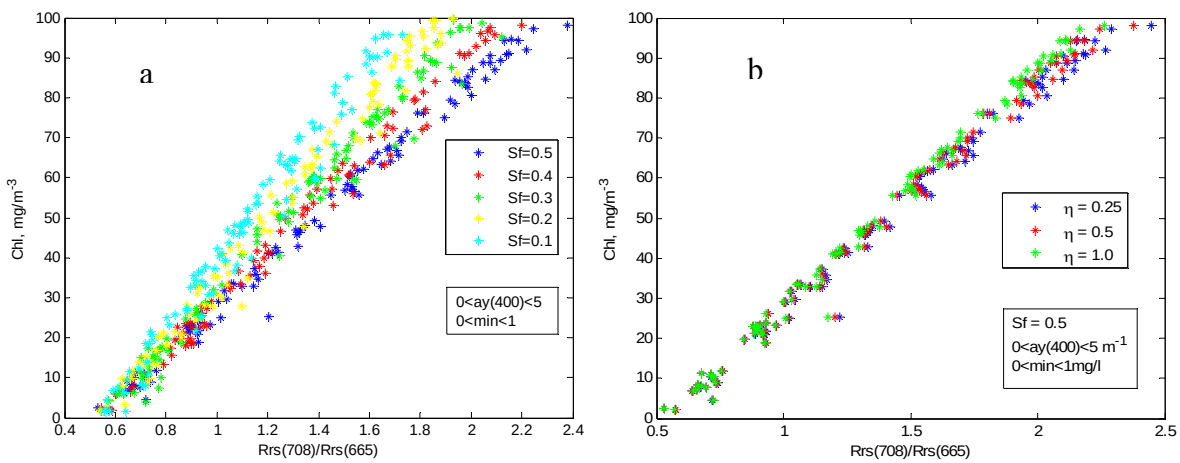

Fig. 3. Chlorophyll-a concentration vs. 2-band Red-NIR algorithm estimates: impact of the specific absorption shape (a) and fluorescence quantum yield (b)

Analysis showed that the use of NIR bands at 753 nm (MERIS) and 748 nm (MODIS) in numerator of Red-NIR algorithm does not provide accurate [Chl] estimates especially for concentrations below 20 mg/m^3. These algorithms are also less accurate with the proximal and especially satellite data due to the low values of reflectance in the bands near 750 nm and associated with that higher uncertainty in reflectance measurements and atmospheric correction. On the other hand, there is no choice for Red-NIR algorithm with MODIS bands. It probably can be used only for the detection of phytoplankton blooms.

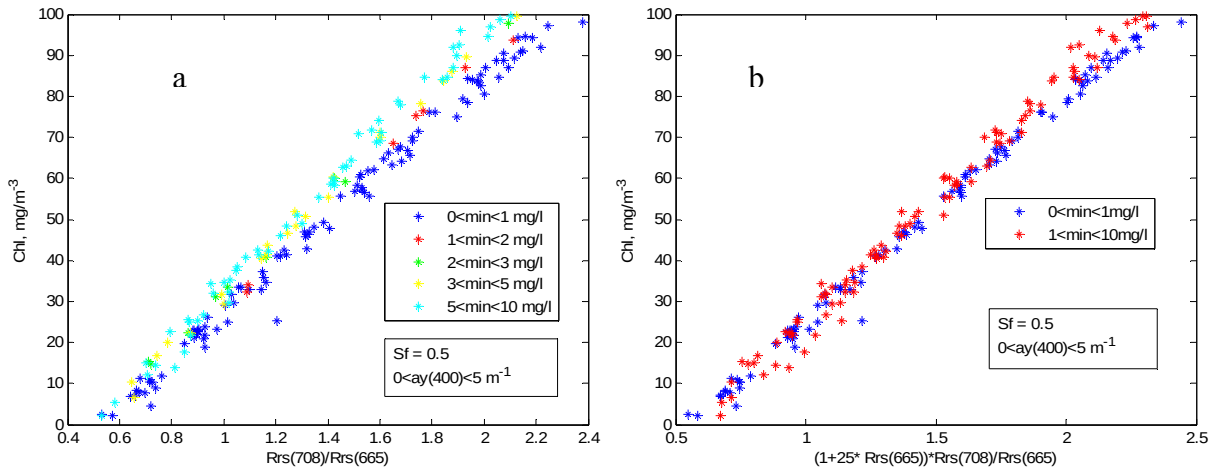

Fig. 4. Chlorophyll-a concentration vs. (a) 2-band Red-NIR algorithm and (b) its modification estimates: impact of C_{NAP} concentrations

Sensitivity of 3 band algorithms to water parameters

Results for 3 band algorithm $[Rrs^{-1}(665) - Rrs^{-1}(708)]\times Rrs(753)$ were found to be very similar to 2 band algorithm Rrs(708)/Rrs(665) in the sensitivity to the specific absorption shape, fluorescence quantum yield and mineral concentrations. However, we were not able to find the simple mechanism similar to the shown above for 2 band algorithm to decrease the sensitivity of this algorithm to change in concentration of mineral particles.

Comparison of NIR and blue-green ratio algorithms

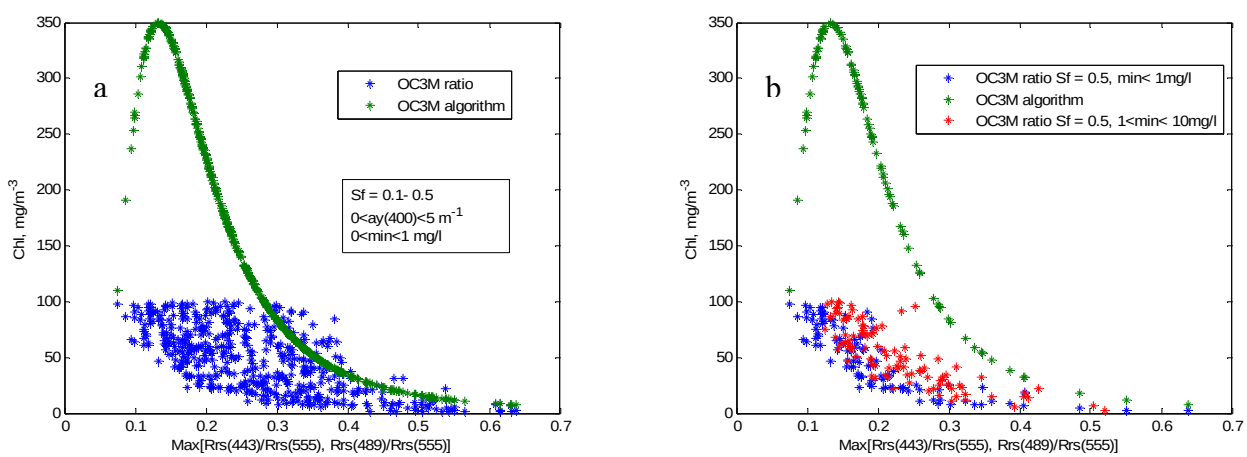

Fig. 5. Tests of OC3M algorithm.

We also analyzed the performance of the blue-green MODIS OC3M algorithm on the same datasets. In Fig. 5a blue points show the known from our dataset [Chl] as a function of the OC3M ratio, green points are [Chl] values determined using OC3M expression for [Chl] as a function of this ratio. Results include all Sf values Sf = 0.1-0.5 and $0<C_{NAP}<1$ mg/l. The spread is extremely high and the data somehow correlate with the expression only for low [Chl] values probably below 10 mg/m^3. Similar results are shown in Fig. 5b but only for Sf = 0.5. We also added results for $1<C_{NAP}<10$ mg/l (red points) to this figure. The spread is lower but the algorithm performance is worse than even for MODIS Rrs(748)/Rrs(667) algorithm.

Comparison with chlorophyll retrieval from MERIS data

Moses et al. [17] calibrated and validated Red-NIR models using MERIS satellite data and {Chl] measured in the field. As a result of calibration following relationships between [Chl] and the models were obtained.
The two-band MERIS algorithm:

$$[\mathrm{Chl}] = 61.026(R_{665}^{-1} \times R_{708}) - 37.76 \qquad (2)$$

The three-band MERIS algorithm:

$$[\mathrm{Chl}] = 239.35[\left(R_{665}^{-1} - R_{708}^{-1}\right) \times R_{753}] + 23.03 \qquad (3)$$

We calculated [Chl] values using 2- and 3-band algorithms (2) and (3) from generated reflectance spectra and plotted them versus actually measured [Chl] values. The results are very close (Figs. 6a and b). Thus, Red-NIR algorithms calibrated using MERIS data are able to estimate chlorophyll-a concentrations using generated spectra in a quite wide range of constituent concentrations.

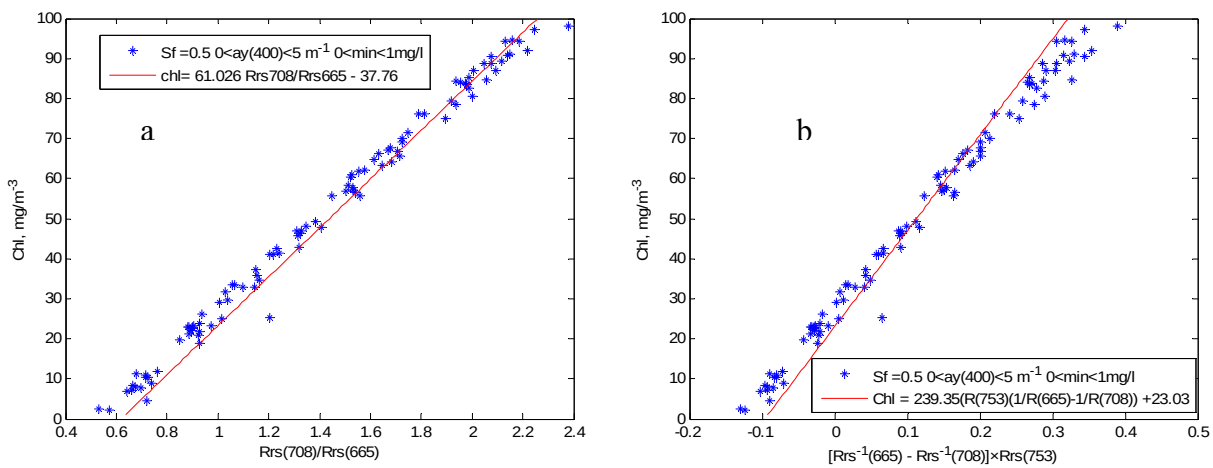

Fig. 6. Estimates of chlorophyll-a concentrations from generated reflectance spectra using calibrated Red-NIR MERIS algorithms: a) 2 band algorithm, b) 3 band algorithm.

Conclusions

1. Synthetic datasets for coastal waters are compared with a very consistent field dataset with [Chl] = 2 - 100 mg/m^3 and showed good match. Further improvement between datasets can be achieved by taking into account more accurately the change of specific chlorophyll absorption with increasing [Chl] due to the packaging effect.

2. 2-band Red-NIR algorithm $R_{rs}(708)/R_{rs}(665)$, which uses MERIS bands, provides a good estimation of chlorophyll concentration for [Chl] > 5 mg/m^3 with a weak dependency on variation in CDOM concentrations. While obvious sensitivity to mineral concentration was observed it can be partially pared by the addition of (1+ 25*Rrs(665)) term to the numerator. Sensitivity to the fluorescence quantum yield in the range 0.25 – 1% is noticeable for [Chl]>60 mg/m^3.

3. 2-band algorithms, which use in numerator MODIS and MERIS bands around 750 nm, showed worse performance. Errors can be even higher on the proximal sensing and satellite data because of the low $R_{rs}(753)$ values.

4. According to the tests on synthetic datasets, 3-band algorithm $[R_{rs}^{-1}(665) - R_{rs}^{-1}(708)]\times R_{rs}(753)$ had similar dependency on CDOM and mineral concentration and fluorescence quantum yield as the 2-band $R_{rs}(708)/R_{rs}(665)$ algorithm. Inclusion of $R_{rs}(753)$ also has a potential of error increase due to the low reflectances at this band. We have not found at this time the mechanism to decrease the sensitivity of the

algorithm to variation in mineral concentration. Advantages of 3-band algorithms should be further studied on the synthetic data with higher [Chl] concentrations as well as on datasets which trace more accurately the change of specific chlorophyll absorption with [Chl] due to the packaging effect.

5. The performance of MODIS blue-green ratio OC3M algorithm in coastal waters is poor and it should be replaced in turbid productive Case-2 waters by Red-NIR algorithm. Exact boundaries for this replacement should be further studied.

6. Relationships of [Chl] vs $R_{rs}(708)/R_{rs}(665)$ and [Chl] vs $[R_{rs}^{-1}(665) - R_{rs}^{-1}(708)]\times R_{rs}(753)$ established recently from MERIS spectra and field data match very well synthetic data which confirms accuracy of the field and synthetic data as well as stability of these relationships.

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