RETRIEVAL OF COLORED DISSOLVED ORGANIC MATTER AND DISSOLVED ORGANIC CARBON IN THE SINGAPORE STRAIT

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ABSTRACT: Monitoring the transport of dissolved organic carbon (DOC) from land to ocean is vital in studying the carbon cycles of terrestrial and aquatic ecosystems. It has been estimated that tropical peatlands in coastal Southeast Asia contribute about 10% of the global land-ocean DOC flux. The use of remote sensing techniques in monitoring DOC would aid in better understanding of biogeochemical processes in this region. We present a quasi-analytical algorithm (QAA) adapted to the Singapore Strait to retrieve colored dissolved organic matter (CDOM) and DOC concentration from the Ocean Land Color Instrument onboard the Sentinel 3A satellite. Our adaptation of the QAA significantly improved retrievals of the water absorption and backscattering coefficients from remote sensing reflectance. Using CDOM absorption as a proxy, the DOC concentration was estimated with a mean absolute percentage error of 5.5%.

1. INTRODUCTION

It has been reported that the tropical peat deposits along the coasts of Borneo and Sumatra in Southeast Asia account for approximately 10% of the global terrigenous dissolved organic carbon (tDOC) flux to the ocean (Baum, 2007; Moore, 2011). Monitoring of DOC in coastal waters is thus important to account for human perturbations of the carbon cycle and to assess its impacts on the functioning of marine ecosystems. In this paper, we develop an algorithm to retrieve the absorption coefficient of colored dissolved organic matter (CDOM) as a proxy for DOC concentration using satellite images acquired by the Ocean and Land Color Instrument (OLCI) on the Sentinel 3 satellite. We chose to parameterize a Quasi-Analytical Algorithm (QAA_v5) (Lee, 2020a) by introducing a backscatter function derived from in-situ data and an appropriate selection of the reference wavelength. We further extended our adaptation of QAA, denoted as QAA_SG, to partition the absorption spectra into the two components due to CDOM and detrital matter (Dong 2013, Zhu, 2011). Thereafter, we established a linear empirical relationship, parameterized according to the monsoon season, to estimate DOC concentration from CDOM absorption.

2. STUDY AREA AND DATA ACQUISITION

Twenty one sets of in-situ bio-optical measurements were collected near two coral reef sites in the Singapore Strait, Hantu Island (1.2250°N, 103.7525°E) and Kusu Island (1.2232°N,

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103.8611°E). Samples were collected one to two times monthly from January 2019 to August 2020. The water at the sampling sites was optically deep such that the remote sensing reflectance would not be influenced by the sea bottom reflectance.

Above water remote sensing reflectance R_{rs} was derived from in-situ radiometric measurements using a system of two spectroradiometers (TriOS RAMSES). One sensor was fitted with a cosine collector to measure the downwelling irradiance and the other measured the subsurface upwelling radiance with a 7 degrees field of view. The backscattering coefficient b_{bp} was measured in situ using a backscattering sensor (Wetlabs ECO-BB9), lowered to ~ 5 m in depth. The backscattering sensor measures b_{bp} at 9 discrete wavelengths. A hyperspectral b_{bp} spectrum was obtained by interpolating between these wavelengths. The absorption coefficient of CDOM, non-algae particles and chlorophyll, (i.e. a_g, a_d, a_φ) were measured using standard protocols in the laboratory from water samples collected at 5 m depth at each site. For a_g, absorbance was measured from 250-800 nm at 1 nm resolution in a 10-cm quartz cuvette on a dual-beam spectrophotometer (Thermo Evolution 300), using ultrapure water as a reference. For a_d, each water sample was filtered onto a 25-mm diameter glass microfiber filter (Whatman GF/F) and measured from 300–900 nm inside an integrating sphere with a spectrophotometer (PerkinElmer Lambda 950) to obtain the total particulate absorption a_p. Filters were then depigmented and remeasured to obtain a_d. The difference between a_p and a_d gave the chlorophyll absorption a_φ.

All hyperspectral measurements ($R_{rs}, a_g, a_d, a_\varphi, b_{bp}$) were convolved with the relative spectral response function (RSR) of Sentinel 3A (ESA Sentinel-3, 2020) to compute the weighted band-average values,

$$R_{rs}(\lambda_j) = \frac{\int R_{rs}(\lambda) RSR_j(\lambda)\, d\lambda}{\int RSR_j(\lambda)\, d\lambda} \quad (1)$$

3. ALGORITHM DEVELOPMENT

In QAA_v5 (Lee, 2020b), the first step is to estimate the total absorption $a_t(\lambda_0)$ at a reference wavelength λ_0 through an empirical relation with the sub-surface water remote sensing reflectance. For Singapore Strait's CDOM-rich waters, we found that shifting λ_0 to 443 nm gave the best results for retrieving a_{t-w} (a_t minus the absorption of pure water) within wavelengths of 400-560 nm and $a_t(\lambda_0=443)$ is thereby empirically determined following the steps in QAA_v5.

In the parameterization of $b_{bp}(\lambda)$, we employed the use of a backscattering basis function $b_{bp}^*(\lambda)$ derived from in situ data to replace the commonly used power law relation. Each in-situ $b_{bp}(\lambda)$ was normalized with its area under the spectral curve and $b_{bp}^*(\lambda)$ was obtained by averaging all the 21 normalized spectra and applying a moving average filter to smoothen the function.

The total absorption a_{t-w} was first partitioned into components due to phytoplankton, a_φ, and the combination of CDOM and detritus a_{dg} following the steps in QAA_v5. Absorption by detritus, a_d was estimated using two algorithms for comparison. In the first method, a_d was obtained from the particulate backscattering by the equation (Zhu, 2011),

$$a_d(440) = C_1 b_{bp}(510)^{C2} \quad (2)$$

The coefficients C_1 and C_2 were obtained by fitting our field data to the equation. In the second method, a_d was obtained by the following set of equations (Dong 2013),

$$a_d = a_d(443)e^{-S(\lambda-443)} \quad (3)$$
$$a_d(443) = 0.6\sigma^{0.9};\ \sigma = 0.05a_{t-w}(443) + b_{bp}(555)1.4^{\frac{Rrs(555)+Rrs(670)}{Rrs(443)}}$$
$$S = 0.0124$$

The CDOM absorption a_g was then obtained by subtracting a_d from a_{dg}.

The DOC concentration is not an optical property of the water. However, CDOM is a large component of DOC and is commonly used as a proxy to determine DOC (eg. Liu, 2013). We estimated DOC using the empirical relation with the coefficients D_1 and D_2 parameterized for the different monsoon seasons,

$$DOC = D_1 a_g(400) + D_2 \quad (4)$$

4. RESULTS AND DISCUSSION

Validation was performed using the leave-one-out cross-validation (LOOCV) method (Stone, 1974). For both a_{t-w} and b_{bp}, we observe significant improvement in the retrievals compared to QAA_v5. First, with respect to a_{t-w}, the root meat square error (RMSE), normalized root mean square error (NRMSE) and mean absolute percentage error (MAPE) are significantly reduced from an average of 0.25, 39.8% and 29.7% for QAA_v5 to 0.062, 10.3% and 11.2% for QAA_SG. This reduction is consistently observed across all bands. Improvement in the retrievals of b_{bp} is also observed across all bands, with a reduction in the average RMSE, NRMSE, MAPE from 0.0103, 21.6%, 31.3% to 0.0051, 10.7%, 16.9%. b_{bp} values retrieved by QAA_v5 are observed to underestimate the field measured b_{bp}.

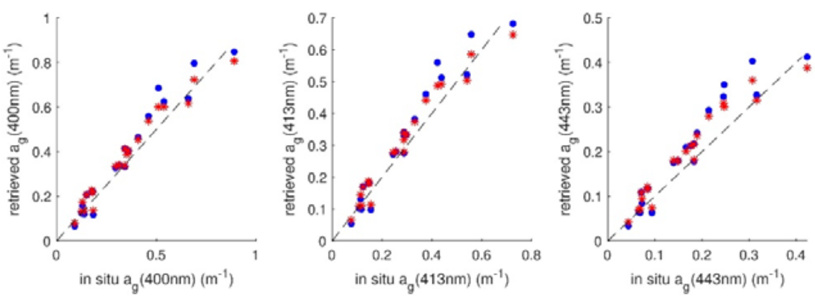

Figure 1. Scatter plot of retrieved *a_g* versus field *a_g* banded to Sentinel 3A. Red stars denote retrievals using Equation 3 (Dong, 2013). Blue dots denote retrievals using Equation 2 (Zhu, 2011). Black dotted line represents the 1:1 line.

The results of CDOM retrieval are shown in Figure 1. The values of a_g obtained using Equation 3 (Dong 2013) show a slightly better RMSE, NRMSE and MAPE of approximately 0.0425, 7.46% and 16.8% as compared to 0.0553, 9.60% and 19.7% for the values obtained using Equation 2 (Zhu 2011). The bias for a_g obtained using Equation 3 is marginally higher, ~0.116, while Equation 2 shows an average bias of 0.113. Because of the inherently low a_d values in our dataset, the slight differences observed in retrieving a_d using either equation do not greatly affect the retrieval of a_g. Furthermore, given the small dataset available, it is difficult to provide an adequate conclusion to which algorithm performs significantly better. Since Equation 3 was designed to fit a wider range of water types, we would suggest its use to retrieve a_d as our current Singapore Strait bio-optical in-situ data does not exhibit properties with high sedimentation and chlorophyll content. However, if one knows that the water type to be retrieved is CDOM-dominated we would advise to use our parameterized Equation 2 to retrieve a_d and a_g.

We parameterized DOC concentration as a function of $a_g(400)$ that depends on the monsoon seasons. The months of Nov to Apr were considered to be the northeast (NE) monsoon season and months of May to Oct were the southwest (SW) monsoon period. During the SW monsoon, DOC and $a_g(400)$ showed a strong, linear relationship over the whole range of the in-situ measurements with $R^2 = 0.74$. However, during the NE monsoon, the DOC concentration and CDOM absorption coefficient were clustered around the lower end of the range resulting in a rather poor correlation between DOC and $a_g(400)$ with R^2=0.28. Despite this, we are still able to obtain a good retrieval of DOC with a MAPE of 5.35% (Figure 2).

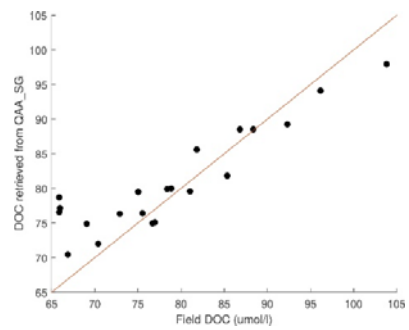

Figure 2. Retrieved DOC versus in-situ DOC concentration (21 data points). Red line denotes the 1:1 line. RMSE = 5.23, NRMSE = 13.8%, MAPE = 5.35%, Bias = 0.0328.

5 CONCLUSIONS

Bio-optical measurements collected in the Singapore Strait were used to parameterize a quasi-analytical algorithm. By shifting the reference wavelength of QAA_v5 to 443 nm and introducing a backscattering basis function $b_{bp}^*(\lambda)$ derived from in situ data, there were significant improvements in the retrievals of the water absorption and backscattering coefficients from remote sensing reflectance. The total absorption was successfully partitioned into the detrital and CDOM components. The DOC concentration was estimated using CDOM absorption as a proxy.

Our QAA_SG algorithm was tested using field data measured at CDOM dominated Singapore Strait and simulated Sentinel 3A OLCI data derived from in-situ radiometric measurements. Continuation of this work will include extending QAA_SG to other water types especially those with higher amount of phytoplankton and non-algal particles. Application of QAA_SG on ocean color satellite imagery will provide us with the capability for real-time and long-term monitoring of surface DOC and CDOM concentrations in coastal waters of Southeast Asia. Implementation of this algorithm will therefore allow for the much needed understanding and direct assessment of the combined effect of natural and anthropogenic processes on DOC and CDOM such as the export of terrigenous matter from South East Asia's peatlands.

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