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Particulate absorption properties in the Red Sea from hyperspectral particulate absorption spectra

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Abstract

This paper aims to describe the variability of particulate absorption properties using a unique hyperspectral dataset collected in the Red Sea as part of the TARA Oceans expedition. The absorption contributions by phytoplankton (a_{ph}) and non-algal particles (a_{NAP}) to the total particulate absorption coefficients are determined using a numerical decomposition method (NDM). The NDM is validated by comparing the NDM derived values of a_{ph} and a_{NAP} with simulated values of a_{ph} and a_{NAP} are found

to be in excellent agreement for the selected wavelengths (i.e., 443, 490, 555, and 676 nm) with high correlation coefficient (R^2), low root mean square error (RMSE), mean relative error (MRE), and with a slope close to unity. Further analyses showed that the total particulate absorption coefficients (i.e., $a_p(443)_{\text{average}} = 0.01995 \text{ m}^{-1}$) were dominated by phytoplankton absorption (i.e., $a_{\text{ph}}(443)_{\text{average}} = 0.01743 \text{ m}^{-1}$) with a smaller contribution by non-algal particles absorption (i.e., $a_{\text{NAP}}(443)_{\text{average}} = 0.002524 \text{ m}^{-1}$). The chlorophyll *a* is computed using the absorption based Line Height Method (LHM). The derived chlorophyll-specific absorption ($a^*_{\text{ph}} = a_{\text{ph}}(\lambda)/\text{Chl}_{\text{LH}}$) showed more variability in the blue part of spectrum as compared to the red part of spectrum representative of the package effect and changes in pigment composition. A new parametrization proposed also enabled the reconstruction of $a^*_{\text{ph}}(\lambda)$ for the Red Sea. Comparison of derived spectral constants with the spectral constants of existing models showed that our study $A(\lambda)$ values are consistent with the existing values, despite there is a divergence with the $B(\lambda)$ values. This study provides valuable information derived from the particulate absorption properties and its spectral variability and this would help us to determine the relationship between the phytoplankton absorption coefficients and chlorophyll *a* and its host of variables for the Red Sea.

Keywords: Red Sea-Particulate absorption properties-Phytoplankton absorption coefficient-Phytoplankton biomass- TARA Oceans expedition.

1. Introduction

The Red Sea is a semi-enclosed, elongated basin, approximately 2000 km long, up to 355 km wide, with a mean depth of 524 m (Edwards, 1987). The Red Sea is one of the warmest and most saline seas on Earth (Raitsos et al., 2015), situated between the African continent and the Arabian Peninsula (Prakash et al., 2015), where the Red Sea exchanges its water with the Arabian Sea and the Indian Ocean via the Gulf of Aden (Edwards, 1987; Sofianos and Johns, 2002). The connection of the Red Sea to the Gulf of Aden is via the strait of Bab-al-Mandab (Edwards, 1987). The Red Sea is an excellent environment for examining the optical variability of phytoplankton pigments as there are major gradients in water mass properties, including temperature, salinity, and nutrients, from south to north (Sofianos & Johns, 2007). Satellite remote sensing has primarily been used to study the large-scale biophysical processes in the upper layer of the Red Sea (Acker et al., 2008; Brewin et al., 2013, 2015; Raitsos et al., 2013; Zhan et al., 2014). However, the potentially wide-ranging importance of optical properties to the upper ocean biogeochemical processes and optics, our current understanding of the particulate absorption properties and its spatial and temporal variability in the Red Sea is limited. The validation and calibration of ocean color satellite sensors are limited due to the lack of in situ optical measurements in the Red Sea, which is essential to improve the ocean color estimates (Brewin et al., 2015).

The spectral shape and magnitude of particulate absorption coefficients ($a_p(\lambda)$) depend on the in-water contents. The complete characterization of particulate absorption spectra is essential for accurate estimation of phytoplankton absorption coefficients ($a_{ph}(\lambda)$), chlorophyll-specific absorption coefficients ($a^*_{ph}(\lambda)$), and to model the primary production (Morel 1991). Optical variability of the open ocean can be determined using the absorption properties of particulate and dissolved fractions.

Therefore, variations in the particulate absorption concerning physical and ecological environmental variability are fundamental to fine-tuning of bio-optical models (Naik et al., 2013). The particulate absorption properties significantly affect the variations of apparent optical properties (e.g., reflectance and diffuse attenuation coefficient).

Light absorption by phytoplankton has a significant influence on the ocean color signal as measured by satellite sensors (Morel & Prieur, 1977; Platt et al., 1988; Morel & Maritorena, 2001) and determines the amount of solar radiation captured by the photosynthesis process (Gordon et al., 1988). Optical variability of the phytoplankton absorption coefficient affects the light attenuation, primary production, pigment biomass and stratification (Morel, 1988; Platt et al., 1988; Hoepffner & Sathyendranath, 1993; Sosik & Mitchell, 1995; Ciotti et al., 2002; Moisan et al., 2011). In the open ocean, optical variability in the upper layer of the open ocean is primarily controlled by phytoplankton pigment concentrations (Platt, 1969; Smith & Baker, 1978) that determines the shades of ocean color. Phytoplankton absorption contributes more to the total absorption in the open ocean, while non-algal particles (NAP) and colored dissolved organic matter (CDOM) contribute a smaller fraction of the total absorption. Changes in the phytoplankton absorption ($a_{ph}(\lambda)$) spectra vary due to differences in phytoplankton community composition, their cell size and pigment package effect (Prieur & Sathyendranath, 1981; Ciotti et al., 2002; Gordon, 2002; Milla-Nuz et al., 2004; Huot et al., 2007).

Optical variations in the a_{ph}^* and its relationships with chlorophyll *a* have been extensively studied and well documented for the open oceans (Yoshimura et al., 2012; and references therein). However, information on the optical variability of a_{ph}^* is understudied for the Red Sea. The few papers that have addressed a_{ph}^* in the Red Sea are limited primarily to the Gulf of Aqaba and northern Red Sea (Stambler, 2005,

2006). Thus, to improve our current knowledge and interpretation of remotely sensed ocean color from the Red Sea, a better understanding of the a_{ph}^* for the Red Sea is required.

Recent advances in the evolution of ocean optical instrumentations, including instruments such as the WETlabs ac-9 meter and ac-s meters, have enabled direct measurements of the spectral absorption coefficients on large time and space scales (Wang et al., 2008). In addition to providing direct measurements of in situ absorption and attenuation, prefiltering the inflow enables differentiation of the contributions from CDOM and suspended particulate matter. The increased availability of high quality in situ measurements has led to the development of inversion models to estimate inherent optical properties from remotely sensed ocean color (IOCCG, 2006).

Fully utilizing this ability to estimate inherent optical properties from ocean color imagery requires knowledge of the absorption coefficients of phytoplankton, non-algal particles, and color dissolved organic matter. This reinforces the need for numerical methods to discriminate the absorption contributions of and the individual constituents from bulk measurements (Wang et al., 2008).

This study focuses on understanding the particulate absorption properties in the Red Sea from hyperspectral particulate absorption spectra. Additionally, in this study, we will examine the role of a_{ph}^* in the Red Sea. To best of our knowledge, the TARA data set is the first comprehensive hyperspectral data set that extends the full extent of the Red Sea, from the Strait of Bab al Mandab in the south to near the Sinai Peninsula in the north. This study aims to (1) partition the total particulate absorption coefficients in phytoplankton (a_{ph}) and non-algal particles (a_{NAP}) contributions using a numerical decomposition method (NDM) and investigate the spectral shape of the

particulate absorption properties to understand its optical variability in the Red Sea, (2) compare the a_{ph}^* obtained from total particulate absorption and the values estimated using the existing algorithms (Lee, 1994; Bricaud et al., 1998), and (3) propose a new parameterization for computing a_{ph}^* .

2. Materials and methods

2.1. TARA Data for the Red Sea

High quality in situ measurements are essential for the calibration and validation of satellite ocean color sensors. An underway system was equipped with a WETLabs ac-s hyperspectral spectrophotometer and Sea-Bird Electronics SBE45 MicroTSG unit was used to measure the hyperspectral particulate absorption coefficients ($a_p(\lambda)$) and particulate attenuation ($c_p(\lambda)$) coefficients during the R/V TARA Oceans expedition traversing the Red Sea during January 2010 (Boss et al., 2013; Werdell et al., 2013, Picheral et al., 2014). To obtain the particulate absorption data, the 0.2 μm filtered data were subtracted from the total absorption data ($a_p(\lambda) = a_t(\lambda) - a_{0.2\mu\text{m}}(\lambda)$) (Chase et al., 2013). Temperature, salinity and GPS location were simultaneously measured using the SBE45 TSG. The data were then averaged to one-minute temporal resolution. A full description of data measurement and processing can be found in Slade et al. (2010), Boss et al. (2013), Werdell et al. (2013), and Brewin et al. (2015). The data were obtained from the NASA SeaBASS web link (<http://seabass.gsfc.nasa.gov/seabasscgi/search.cgi>) where the spectral data is provided at ~ 4 nm intervals between 404 and 736 nm (Brewin et al., 2015). The in situ optical properties have been validated against ocean color estimates (Werdell et al., 2013). Fig. 1 shows the TARA Oceans expedition transect overlaid on the

Moderate Resolution Imaging Spectroradiometer (MODIS) true color (RGB) satellite image acquired over the Red Sea on 10 January 2010.

Fig. 1. Map of the study region showing the location of stations where optical measurements were made during the TARA Oceans expedition in January 2010. These measurements give valuable insights into the particulate absorption properties of the Red Sea.

2.2. Simulated data

The inherent and apparent optical properties were simulated for the Red Sea using the Hydrolight 5.1.4 radiative transfer model (Mobley and Sundman, 2008). Here the essential informations are briefly outlined, which is required to run the radiative transfer simulation. Four component bio-optical models and ancillary information on solar zenith angle, sky conditions, wind speed, and ocean bottom depth are incorporated as input to the Hydrolight radiative transfer model (Li et al., 2016). In this simulation, pure water absorption is taken from Pope and Fry (1997).

For every simulation, the solar zenith angle was set to at 30° with clear sky conditions. A constant wind speed was considered to 5 ms^{-1} , and the water body is assumed

homogeneous with an infinitely deep ocean. The inelastic processes (Chlorophyll a fluorescence, CDOM fluorescence, and Raman Scattering) were omitted in our simulation. Backscattering ratios for phytoplankton particles and non-algal particles are assumed to be 0.01 and 0.03 (Mobley & Stramski, 1997) respectively. The simulation of the radiative transfer is carried out for the ranges: $[\text{Chl}] = 0.01 \sim 1.0$ $[\text{mg m}^{-3}]$; $C_{\text{NAP}} = 0 \sim 0.1$ $[\text{g m}^{-3}]$; $a_{\text{CDOM}}(443) = 0 \sim 0.15$ $[\text{m}^{-1}]$; $S_{\text{CDOM}} = 0.01 \sim 0.02$ $[\text{nm}^{-1}]$; $S_{\text{NAP}} = 0.007 \sim 0.03$ $[\text{nm}^{-1}]$.

2.3. Estimation of chlorophyll a using line-height method (LHM)

The values of a_p are extracted at three wavelengths (i.e., 650, 676, and 715nm) to estimate the chlorophyll a in the Red Sea. The LHM uses the pigment absorption peak in the red band (i.e., 676 nm) of a_p spectra, which is considered to be little influenced by the colored dissolved organic matter (CDOM) and non-algal particles (NAP). Therefore, the LHM is a very effective method for an accurate estimation of chlorophyll a (Roesler & Barnard, 2013).

2.3.1. Computation of absorption line height

A linear equation presents the absorption value of a baseline at a reference wavelength at 676 nm between the 650 and 715 nm and, $y = mx + c$:

$$a_{BL}(\lambda_{ref}) = \frac{a_p(715) - a_p(650)}{715 - 650} \times (\lambda_{ref} - 650) + a_p(650) \quad (1)$$

where m is the slope and c is the intercept. To obtain the value of absorption line height at 676 nm, we subtracted the baseline absorption from the total particulate absorption at 676 nm:

$$a_{BL}(\lambda_{ref})(m^{-1}) = a_p(676) - a_{BL}(676) \quad (2)$$

The baseline value of absorption at 676 nm obtained from Eq. (1) is substituted in Eq. (2) to derive the a_{LH} at 676 nm. This approach serves not only to remove the measured null absorption value at wavelength > 715 nm (i.e., associated with a scattering offset in the absorption meter) but also eliminates the tail of absorption by pigments which are near to the peaks of chlorophyll b and some phycobilipigments absorption spectra (Roesler & Barnard, 2013). Nardelli and Twardowski (2016) conducted a thorough study using the data collected in a broad range of water types and suggested the $a^*_{LH} = 0.0108 \text{ [m}^2 \text{ (mg Chl a)}^{-1}\text{]}$. However, in this study the value of chlorophyll-specific absorption line height, $a^*_{LH} (\approx 0.0104 \text{ [m}^2 \text{ (mg Chl a)}^{-1}\text{]})$ is taken from Roesler and Barnard (2013) to derive the absorption based chlorophyll concentration as given below:

$$Chl_{LH} = \frac{a_{LH}(676)}{a^*_{LH}(676)} \quad (3)$$

It is essential to remove the contributions by pure water and colored detritus absorption to achieve accurate values of chlorophyll a in optically complex seawaters. The LHM is relatively insensitive to instrument drift, incident irradiance and non-photochemical quenching (Roesler & Barnard, 2013). Brewin et al. (2015) reported that the LHM has also been found to perform well when compared with discrete *in situ* HPLC chlorophyll a data and diverse phytoplankton cultures (Dall'olmo et al., 2009; Westberry et al., 2010; Dall'olmo et al., 2012; Chase et al., 2013; Boss et al., 2013; Roesler & Barnard, 2013).

2.4. Decomposition of total particulate absorption

The numerical decomposition method (NDM) developed by Bricaud & Stramski (1990) is based on the shape of the $a_p(\lambda)$ spectrum. The exponential function was used

to model the shape and magnitude of $a_{NAP}(\lambda)$ in the decomposition of $a_p(\lambda)$ spectra. The pairs of wavelengths were selected to formulate the expressions to estimate the NAP spectral slope and NAP at reference wavelength. The rationale for choosing the ratios (505/380 and 580/692 or λ_2/λ_1 and λ_3/λ_4) for which the absorption ratios by accessory pigments should be minimal (i.e., ratios must be free from influence of variations in pigment composition), and must be close to 1 (i.e., not affected by package effect). The ratio of phytoplankton absorption was computed at the two pairs of wavelengths ($r\phi_1$ and $r\phi_2$) from the in situ samples collected, on which the a_{ph} is estimated using a chemical bleaching method (Oubelkheir et al., 2007). The particulate absorption ratio at the two pairs of wavelengths, determined on a given sample, are supplied as inputs to a set of equations with two unknowns (Eq. 5 in Bricaud and Stramski 1990 and Eq. 3 in Oubelkheir et al., 2007) to extract S_{NAP} and $a_{NAP}(\lambda_o)$, the parameters required to describe $a_{NAP}(\lambda)$ and is written as:

$$r\phi_1 a_{NAP}(\lambda_o) e^{(-\lambda_1 * S_{NAP})} - a_{NAP}(\lambda_o) e^{(-\lambda_2 * S_{NAP})} = r\phi_1 a_p(\lambda_1) - a_p(\lambda_2) \quad (4a)$$

$$a_{NAP}(\lambda_o) e^{(-\lambda_3 * S_{NAP})} - r\phi_2 a_{NAP}(\lambda_o) e^{(-\lambda_4 * S_{NAP})} = a_p(\lambda_3) - r\phi_2 a_p(\lambda_4) \quad (4b)$$

Finally, the difference between the particulate and non-algal fractions ($a_{ph}(\lambda) = a_p(\lambda) - a_{NAP}(\lambda)$) given the values of phytoplankton absorption coefficient.

The NDM is thoroughly validated in a wide range of oligotrophic and mesotrophic waters, therefore, its considered to be a reliable method to partition the $a_p(\lambda)$ spectra (Wang et al., 2008). In the present study, we applied NDM (R-script) to the hyperspectral $a_p(\lambda)$ data to estimate the contributions of a_{ph} and a_{nap} . The a^*_{ph} can be derived by dividing the $a_{ph}(\lambda)$ by $[Chl]_{LH}$. The root mean square error computed on $a^*_{ph}(440)$ is 3-8% (Bricaud and Stramski 1990).

Fig. 2. Frequency distributions of the a) $a_{ph}(440)$, b) $a_{ph}(676)$, and c) Chl a in the Red Sea. Presented data are obtained from the numerical decomposition and line height methods applied on the TARA data.

Fig. 2 presents frequency distributions of the $a_{ph}(440)$, $a_{ph}(676)$, and Chl-a in the Red Sea. The histograms of $a_{ph}(440)$ peak near the 0.01 m^{-1} , $a_{ph}(676)$ peak near the 0.0025 m^{-1} , and Chl a near the 0.015 mg m^{-3} in the Red Sea.

2.5. Parameterization of chlorophyll-specific absorption

The phytoplankton absorption coefficient is directly proportional to the chlorophyll pigment concentration:

$$a_{ph}(\lambda) \propto \langle Chl \rangle \quad (5)$$

It is expressed as,

$$a_{ph}(\lambda) = a_{ph}^*(\lambda) \langle Chl \rangle \quad (6)$$

where $a_{ph}^*(\lambda)$ is the phytoplankton-specific absorption coefficient (that varies widely depending on light intensity, nutrient availability, and species composition).

A more robust relationship can be expressed based on the previous work of Bricaud et al. (1981, 1995, and 1998):

$$a_{ph}^*(\lambda) = A(\lambda) < Chl >^{-B(\lambda)} \quad (7)$$

where $A(\lambda)$ and $B(\lambda)$ are the spectral coefficients. The constants A and B give the a_{ph}^* per unit Chl a and deformations of a_{ph}^* spectrum with the increase in Chl a. The spectral coefficients are computed when Eq. (7) is applied to the a_{ph}^* and Chl a data (**Table 1**). The spectral constant $A(\lambda)$ derived in this study is very close to the Bricaud et al. (1995) study, a noticeable difference was observed in the blue region and a little deviation in the red part of the spectrum (Fig. 3). A shoulder was evident in the green region (510 and 560 nm), which is a typical feature of phycoerythrin (PE) pigment and cyanobacteria. The parameter B is high around 406-500 nm where the chlorophyll-specific absorption spectra exhibit shoulders between 470 and 490 nm due to the influence of various carotenoid accessory pigments. At minimum a_{ph}^* , the values of B become unstable in the region of 525-700 nm due to changes in the phytoplankton community structure in the Red Sea.

Fig. 3. Spectral constants $A(\lambda)$ and $B(\lambda)$ are derived using the power function fitted on the chlorophyll-specific absorption coefficient versus Chl_{LH} .

Table1: Spectral values of the numerical constants $A(\lambda)$ and $B(\lambda)$ obtained when power function fitting applied to the $a^*_{\text{ph}}(\lambda)$ versus Chl_{LH} in the Red Sea and the coefficient of determination (R^2) calculated from power regression.

λ (nm)	$A(\lambda)$	$B(\lambda)$	R^2	λ (nm)	$A(\lambda)$	$B(\lambda)$	R^2
400	0.0299	0.1545	0.0938	488	0.0258	0.2472	0.7272
402	0.0301	0.1609	0.1090	490	0.0253	0.2480	0.7237
404	0.0303	0.1670	0.1250	492	0.0246	0.2443	0.7207
406	0.0305	0.1727	0.1417	494	0.0239	0.2403	0.7074
408	0.0313	0.1811	0.1699	496	0.0231	0.2355	0.7028
410	0.0320	0.1916	0.2135	498	0.0223	0.2302	0.6902
412	0.0327	0.2029	0.2402	500	0.0215	0.2231	0.6763
414	0.0336	0.2039	0.2731	502	0.0206	0.2135	0.6579
416	0.0346	0.2018	0.2713	504	0.0197	0.2024	0.6317
418	0.0352	0.2061	0.3061	506	0.0189	0.1894	0.6030
420	0.0357	0.2130	0.3345	508	0.0181	0.1747	0.5558
422	0.0360	0.2241	0.3812	510	0.0174	0.1595	0.5131
424	0.0362	0.2379	0.4227	512	0.0168	0.1427	0.4547
426	0.0364	0.2497	0.4521	514	0.0163	0.1246	0.3799
428	0.0366	0.2584	0.5165	516	0.0158	0.1063	0.3080
430	0.0368	0.2668	0.5188	518	0.0153	0.0859	0.2160
432	0.0371	0.2731	0.5727	520	0.0148	0.0655	0.1326
434	0.0373	0.2791	0.5657	522	0.0145	0.0443	0.0618
436	0.0372	0.2836	0.6121	524	0.0141	0.0211	0.0133
438	0.0370	0.2881	0.6122	526	0.0138	-0.0017	0.0001
440	0.0363	0.2953	0.6640	528	0.0136	-0.0267	0.0179
442	0.0356	0.3026	0.6758	530	0.0133	-0.0456	0.0473
444	0.0352	0.3064	0.6908	532	0.0131	-0.0629	0.0800
446	0.0348	0.3089	0.7071	534	0.0129	-0.0820	0.1173
448	0.0344	0.3114	0.7123	536	0.0128	-0.1038	0.1623
450	0.0340	0.3139	0.7096	538	0.0126	-0.1270	0.2006
452	0.0327	0.3169	0.7279	540	0.0123	-0.1369	0.2167
454	0.0323	0.3154	0.7391	542	0.0120	-0.1459	0.2253
456	0.0320	0.3132	0.7383	544	0.0118	-0.1545	0.2364
458	0.0317	0.3086	0.7419	546	0.0115	-0.1634	0.2485
460	0.0313	0.3025	0.7420	548	0.0112	-0.1729	0.2556
462	0.0311	0.2952	0.7384	550	0.0107	-0.1694	0.2492
464	0.0309	0.2868	0.7363	552	0.0102	-0.1656	0.2367
466	0.0308	0.2781	0.7205	554	0.0097	-0.1643	0.2311
468	0.0303	0.2690	0.7262	556	0.0092	-0.1654	0.2303
470	0.0299	0.2595	0.7120	558	0.0087	-0.1656	0.2228
472	0.0296	0.2560	0.7216	560	0.0082	-0.1588	0.2106

474	0.0293	0.2524	0.7210	562	0.0077	-0.1514	0.1886
476	0.0289	0.2504	0.7223	564	0.0072	-0.1438	0.1720
478	0.0284	0.2501	0.7279	566	0.0068	-0.1357	0.1519
480	0.0279	0.2498	0.7242	568	0.0064	-0.1257	0.1272
482	0.0274	0.2483	0.7282	570	0.0060	-0.1131	0.1013
484	0.0269	0.2468	0.7248	572	0.0056	-0.0982	0.0718
486	0.0264	0.2464	0.7239	574	0.0053	-0.0783	0.0470
λ (nm)	A(λ)	B(λ)	R ²	λ (nm)	A(λ)	B(λ)	R ²
576	0.0050	-0.0566	0.0233	640	0.0052	-0.1343	0.1146
578	0.0049	-0.0519	0.0212	642	0.0053	-0.1348	0.1188
580	0.0047	-0.0481	0.0183	644	0.0054	-0.1322	0.1206
582	0.0045	-0.0341	0.0085	646	0.0056	-0.1267	0.1198
584	0.0044	-0.0182	0.0021	648	0.0058	-0.1210	0.1157
586	0.0043	-0.0118	0.0009	650	0.0061	-0.1105	0.1123
588	0.0042	-0.0065	0.0003	652	0.0064	-0.1012	0.1047
590	0.0041	-0.0060	0.0002	654	0.0070	-0.0935	0.1105
592	0.0040	-0.0063	0.0002	656	0.0076	-0.0872	0.1172
594	0.0040	-0.0072	0.0003	658	0.0083	-0.0770	0.1142
596	0.0039	-0.0083	0.0004	660	0.0091	-0.0644	0.1013
598	0.0038	-0.0103	0.0006	662	0.0099	-0.0532	0.0852
600	0.0038	-0.0124	0.0008	664	0.0112	-0.0392	0.0653
602	0.0038	-0.0102	0.0005	666	0.0133	-0.0280	0.0489
604	0.0038	-0.0089	0.0004	668	0.0139	-0.0272	0.0527
606	0.0038	-0.0098	0.0005	670	0.0144	-0.0273	0.0571
608	0.0038	-0.0108	0.0005	672	0.0145	-0.0283	0.0666
610	0.0038	-0.0105	0.0005	674	0.0144	-0.0300	0.0799
612	0.0039	-0.0102	0.0005	676	0.0140	-0.0322	0.0870
614	0.0039	-0.0167	0.0014	678	0.0133	-0.0352	0.0865
616	0.0040	-0.0230	0.0028	680	0.0125	-0.0384	0.0841
618	0.0041	-0.0328	0.0059	682	0.0115	-0.0418	0.0822
620	0.0042	-0.0458	0.0116	684	0.0105	-0.0454	0.0766
622	0.0043	-0.0523	0.0154	686	0.0092	-0.0472	0.0668
624	0.0044	-0.0587	0.0192	688	0.0079	-0.0504	0.0557
626	0.0044	-0.0692	0.0270	690	0.0067	-0.0580	0.0528
628	0.0045	-0.0819	0.0378	692	0.0055	-0.0689	0.0483
630	0.0046	-0.0944	0.0498	694	0.0045	-0.0832	0.0471
632	0.0047	-0.1064	0.0660	696	0.0036	-0.1042	0.0457
634	0.0048	-0.1178	0.0815	698	0.0029	-0.1334	0.0483
636	0.0049	-0.1260	0.0962	700	0.0023	-0.1750	0.0478
638	0.0051	-0.1339	0.1070				

3. Results

3.1. Variations in spectral particulate absorption spectra

This section presents and discusses spectral variations of the particulate absorption properties for the Red Sea. Fig. 4 shows hyperspectral spectra for the a_p , a_{ph} , and a_{NAP} in the north and south of Red Sea. Two distinct peaks can be seen for both a_p and a_{ph} spectra, with the primary peak around at the blue wavelength 443 nm and the secondary peak in the red region (i.e., 676 nm). Both peaks are representative of the absorption by chlorophyll a pigment.

The shape and magnitude of a_{ph} spectra are nearly identical to the a_p spectra. A high blue to red peak ratio ($a_{ph}(440):a_{ph}(675) = 1.91-7.25$) is characteristic of a phytoplankton community dominated by small celled organisms. The non-algal particles (i.e., $a_{NAP}(443)_{average} = 0.002524 \text{ m}^{-1}$) do not provide a significant contribution to the a_p spectra. Thus, our analyses confirm that phytoplankton absorption (i.e., $a_{ph}(443)_{average} = 0.01743 \text{ m}^{-1}$) is the primary contributor to the total particulate absorption (i.e., $a_p(443)_{average} = 0.01995 \text{ m}^{-1}$) in the Red Sea.

Fig. 4. The variability in hyperspectral spectra for the particulate absorption properties (a_p , a_{ph} , and a_{NAP}) in the north and south of Red Sea. These data are from the in situ TARA measurements and decomposed for the Red Sea.

3.2. Validation of NDM with simulated data

The simulated a_{ph} and a_{NAP} are used to validate NDM in the Red Sea. Statistical matrices such as Root Mean Square Error (RMSE), Mean Relative Error (MRE), and the linear regression analysis are used to quantify the performance of the NDM. Fig. 5 shows comparisons of a_{ph} and a_{NAP} values derived from the decomposition method against the simulated data. We found a good correlation between the derived and simulated dataset of a_{ph} and a_{nap} , with low root mean square error (RMSE = 0 ~ 0.004 for a_{ph} and RMSE = 0 ~ 0.004 for a_{nap}), mean relative errors (MRE = -0.019 ~ 0.085 for a_{ph} and MRE = -0.006 ~ 0.162 for a_{nap}), and a regression slope close to unity. Outliers are seen in the a_{nap} scatter plots, where a_{nap} does not show good matchups with the simulated a_{nap} . Overall, the validation of decomposition method with simulated data is found excellent for the selected visible wavebands.

3.3. Chlorophyll-specific phytoplankton absorption coefficient

The $a_{ph}^*(\lambda)$ spectra showed high variability in the blue part of the spectrum as compared to the red part of spectrum indicative of the small cell size phytoplankton (Ciotti et al., 2002; Devred et al., 2006). The high values of $a_{ph}^*(\lambda)$ are mostly found in the Northern Red Sea (NRS), dominated by the diverse phytoplankton community (Kheireddine et al., 2017) with low chlorophyll concentrations. On the other hand, the low values of $a_{ph}^*(\lambda)$ perceived in the Southern Red Sea (SRS), where chlorophyll concentrations are comparatively higher than the NRS.

Fig. 5. Comparisons between the NDM-derived (a_{ph} and a_{NAP}) and simulated (a_{ph} and a_{NAP}) values for the selected wavelengths (i.e., 443, 490, 555, and 676 nm). The simulated data is close to the Red Sea environment and covers the optical variability of the Red Sea.

The $a_{ph}^*(\lambda)$ decrease from NRS (oligotrophic) to SRS (mesotrophic), spanning over more than one order of magnitude (0.12 to 0.01 [m^2 (mg Chl a) $^{-1}$]) at the blue absorption maximum. The mean a_{ph}^* (Fig. 6, solid black color line) shows that a_{ph}^* varied from 0.038 to 0.052 [m^2 (mg Chl a) $^{-1}$] at the blue (i.e., 443 nm) waveband.

Fig. 6. Spectral variability of chlorophyll-specific phytoplankton absorption coefficient ($a_{ph}^*(\lambda)$) and mean ($a_{ph}^*(\lambda)$) in the Red Sea. The $a_{ph}^*(\lambda)$ spectra is derived by normalizing the phytoplankton absorption by chlorophyll a.

3.4. Relationship between phytoplankton absorption coefficient and chlorophyll a

Fig. 7 shows the relationships for the a_{ph} at selected wavebands (i.e., 443 , 490 , 555 , and 676 nm) with Chl a, which can be well described by a power-law function:

$$a_{ph}(443) = 0.037 \times <Chl_{LH}>^{0.75}; R^2 = 0.94 \quad (8)$$

$$a_{ph}(490) = 0.026 \times <Chl_{LH}>^{0.78}; R^2 = 0.96 \quad (9)$$

$$a_{ph}(555) = 0.0083 \times <Chl_{LH}>^{0.998}; R^2 = 0.92 \quad (10)$$

$$a_{ph}(676) = 0.014 \times <Chl_{LH}>^{1.019}; R^2 = 0.996 \quad (11)$$

The variations of $a_{ph}(443)$ and Chl a relationship suggest that a_{ph} does not include much contribution by absorbing detrital matter (Bricaud et al., 1995). The power formula found between the $a_{ph}(443)$ and Chl a also held at other wavelengths (i.e., 490 , 555 , and 676 nm).

Fig. 7. The relationship between Chl_{LH} and a_{ph} for the selected wavelengths (443, 490, 555, and 676 nm). Presented data are obtained from the numerical decomposition and line height methods applied on the hyperspectral in situ TARA data collected in the Red Sea.

Fig. 8 shows the inverse relationship between $a^*_{ph}(440)$ and chlorophyll a and expressed as the power law function:

$$a^*_{ph}(443) = 0.036 \times <Chl_{LH}>^{-0.303}; R^2 = 0.68 \quad (12)$$

The similar relationship with different constants was reported in global waters (e.g., Bricaud and Stramski, 1990, Bricaud et al., 1995, 1998).

The high values of $a^*_{ph}(443)$ found in the NRS for low concentration of chlorophyll ($0.01 < Chl a < 0.1$) and low values of $a^*_{ph}(443)$ observed in the SRS for high chlorophyll concentration ($0.1 < Chl a < 1.6 \text{ mg m}^{-3}$). This kind of trend is caused by an increasing package effect from low to high chlorophyll concentrations (Morel & Bricaud, 1981) and inverse co-variation between the relative abundance of accessory

pigments (Chl b, Chl c, and carotenoids) and Chl a level (Bricaud et al., 1995). The R^2 is relatively weak because of the NDM uncertainty associated with the decomposed data.

Fig. 8. The scatter plot showing the relationship between the Chl_{LH} and $a_{ph}^*(443)$ in the Red Sea. The relationship presented here derived from TARA data collected in the Red Sea.

3.5. Comparison between the NDM- a_{ph}^* and derived a_{ph}^*

Bricaud et al. (1998) have established a global relationship for a_{ph}^* using a large data collected in a wide range of oligotrophic oceanic waters. In this study, Lee (1994) and Bricaud et al. (1998) a_{ph}^* relationships at 443 nm were tested in the Red Sea and compared against the NDM- $a_{ph}^*(443)$ (Fig. 9). It is clear from the scatter plot that the values of $a_{ph}^*(443)$ obtained from Bricaud et al. (1998) are overestimated compared with the values of NDM- $a_{ph}^*(443)$ while the $a_{ph}^*(443)$ values of Lee (1994) are overestimated for low values of NDM- $a_{ph}^*(443)$ and underestimated at high values of NDM- $a_{ph}^*(443)$. The coefficient of determination, $R^2 = 0.67$, is almost same for both the algorithms. It is worth noting that the Red Sea is an oligotrophic clear water body with low concentrations of chlorophyll and unique regional environmental conditions (e.g., Brewin et al., 2015). We note that both algorithms, Bricaud et al. (1998) and

Lee (1994), are designed for global open ocean waters. The Bricaud et al. (1998) algorithm is based on a large data set which covers a wide range of global oceanic water types while Lee's (1994) model is constructed with a limited data set that may not have used the sufficient data from clear ocean waters. It could be possible reason of the deviations in the models against the observations.

Fig. 9. Comparison of Bricaud et al. (1998) and Lee (1994) derived chlorophyll-specific absorption values at 443 nm with NDM specific absorption values in the Red Sea.

3.6. Latitudinal variations in CHL_{LH} with respect to Water temperature $[T]$, Salinity $[S]$, and chlorophyll-specific absorption coefficient $[a^*_{ph}(443)]$

Latitudinal gradients (from 12°N to 28°N) of sea surface temperature, surface salinity, chlorophyll a, and $a^*_{ph}(443)$ were observed. Surface salinity increased from south to north along the Red Sea axis during January 2010 while the surface temperature rose to a mid-basin maximum then declined to minimum values in the north (Fig 10a). During the winter, the Red Sea characterized by a standard two-layer exchange flow through the Strait of Bab al Mandab, (Siedler, 1968, Morcos, 1970, Sofianos 2001) when there is a surface inflow of fresher Gulf of Aden Surface Water (GASW) and

an underlying (Sofianos & Johns, 2002, 2003). Fig. 10a shows the complexity of the thermohaline characteristics in the upper layer of Red Sea. During the horizontal advection to the north, the thermohaline characteristics of GASW are modified due to mixing, heating, and evaporation as it advects northward along the basin.

Fig. 10. Latitudinal distributions (from 12°N to 28°N) of the surface temperature, surface salinity, chlorophyll a, and $a_{ph}^*(443)$ in the Red Sea. a) Variations in chlorophyll a with respect to surface temperature and surface salinity, b) latitudinal variations in chlorophyll a with $a_{ph}^*(443)$ shown in color, c) latitudinal variations in salinity with chlorophyll concentration indicated by symbol color and d) latitudinal variations in potential temperature (Theta) with chlorophyll concentration indicated by color.

The surface salinity shows a nearly linear increase from south (12°N) to north (28°N) of the Red Sea (Fig. 10b). The maximum salinity coincides with minimum chlorophyll and high a_{ph}^* in the northern Red Sea (Fig. 10c). The wind forcing likely affects the range of northward transport of GASW (Bower & Farrar, 2015). The highest chlorophyll concentrations are found in the southern half of the Red Sea while the highest a_{ph}^* occur the northern Red Sea (above 22°N) that is considered to be the most oligotrophic portion of the sea (Raitsos et al., 2013).

The high values of a_{ph}^* in the northern Red Sea are indicative of small cell phytoplankton communities with high a_{ph}^* while larger phytoplankton having lower $a_{ph}^*(443)$ occur in the south, likely advected in from the Gulf of Aden. The variation in cell size and pigment composition with changing temperature and light intensity can lead to variation in a_{ph}^* . Different types of phytoplankton species, which exhibit a wide range of cell sizes and accessory pigments and are in association with other phytoplankton communities, together could affect the magnitude and spectral shape of the a_{ph}^* (Zhang et al., 2012). Kheirredine et al. (2017) have described along-basin variations in phytoplankton size and community composition based on pigment composition during the late winter and early spring. The distributions show diatoms at either end of the basin and dominance of nanoplankton in the Central and North Central Red Sea. The surface temperature is more complicated within the basin, and less warm water observed in the south of the Red Sea that gradually gains heating towards the northward. The peak of surface temperature reaches to 28.5 °C at 20 °N due to a strong evaporation that occurred in the southern Red Sea. On the other hand, the temperature dropped to 24 °C at 26.2 °N due to the wintertime cooling in the northern Red Sea (Fig. 10d).

The MODIS-Aqua satellite remote sensing data (L1A, calibrated spectral radiance, 1.1x1.1 km resolution) acquired over the Red Sea on 10 Jan 2010, to understand the distribution patterns of the different types of the phytoplankton (Fig. 11). For brevity, Hirata et al. (2008) algorithm inbuilt within the NASA SeaDAS (the ocean color data processing software) was used to process the satellite data to gain the further insights on the phytoplankton biomass. The processed data showed the consistent pattern of the distinct phytoplankton features in the Red Sea.

Fig. 11. MODIS-Aqua satellite remote sensing image acquired on 10 January 2010 over the Red Sea, showing distribution patterns of the different types of phytoplankton in the Red Sea. The satellite images were processed using NASA SeaDAS ocean color data processing software.

3.7. Non-algal particle absorption coefficient

Fig. 12 shows the examples of the exponential model fitted on the NDM derived $a_{NAP}(\lambda)$ spectra. The spectral slope of NAP absorption spectrum (S_{NAP}) is estimated by fitting an exponential function to the data over the 400-650 nm wavelength range with an average slope (S_{NAP}) of 0.017 nm^{-1} . The average value of S_{NAP} in the Red Sea altered from the value of S_{NAP} in the clear open oceans (Bricaud et al., 1998).

From the least square analysis, $a_{NAP}(\lambda)$ can be expressed as:

$$a_{NAP}(\lambda) = a_{NAP}(412)e^{(-0.017(\lambda-412))} \quad (13)$$

where $a_{\text{NAP}}(\lambda)$ and $\lambda_r = 412\text{nm}$ are the NAP absorption coefficient at the desired wavelength and a reference wavelength respectively.

Fig. 12. Examples of the NDM derived NAP absorption spectra (dotted black color lines) and the corresponding exponential fits (solid red color lines) for the Red Sea.

Fig. 13 shows the scatterplot of S_{NAP} as a function of $a_{\text{NAP}}(412)$. There is no clear inverse relationship found between them, it can be seen from the scatter points that a larger variability in S_{NAP} at smaller values of $a_{\text{NAP}}(412)$ and lower variability at higher values. S_{NAP} is greater during January 2010. Hence, it suggests the predominance of inorganic particles in the Red Sea.

Fig. 13. Scatterplot of S_{NAP} as a function of $a_{\text{NAP}}(412)$ in the Red Sea.

4. Discussion and conclusion

In this paper, we have examined the hyperspectral particulate absorption spectra in the Red Sea. The TARA data presented in this study show latitudinal variability in the particulate absorption properties and is illustrative of local, regional and winter conditions. This research has made a valuable contribution to study the optical characterization of particulate absorption properties in the Red Sea. Thus, the results of our study can be used as a good approximation for examining the relationship between the a_{ph} and Chl *a*.

Until now, information on particulate absorption properties and its variations in the Red Sea has been lacking. In the present study, NDM was used to decompose the total particulate absorption spectra into the contributions by phytoplankton and non-algal particles. To confirm the validity of NDM, the method was validated with the independently simulated data, and statistical matrices were computed. The validation results are excellent with low RMSE, MRE, and a slope close to unity. The statistical analyses of the derived and simulated data have shown errors are somewhat high for the decomposed values of a_{nap} . Overall, the performance of NDM is excellent with acceptable uncertainty in the Red Sea. Further analysis of the hyperspectral decomposed data revealed that phytoplankton light absorption contributed a significant portion to the total particulate absorption spectra. The decomposed spectra shown in Fig. 5 clearly show that the contribution of phytoplankton absorption to the total particulate absorption is much higher than the non-algal particles.

The a^*_{ph} varies from one water body to another due to changes in the phytoplankton composition. In the blue spectral region, Bricaud et al. (1995) determined that $a^*_{ph}(443)$ varies from 0.01 to 0.18 [$m^2 (mg\ Chl\ a)^{-1}$] for the open ocean, while Staehr et al. (2004) extended this range to 0.015-0.19 [$m^2 (mg\ Chl\ a)^{-1}$] for estuarine and

coastal waters. The red portion of the $a_{ph}^*(\lambda)$ spectrum is less affected by changes in phytoplankton composition or pigment composition than the blue region of the spectrum.

The a_{ph}^* values at 443 nm from the present study ranged from 0.01 to 0.12 [m^2 (mg Chl a) $^{-1}$]. High values of a_{ph}^* in the northern Red Sea is an indicate significance of small phytoplankton in this region. The small size phytoplankton is consistent with our understanding of the northern Red Sea which is considered to be oligotrophic (Raitsos et al., 2013). Phytoplankton composition may change in response to changes in salinity, temperature, and nutrient supply, phenology (timing of major events in the annual cycle of phytoplankton dynamics) and their total abundance. Understanding the effects of cell size, intercellular pigment concentration, and composition could contribute to our understanding of the variations of $a_{ph}^*(\lambda)$ in the Red Sea.

The NAP absorption spectra showed an exponential decay towards the longer (red) wavelengths. Additionally, the relationship between the S_{NAP} and $a_{NAP}(412)$ showed more substantial variability in S_{NAP} at lower values of $a_{NAP}(412)$ and lower variability in S_{NAP} at higher values of $a_{NAP}(412)$. Therefore, the average spectral slope ($S_{NAP} = 0.017 \text{ nm}^{-1}$) value derived for the Red Sea is higher than the global average spectral slope ($S_{NAP, average} = 0.0123 \text{ nm}^{-1}$; (Babin et al., 2003)). It should be noted that Chl_{LH} , a_{ph} , a_{ph}^* , and a_{NAP} are derived parameters using two different methods (i.e., NDM and LHM) and both methods are subject to uncertainties (Brewin et al., 2015). However, accuracies for both methods were still within acceptable limits.

In conclusion, this is first attempt to understand particulate absorption properties from a unique hyperspectral dataset collected in the Red Sea providing real insight into the optical variability of the absorption coefficients. The NDM and LHM were applied to

the hyperspectral data to study the particulate absorption properties in the Red Sea. Further, the presented validation between the derived and simulated phytoplankton and NAP absorption coefficients have proven the method applicability with excellent correlation coefficient, low statistical errors (RMSEs and MREs), and a slope close to unity for the selected wavelengths. Our results showed that the contribution of NAP absorption to total particulate absorption is less than phytoplankton absorption in the Red Sea. High values of a^*_{ph} occurred in the northern Red Sea, where picophytoplankton communities are understood to dominate much of the year. Picophytoplankton communities are consistent with our understanding of the Red Sea where small cyanobacteria (e.g., *Prochlorococcus* and *Synechococcus*) are thought to dominate productivity, as their small size contributes to efficient uptake at deficient nutrient concentrations (Pearman et al., 2017). The variability of a^*_{ph} in the northern Red Sea is consistent with distinct phytoplankton spatial features obtained from the satellite remote sensing data. The results of this study improve our knowledge regarding characteristics of particulate absorption properties and will contribute to determine the variability in phytoplankton and NAP absorption coefficients in the Red Sea.

Future research should address the seasonal variability of the a^*_{ph} in the Red Sea and the impacts of this variability on estimates of remote sensing reflectance spectra.

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