New parameterization to Inversion model to derive optical properties for global waters

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Abstract

The optical constituents like chlorophyll-a (Chl-a), coloured dissolved organic matter (ag) and particulate matter play significant role in presence of light field within the water bodies. The apparent optical perturbations take place in the varying inherent optical properties of the medium. The present study elaborates the importance of parameterizations for bio-optical algorithms in order to isolate the detritus absorption coefficient (ad) unlike the integrated response of absorption coefficient due to coloured dissolved organic matter and detritus/degraded matter at 443nm. Here attempt has been made to meet the two major limitations, ie, choosing the right parameterizations for the model and also for isolating detritus absorption coefficient from remote sensing reflectance. Detritus absorption coefficient (ad) at 443nm was derived from remote sensing reflectance (Rrs) with a mean absolute percentage difference (MAPD) of 40% and coloured dissolved organic matter(ag) at 443nm with MAPD of 30% using NASA Bio-optical marine algorithm (NOMAD) dataset for global waters.

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Key Points:

- Isolation of detritus absorption coefficient(a_d)(1/m) from marine optics.
- Simultaneous retrievals of bio optical constituents were carried out using new parameterization to the inversion model.
- Inversion model is adopted for its further implementation on Sentinel-3A OLCI data of Arabian Sea (Date: Oct 06,2018).

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Abstract
The optical constituents like chlorophyll-a (Chl-a), coloured dissolved organic matter (a_g) and particulate matter play significant role in presence of light field within the water bodies. The apparent optical perturbations take place in the varying inherent optical properties of the medium. The present study elaborates the importance of parameterizations for bio-optical algorithms in order to isolate the detritus absorption coefficient (a_d) unlike the integrated response of absorption coefficient due to coloured dissolved organic matter and detritus/degraded matter at 443nm. Here attempt has been made to meet the two major limitations, ie, choosing the right parameterizations for the model and also for isolating detritus absorption coefficient from remote sensing reflectance. Detritus absorption coefficient (a_d) at 443nm was derived from remote sensing reflectance (Rrs) with a mean absolute percentage difference (MAPD) of 40% and coloured dissolved organic matter(a_g) at 443nm with MAPD of 30% using NASA Bio-optical marine algorithm (NOMAD) dataset for global waters.

Plain Language Summary

The present study focuses on not only global challenging problem of retrieval of bio optical constituents in optically complex waters in coastal region but also on the new parameterization to the inversion model, dealing with the modulation of light field with optical constituents within the oceanic waters. Since the apparent optical properties of the oceanic medium depend on bio optical constituents as well. Here, bio optical characterization was carried out in terms of simultaneous retrieval of chlorophyll-a (mg/m^3), coloured dissolved organic matter(CDOM) absorption coefficient (1/m), detritus absorption coefficient(1/m) and back scattering coefficient for global waters using NASA bio optical marine algorithm datasets (NOMAD). It is inferred from the results that the suitable parameterization to the inversion model may lead to the simultaneous retrieval of the bio-optical constituents with better accuracy. In addition, the current parameterization to the inversion model leads to the isolation of the detritus absorption coefficient(a_d) at 443nm too from the combined absorption coefficient i.e. CDOM (a_g) and detritus (a_d) at 443nm during retrieval process unlike the global bio optical model. These adaptations of the parameterization to the inversion model may change the retrieval process significantly over traditional one.

1 Introduction

Life in the aquatic ecosystems are dependent on components such as phytoplankton, detritus and CDOM (Colored Dissolved Organic Matter)(Sarthyendranath, 2000). Phytoplankton absorbs visible radiation for converting inorganic carbon into organic carbon via photosynthesis, whereas CDOM & detritus strongly absorbs ultraviolet (UV) radiation providing protection to living organism (Sarthyendranath, 2000). Therefore, an improved estimation of dissolved and suspended matter (including detritus) in the coastal and open ocean waters will help in understanding the light limitation on the growth of phytoplankton. This will also improve our knowledge on the amount of terrestrial materials flowing from rivers to the coastal environment.

The legacy of ocean colour sensors started with Coastal Zone Colour Scanner (CZCS) in 1978, that laid the foundation for subsequent ocean colour satellites to address the scientific problem for biological oceanography. This provided a great opportunity to use the space borne measurements in both spatial and temporal domain for retrieving bio-optical parameters. Later on, number of its successors like SeaWiFS, MODIS, VIIRS, OCM-1, OCM-2 etc. came into reality with a common objective of retrieving the optical parameters for different water types with the desired uncertainty. Gordon (1990) introduced first empiricism for deriving chl-a based on the radiance ratio of two channels - blue and green bands with an uncertainty of ±20%. O Reilly et al.(1998,2000) formulated the two well-known algorithms OC2 and OC4 for SeaWiFS to estimate chl-a. In addition, semi analytical bio optical model was adopted for the simultaneous estimation of bio optical constituents like chlorophyll-a concentration, back scattering coefficient due to particulate matter and the combined response of CDOM (a_g) and detritus absorption coefficient (a_d). Its performance till today has been remarkable with suitable parameterizations for both case-1 and case-2 waters. The semi analytical model has been carried further for bio optical characterization using nonlinear optimization e.g. Levenburg-Marquardt local optimization which is quasi sensitive to the initial guess. The algorithm assumes constant parameterizations of CDOM absorption slope 'S', back-scattering power exponent η and Chl-a specific absorption coefficient a^*_{ph} obtained using global optimization i.e. simulated annealing (Maritorena et al., 2002).

The relationship between apparent optical properties and inherent optical properties was established by Gordon et al (1988) with the model being insensitive to polarization. Later, Lee et al (2004) adopted the concept given by Morel and Loisel (1998), and suggested that the response collected just below the water surface is the resultant of two nonlinear terms i.e. the upwelling light field scattered through molecular scattering and upwelling light field scattered through particulate matter. Further, the model developed by Gupta et al (2020) suggested suitable parameterizations for Lee et al, (2004) model that helps in retrieving chl-a, back scattering coefficient at 443nm and absorption due to colored dissolved organic matter at 443nm instead of combined response of absorption due to colored dissolved organic matter and absorption due to detritus at 443nm. Semi- analytical models are associated with certain limitations, firstly choosing the right parameterizations for the model, secondly model being insensitive to the polarization of light field and lastly, the isolation of detritus absorption coefficient from remote sensing reflectance. The study presented here focuses on two limitations, i.e., for choosing right parameterizations for the model and also for the isolation of detritus absorption coefficient from remote sensing reflectance, which has been discussed in detail in the following sections.

2 In-situ data Used

The global in-situ dataset i.e. NOMAD (NASA Bio optical marine algorithm dataset) was used in this study(Werdell & Bailey, 2005). Parameters that were used from NOMAD, includes water leaving radiance just above the surface (Lw(0^+, λ)) and down welling irradiance at the water surface (Ed(0^+, λ)), Chl-a concentration, CDOM absorption coefficient and detritus absorption coefficient in Coastal waters. Remote sensing reflectance was derived through the ratio of water leaving radiance just above the surface (Lw(0^+, λ)) and down welling irradiance at the water surface (Ed(0^+, λ)).

3 Bio optical Models

The semi analytical bio optical models as Garver, Siegel and Maritorena (GSM) model, LeeMorel-Bricaud (LMB) model and New parameterized bio optical model are explained in the following sections.

3.1 GSM Model

GSM model is named after the three scientists as Garver, Siegel and Maritorena with their novel contribution to semi analytical bio optical model in 2002. The model adaptation is based on the assumption of scattering in forward direction. The light field exiting the water column, emanates in variable colours and shapes due to absorption and single scattering at large angles. This assumption has led to the development of a number of analytical models. The fundamental base of all semi analytical models

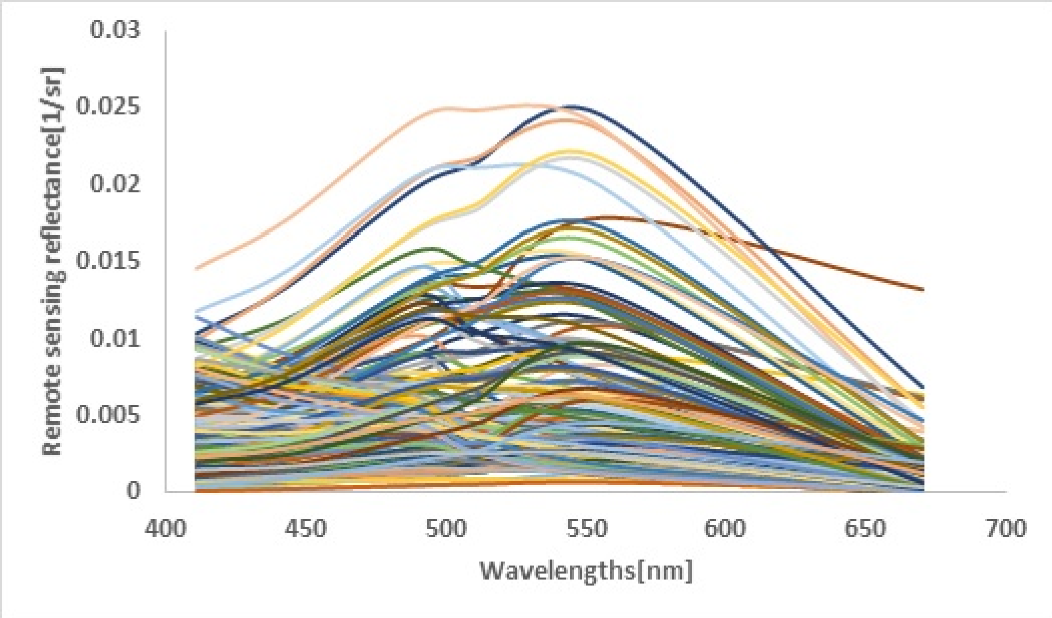

Figure 1. Remote sensing reflectance(1/sr) at different geographic location dealing with mostly all types of coastal waters
(Werdell & Bailey, 2005)

is the color and shape of the upwelling light which is the resultant of absorption and scattering of downwelling light via modulation with optical constituents in the water column. The apparent optical properties 'AOPs' depend on inherent optical properties of the media and distribution of light field therein i.e. light absorption coefficient due to sea water, absorption due to coloured dissolved organic matter and detritus, absorption due to phytoplankton, back scattering due to sea water and due to particulate matter (Morel & Prieur, 1977; Gordon et al., 1988) as well. The model equations as follow:

The cost function is mean square difference (msd) between modelled remote sensing reflectance $Rrs(\lambda_i, \theta, \phi)$ and in-situ $Rrs(\lambda_i)$ data to be optimized.

$$Rrs(\lambda) = \frac{t^2}{n_w^2} \sum_{i=1}^{2} g_i \left(\frac{b_b(\lambda)}{b_b(\lambda) + a(\lambda)} \right)^i \tag{1}$$

where $Rrs(\lambda_i, \theta, \phi)$, is modelled remote sensing reflectance, having a function of $\theta = [a_{cdm}(\lambda_0), Chl, (b_{bp}(\lambda_0)]$ i.e. absorption due to coloured dissolved organic matter (CDOM) and detritus in integrated mode(CDM), chlorophyll-a and back scattering coefficient at reference wavelength λ_0 respectively and $\phi = [S, \eta, a^*_{ph}(\lambda_0)...a^*_{ph}(\lambda_N)]$ i.e. CDM slope(S), power exponent and spectral chl-a specific absorption coefficient respectively. In addition, t is the sea–air transmission factor, n_ω is the index of refraction of the water, $b_b(\lambda)$ is the total back scattering coefficient and $a(\lambda)$ is total absorption coefficient.

$$a_{ph}(\lambda) = Chl * a^*_{ph}(\lambda) \tag{2}$$

where $a^*_{ph}(\lambda)$ is chl-a specific absorption coefficient and $a_{ph}(\lambda)$ is the phytoplankton absorption.

$$a_{cdm}(\lambda) = a_{cdm}(\lambda_0) * exp[-S(\lambda - \lambda_0)] \quad (3)$$

Where $a_{cdm}(\lambda_0)$ absorption due to coloured dissolved organic matter (CDOM) and detritus in integrated mode(CDM) at reference wavelength λ_0.

$$b_{bp}(\lambda) = b_{bp}(\lambda_0) * \left(\frac{\lambda}{\lambda_0}\right)^{\eta} \quad (4)$$

Where $b_{bp}(\lambda_0)$ is the back scattering coefficient of particulate matter at reference wavelength (λ_0).

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda) \quad (5)$$

Where $b_b(\lambda)$ is the total back scattering coefficient and $b_{bw}(\lambda)$ is the back scattering coefficient of sea water.

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{cdm}(\lambda) \quad (6)$$

Where $a_w(\lambda)$ is the absorption coefficient of pure sea water.

$$costfunction = \sum_{i=1}^{N}(Rrs(\lambda_i, \theta, \phi) - Rrs(\lambda_i))^2 \quad (7)$$

Where $Rrs(\lambda_i)$ is the in-situ water leaving radiance measurements and $Rrs(\lambda_i, \theta, \phi)$ is modelled remote sensing reflectance. The equation (7) is for the cost function with number of wavelengths $N(\lambda)$.

3.2 Lee-Morel-Bricaud model

(Lee et al., 2004) explained very clearly for the effect of phase function due to molecular and particulate scattering (Morel & Loisel, 1998). The equation is as such

$$rrs(\lambda) = C1(\frac{b_w(\lambda)}{b_b(\lambda) + a(\lambda)}) + C2(\frac{b_b p(\lambda)}{b_b(\lambda) + a(\lambda)}) \quad (8)$$

$$C1 = 0.113 \quad (9)$$

$$C2 = 0.197[1 - 0.636 * exp(-2.552(\frac{b_p(\lambda)}{b(\lambda) + a(\lambda)}))] \quad (10)$$

Lee et al. (2002) established a relation between remote sensing reflectance 'rrs' just below the water surface to remote sensing reflectance 'Rrs' in equation (11). Since rrs(λ), the function of IOPs was illustrated in equation (8)(Morel & Loisel, 1998; Mobley et al., 2002; Lee et al., 2004). The cdom + detritus slope w.r.t. optical bands relationship was developed using global datasets(Lee et al., 2009) expressed in equation (13).

$$rrs(\lambda) = \frac{Rrs(\lambda)}{0.52 + 1.7 * Rrs(\lambda)} \quad (11)$$

$$\eta = 2.2 * (1.0 - 1.2 * exp(-0.9 * (\frac{rrs(440)}{rrs(555)}))) \quad (12)$$

$$S = 0.015 + \frac{0.002}{0.6 + \frac{rrs(440)}{rrs(555)}} \quad (13)$$

Gupta et al, (2020) made some changes in parameterizations for the inversion model of Lee et al (2004) for optically complex waters such as:

1. Replacement of slope of cdom + detritus (Lee et al., 2009) with the relation between Slope of CDOM Absorption and CDOM Absorption at 443nm based on global dataset with ≤50 m depth, basically coastal waters.

$$S_g = 0.0099 * a_g^{-0.226} \tag{14}$$

2. Use of Chl-a specific absorption coefficient (Bricaud et al., 1995) in inversion model (Lee et al., 2004).

$$a_{ph}(\lambda) = A(\lambda) * Chl^{-B(\lambda)} \tag{15}$$

where A & B are spectral constants.

3.3 New parameterized model

Lee et al. (2004) was updated again with further addition of new parameterizations mostly applicable to all kinds of coastal waters. A few changes in parameterizations to inversion model (Lee et al., 2004) are as such:

Replacement of slope of CDOM(a_g)+detritus(a_d) (Lee et al., 2009) with mean Slope of CDOM(a_g)+detritus(a_d) Absorption based on global dataset. The integrated slope of cdom and detritus for global waters was observed with a linear trend of 0.016±0.0025. The observation is based on NASA Bio optical marine algorithm (NOMAD) dataset (Werdell & Bailey, 2005). The requisite number of data points (321) were filtered from 4459 data pool of global points depending upon the availability of optical bands i.e. 411, 443, 489, 510, 555, 670 nm and most importantly reducing the unnecessary data redundancies. The Figure (2) illustrates the distribution of CDOM(a_g)+detritus(a_d) slope with respect to different geographic locations, converges to 0.016±0.0025. So this change in parameterization was implemented for simultaneous estimations of bio optical constituents using rrs just below the water column.

Implementation of global relation between integrated response of CDOM and detritus (a_d+a_g) at 443nm and detritus at 443nm in inversion model (Lee et al., 2004). Since the global models fail in the simultaneous retrievals of the sub components of the IOPs like detritus absorption coefficients because of similar spectral signature with the cdom absorption coefficients. So to overcome this limitation, the global data points were pooled altogether to come up with a concrete decision to make sense. As a consequence, it is an additional change to parameterizations to the model.

Use of Chl-a specific absorption coefficient (Bricaud et al., 1995) in inversion model (Lee et al., 2004).

The fundamental conceptualization adopted, was given by Lee et al. (2004) which integrates the angular distribution of light field within the water column either from molecular or particle scattering.The retrieval of all the optical constituents using the semi-analytical models elucidate the cost function minimization between apparent optical properties and IOPs using Levenberg-Marquardt (LM) technique in a least square sense.

4 Results and Discussions

The performance of the global models was illustrated in Table1 for deriving absorption coefficients due to coloured dissolved organic matter, detritus and their integrated response at 443nm. The limitation of the Lee-Morel-Bricaud model and GSM model is to derive the integrated response of CDOM and detritus only with 33% and 30% uncertainty respectively. However, the above limitation was partially

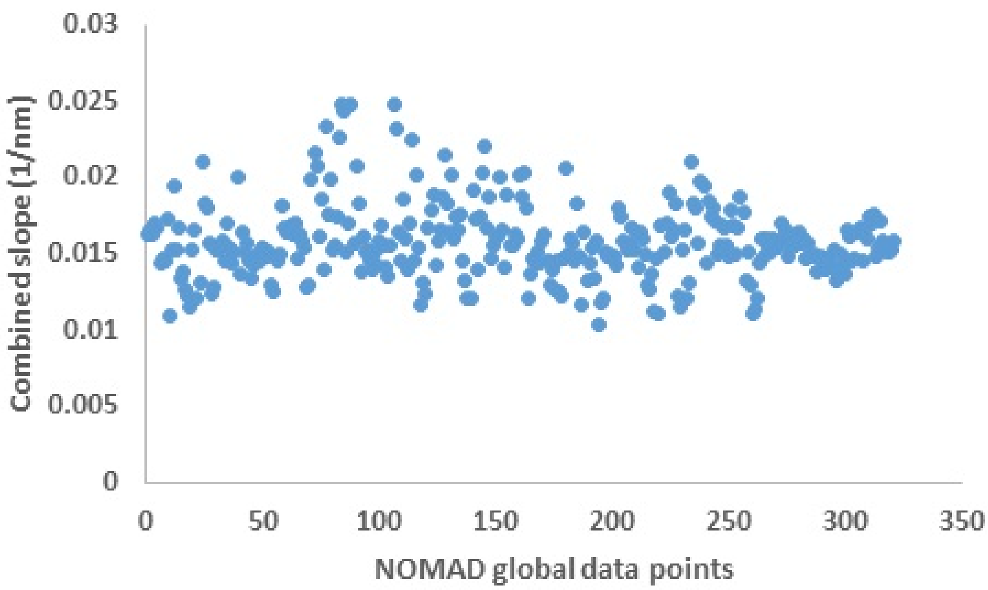

Figure 2. The integrated slope response of the CDOM and detritus distribution in Global scenario

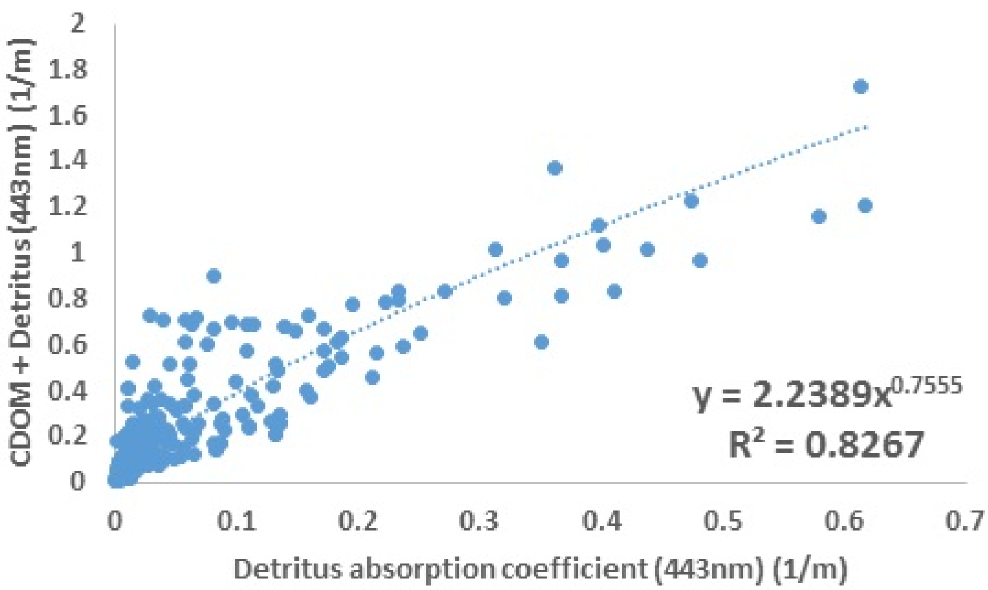

Figure 3. A relationship between the integrated response of the CDOM and detritus i.e. CDOM+detritus and detritus for Global dataset

solved using (Gupta et al., 2020) i.e. the model is capable to derive the absorption coefficient due to coloured dissolved organic matter at 443nm with 36% uncertainty in optically complex waters. While the new parameterized model is able to address the above described limitations of deriving absorption coefficients due to coloured dissolved

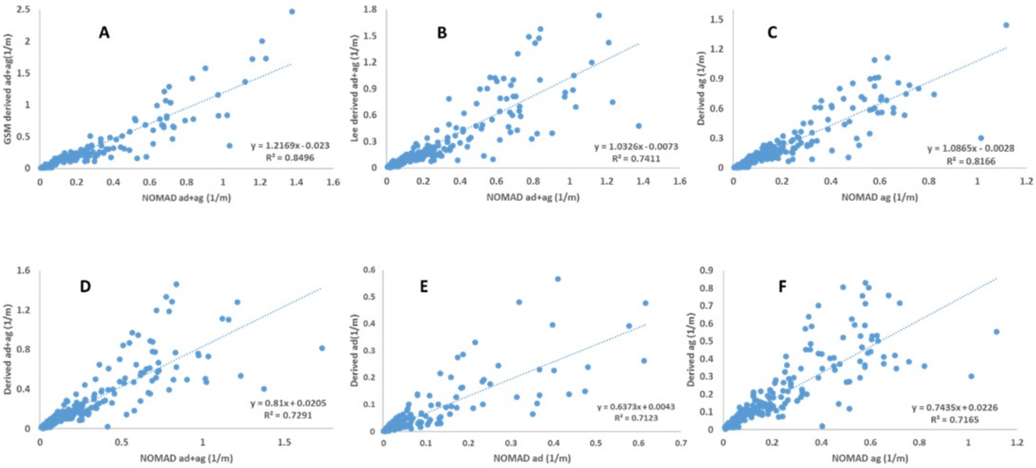

Figure 4. A) GSM derived (a_d+a_g) at 443 nm versus NOMAD (a_d+a_g) at 443nm, B) Lee derived (ad+ag) at 443 nm versus NOMAD (a_d+a_g) at 443nm, C) Gupta et al, 2020 derived ag at 443 nm versus NOMAD ag at 443nm, D), E) and F) new parameterized based model derived a_d, a_g and (a_d+a_g) at 443 nm versus NOMAD a_d, a_g and (a_d+a_g) at 443nm respectively.

organic matter, detritus and their integrated response at 443nm with 30%, 40% and 29% uncertainties respectively.

In addition to that, Statistics of the performance of the global models for deriving CDOM (a_g), detritus (a_d) absorption coefficients and their integrated response at 443nm, have been illustrated in Table 2. The important point here is to note that the mean values of NASA bio optical marine algorithm datasets [NOMAD] for absorption due to CDOM, detritus and their integrated response are 0.18 (1/m), 0.06 (1/m) and 0.24 (1/m) respectively. LMB and GSM derived integrated responses are 0.21 (1/m) as compared to NOMAD i.e. 0.24 (1/m) while New model derived response is very close to NOMAD i.e. 0.23 (1/m). Further, new model derived individual response i.e. absorption due to CDOM and detritus 0.17 (1/m) and 0.06 (1/m) respectively are very close to the mean values of NOMAD.Similarly, Gupta et al (2020) also works very well for CDOM showing close proximity to NOMAD mean CDOM at 443nm.

From the outputs of validation shown in Figure (4), it could be concluded that integrated response a_d+a_g at 443nm is slightly underestimated with respect to NOMAD in-situ data while other two models like GSM and Lee-Morel-Bricaud are overestimated with respect to NOMAD in-situ data. Also, Gupta et al (2020) derived only cdom (a_g) at 443nm with slope tending to unity and R-square and RMSE, 0.82 and 0.10, respectively. Whereas, the new parameterized model derived cdom and detritus at 443nm, are much underestimated with respect to NOMAD ag and ad at 443nm while their integrated response at 443nm is slightly better than their individual ones. The approach adopted in the current model for the isolation of detritus absorption from remote sensing reflectance is novel and can be used globally.

5 Implementation on Satellite data

An attempt was made to implement the newly parameterized algorithm on Sentinel-3A OLCI data of Arabian Sea (Date: Oct 06,2018) to capture the spatial variability of bio-optical parameters. The top of the atmosphere radiance was downloaded from Copernicus ESA website. Then data was processed using ESA toolbox

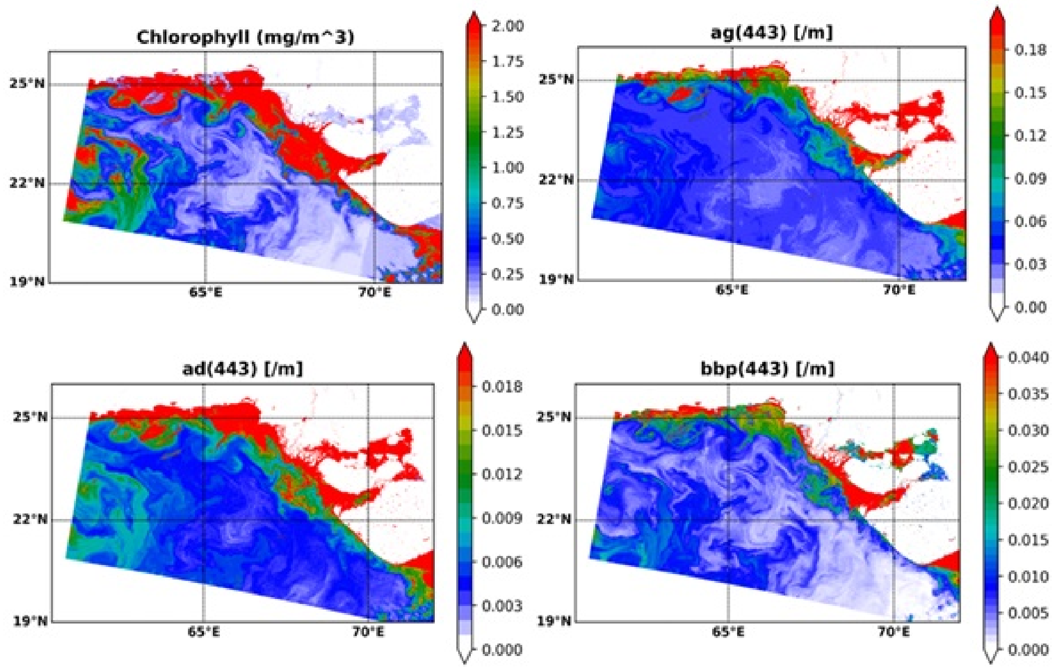

Figure 5. Clock wise figure shows the spacial distribution of chl-a (mg/m^3) in Arabian sea followed by absorption due to coloured dissolved organic matter(1/m) at 443nm then back scattering coefficient (1/m) at 443nm and detritus absorption coefficient (1/m) at 443nm near coastal boundaries of India and in Arabian sea.

Table 1. Performance of the global models for deriving CDOM (a_g) and detritus (a_d) absorption coefficients at 443 nm with their uncertainties

Models	Detritus(a_d) at 443 nm(%)	CDOM at 443nm((%))	(a_d + a_g) (%)
Lee-Morel-Bricaud (LMB)	N/A	N/A	33%
GSM	N/A	N/A	30
Gupta et al. 2020	N/A	36%	N/A
New	40%	30%	29%

named as SNAP to get remote sensing reflectance (rrs). Algorithm was applied on remote sensing reflectance (rrs) to derive further bio-optical constituents as well. The maps of chl-a, ag(443), ad(443) and bbp(443) thus derived, are shown in Figure(5).

Table 2. Statistics of the performance of the global models for deriving CDOM (a_g), detritus (a_d) absorption coefficients and their integrated response at 443nm

Models	R-Square	RMSE	Slope	Intercept	Mean (a_d, a_g, $a_d + a_g$)
LMB [$a_d + a_g$]	0.74	0.16	1.03	-0.007	0.21
GSM [$a_d + a_g$]	0.84	0.14	1.22	-0.023	0.21
Gupta et al. 2020 [a_g]	0.82	0.1	1.09	-0.003	0.17
New[a_d, a_g, $a_d + a_g$]	0.71,0.72,0.7	0.07,0.11,0.16	0.64,0.74,0.82	0.004,0.023,0.028	0.06,0.17,0.23

6 Conclusions

The present study attempted to bring about improvement in the parameterization of Lee at al (2004) inversion model using the global NOMAD in-situ dataset. The parameterization to inversion model successfully estimated detritus and CDOM absorption coefficients with uncertainty of 40% and 30%, respectively. Also, the integrated response of CDOM and detritus after parameterization, had a lesser uncertainty of 29% as compared to GSM and Lee-Morel-Bricaud (LMB) model whose uncertainties were 30% and 33%, respectively. Similar results can be obtained globally by introducing a new parameterization to inversion model for deriving detritus absorption. This might be quite significant in deriving the sub components of inherent optical properties (IOPs) within the acceptable uncertainty.

Acknowledgments

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Data Availability Statement

Sentinel-3A OLCI data was downloaded from website "https://scihub.copernicus.eu/dhus/#/home" and ESA Science Toolbox Exploitation Platform (SNAP) was downloaded from website "https://step.esa.int/main/download/snap-download/".

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