SAC/EPSA/AOSG/BOD

Algorithm Theoretical Basis Document

Inherent optical properties derived using Ocean colour monitor onboard EOS-06

S. No.	Product Name	Spatial Resolution (m)	Temporal Resolution
1	IOP_YYYYMMDD_D.nc	360X360	Alternate day

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1. Algorithm Configuration Information

1.1 Algorithm Name

Analytical bio-optical model (ABOM).

1.2 Algorithm Identifier

IOP_YYYYMMDD_D.nc

1.3 Algorithm Specification

Version	Date	Prepared by	Description
1.0.0	03/08/2024	Anurag Gupta, Debojyoti Ganguly, Syed Moosa Ali and K.N. Babu	Derivation of Inherent optical properties like chl-a, phytoplankton absorption coefficient at 443nm, back scattering coefficient, CDOM and detritus absorption coefficients at 443nm in optically complex waters

2.1 Introduction

ALGORITHMS for the retrieval of chlorophyll-a (chl-a) from ocean color sensors have evolved to a great extent over past few decades. Simplest form of the algorithm is based on empirical regression, in which chl-a concentration is correlated with the reflectance ratio at blue and green wavelength bands (O' Reilly et al., 1998 & 2000). Empirical-based methods have been used operationally to generate global chl-a products from satellites such as Coastal Zone Color Scanner (CZCS), SeaViewing Wide Field-of-View Sensor (SeaWifs), Moderate Resolution Imaging Spetroradiometer (MODIS), Visible Infrared Imaging Radiometer Suite (VIIRS), and so on. Constant improvement has been made in such algorithms to increase their accuracy even in low chlorophyll oligotrophic waters [3]. Although reliable and easy to implement, retrieval from these global algorithms may not be accurate in all parts of the ocean. Empirical algorithms for chl-a retrieval work on the assumption that the remote-sensing reflectance (Rrs) is mainly influenced by phytoplankton and its degraded products. However, this assumption does not hold for Case-2 waters where the optically active constituents do not covary (Dierssen 2010). Due to overlapping nature of absorption spectra of various independently varying constituents, relative change in reflectance value at blue and green bands cannot be linked directly to chl-a and therefore, results in the failure of empirical methods. Also, during phytoplankton blooms of a particular species, the empirical based method fails to accurately retrieve chla. This is because most empirical relationships are derived from Case-1 waters constituting a large number of other phytoplankton species.

Another set of algorithms are based on semi analytical (SA) inversions of optical closure relationship derived from radiative-transfer theory (Gordon et al., 1988; Carder et al., 1999; Maritorenna et al., 2002; Lee et al., 2004). The model relates Rrs spectra to the inherent optical properties (IOPs) of a water column. The IOPs include (A) total absorption coefficient, which is the sum of absorption by seawater (aw), phytoplankton (aph), colored dissolved organic matter (CDOM) + detritus (acdm); and (B) total backscattering coefficient, which includes backscattering by seawater (bbw) and suspended particles (bbp). Proper inversion of such model allows accurate retrieval of bio-optical parameters including chl-a concentration and various IOPs.

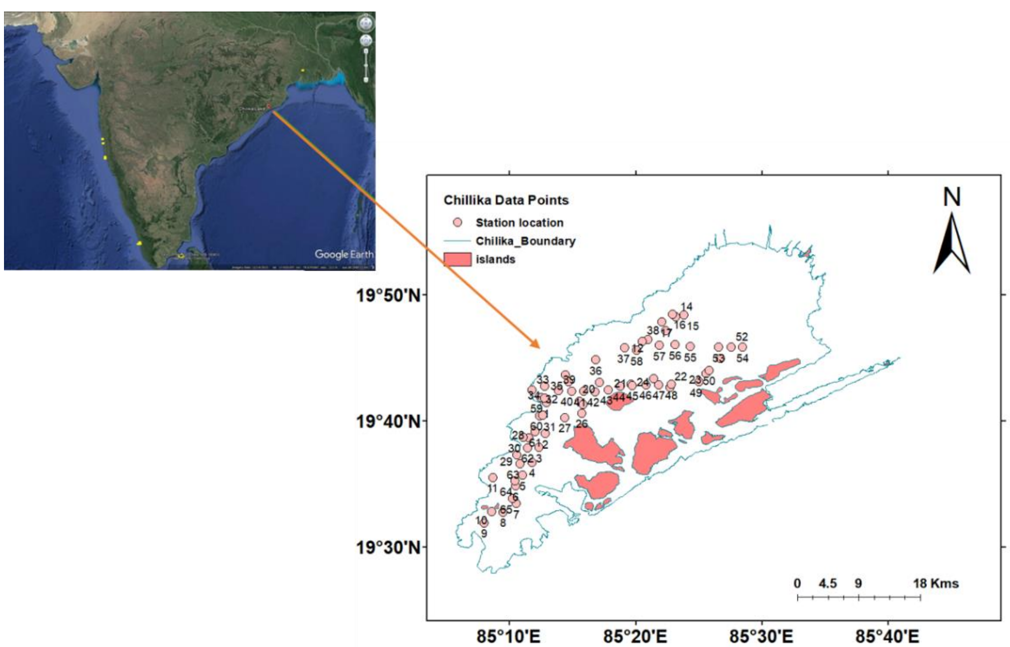


Fig. 1. Map of Chilika with station locations (The numbers indicate station locations where repeated observations were taken in years 2014 and 2015, N = 64 points).

Advantage here is that several parameters can be retrieved simultaneously. To mathematically solve SA equation, spectral models for the three IOPs (i.e., aph(λ), $a_{cdm}(\lambda)$, and $b_{bp}(\lambda)$) must be known. To define spectral absorption of CDOM+detritus (CDM), exponential decay function is used which depends on spectral slope “S” whereas, particle backscattering is defined in terms of a power-law function of wavelength that depends on exponent “η.” On the other hand, phytoplankton absorption is spectrally defined in terms of its specific absorption coefficient, which may vary based on community structure and pigment composition. Therefore, complete formulation of a SA algorithm requires certain model parameters to be hardcoded. However, these parameters show a nonlinear behavior and vary on a global scale. Accuracy of the algorithm, therefore, depends on the accuracy with which parameters such as specific absorption coefficient of phytoplankton ($a^*ph(\lambda)$), spectral slope “S” and exponent “η” are defined. If the model parameters are accurate, SA algorithm performs well even in Case-2 waters, where optically active constituents modify the light field independently.

To use the model for any set of wavelengths, major difficulty arises in parametrization of $a^*ph(\lambda)$ (Maritorena et al., 2002). Many researchers have expressed $a^*ph(\lambda)$ as a representative spectrum for doing the inversion„ whereas the coefficient is widely known for its variability. A general representation of $a*$ ph(λ) should account for its variations due to community structure shifts, pigment composition, package effect, and irradiance level (Bricaud et al., 1995; Fujiki et al., 2002). Therefore, there is a need to fine-tune the existing SA algorithms in order to account for the variations in specific absorption coefficient, which would allow the retrieval of bio-optical parameters (e.g., Chl-a) simultaneously in both Case-1 and Case-2 waters. One of the important parameters that affects the retrieval of bio-optical constituents, in optically complex waters, is the slope S of $a_{cdm}(\lambda)$. Meler et al. 2016 explained the distribution of the CDM slope (S) as a function of $a_{cdm}(440)$. It is was shown to be nonlinearly related to CDM absorption coefficient (Meler et al. 2016; Kowalczuk et al., 2006) and governs the spectral shape of $a_{cdm}(\lambda)$. The CDM-absorption affects the attenuation of light in ultraviolet (UV) and blue wavelengths thereby shielding the aquatic life from harmful UV radiation (Wei et al., 2016). In this study, we propose a SA approach with improved CDOM slope estimate for calculating bio-optical parameters with good accuracy in optically complex waters.

3. Datasets

3.1 NASA Bio-optical marine algorithm datasets (NOMAD)

The relationship between CDOM slope “S” (1/nm) and CDOM absorption coefficient ag at 443 nm was established based on the combined data set of NOMAD and Indian coastal data as shown in Fig-3 & 4.

3.2 Validation data set

Chilika Lagoon is a good site to study optically complex waters. Chilika lagoon on the east coast of India ($19^0 28'$ N – $19^0 54'$ N; $85^0 06'$ E−$85^0 35'$ E) is one of the important wetlands in the country and is the largest brackish water lagoon in Asia. In the northern side of the lagoon, tributaries of the Mahanadi River such as Daya, Nuna, and Bhargavi bring a lot of sediment and freshwater influx with terrestrial inputs into the lagoon.

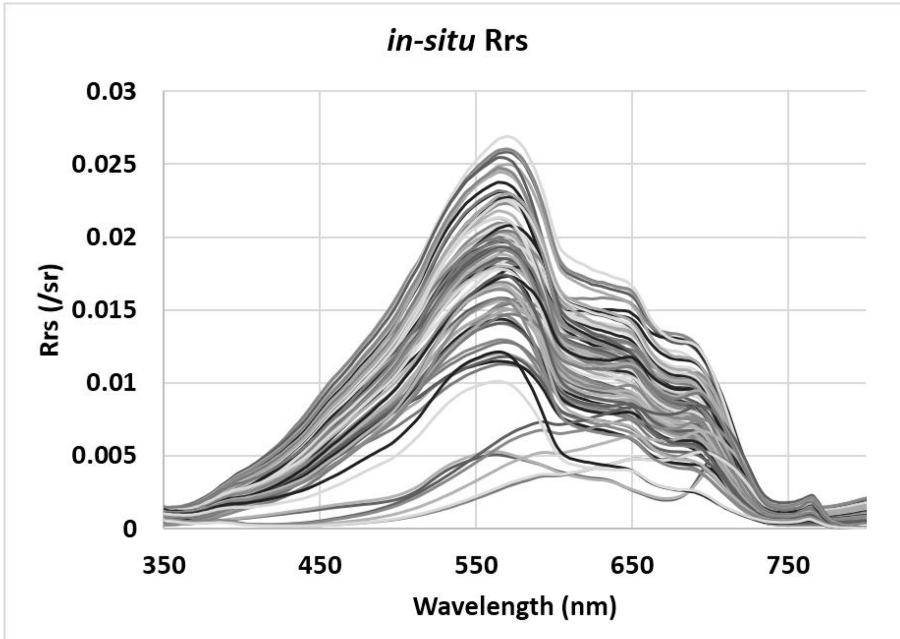


Fig. 2. Remote-sensing reflectance spectra (Rrs(λ)) measured during field data collection.

A mouth open in the northern side of the Fig. 2. Remote-sensing reflectance spectra (Rrs(λ)) measured during field data collection. Lake exchanges seawater with Lagoon making it optically complex system. Fig. 1 shows the map of study area with station locations used for collecting in situ data. Corresponding reflectance spectra is shown in Fig. 2.

4. Background and Methodology

4.1 Bio-Optical Inversion Model

Gordon developed the first simplified analytical model in 1973 for ocean color applications. The model was based on the assumption that most of the scattering takes place in forward direction, and the color and shape of the upwelling light field are the consequences of absorption and single scattering at large angles (Gordon and Evans, 1993). Based on this assumption number of analytical models have been developed. The Rrs in water column is the function of total absorption coefficient and backscattering coefficients (Gordon et al., 1988; Morel 1988; Morel and Prieur 1977). The SA ocean color models by Gordon et al. 1988, Maritorena et al. 2002, and Garver and Siegel 1997 are described below through the following equations:

$$Rrs(\lambda, \theta, \psi) = \frac{t^2}{n_\omega^2} \sum_{i=1}^{2} g_i \left(\frac{b_b(\lambda)}{b_b(\lambda)+a(\lambda)}\right)^i \quad (1)$$

$$a(\lambda) = a_\omega(\lambda) + a_{ph}(\lambda) + a_{cdm}(\lambda) \quad (2)$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda) \quad (3)$$

$$a_{ph}(\lambda) = Chl\ a_{ph}^*(\lambda) \quad (4)$$

$$a_{cdm}(\lambda) = a_{cdm}(\lambda_0)\exp(-S(\lambda - \lambda_0)) \quad (5)$$

$$b_{bp}(\lambda) = b_{bp}(\lambda_0)\left[\frac{\lambda_0}{\lambda}\right]^\eta \quad (6)$$

4.2 Solving the Model

The above set of equations show that the Rrs is a function of six unknowns S, η, $a^*ph(\lambda)$, chl, $a_{CDM}(\lambda_0)$, and $b_{bp}(\lambda_0)$. The vector θ = [chl, $a_{cdm}(\lambda)$, $b_{bp}(\lambda)$] represents variables to be retrieved, whereas ϕ = [$a^*ph(\lambda_1)..a^*ph(\lambda_N)$, S, η] is the vector of modeled parameters. Maritorena et al. 2002 solved the bio-optical model [known as Garver–Seigel–Maritorena (GSM) algorithm] by minimizing the cost function described in (7). The model parameter vector (ϕ) was optimized from global data set using simulated annealing technique. The value of vector ϕ in the GSM algorithm is kept constant throughout the scene which may create a strong bias while solving for the unknown vector (θ), especially in optically complex waters. Likewise, Lee et al. [18] proposed quasi-analytical algorithm (QAA) for deriving IOPs from Rrs in which he used empirical relations for estimating the parameters S and η [see (8) and (9). Limitation of QAA algorithm is with the parameterization of CDM slope S [see (8)]. The equation for S makes sense as it exploits the Rrs explicitly, but is not sufficient to deal with all kinds of waters, thus affecting the retrieval outcome. In case of optically complex waters, S takes much lower value for waters with high CDOM absorption at 443 nm. In addition, the presence of other constituents may change the slope value significantly

$$cost = \frac{1}{(N_\lambda - 1)} \sum_{i=1}^{N_\lambda} [Rrs(\lambda_i, \theta, \psi) - Rrs(\lambda_i)]^2 \quad (7)$$

$$S = 0.015 + \frac{0.002}{0.6 + \frac{\mathrm{rrs}(443)}{\mathrm{rrs}(555)}} \quad (8)$$

$$\eta = 2.2 * (1.0 - 1.2 * \exp(-0.9 * (r_{rs}[440] / r_{rs}[555]))) \quad (9)$$

where rrs is the remote sensing reflectance just below the water surface and is related to Rrs by the following equation:

$$\mathrm{rrs}(\lambda) = \frac{\mathrm{Rrs}(\lambda)}{0.52+1.7*\mathrm{Rrs}(\lambda)} \tag{10}$$

Both GSM and QAA uses SA model described in (1), with the two coefficient g1 and g2 fixed for nadir viewing geometry. Many ocean color sensors are looking at the ocean away from nadir to avoid sunglint making Rrs to be anisotropic in nature, having an angular distribution (Lee et al., 2004). Therefore, an inversion of satellite-derived reflectance with good accuracy using (1), specially for coastal waters, have always been a challenging task.

4.3 ABOM/ABOM2 Model Description

The basic formalism of QAA (quasi-analytical model) by Lee et al. 2004 has been adopted in analytical bio optical model (ABOM) model which accounts for the cumulative response of angular distribution of light field and multiple scattering within the water column (due to molecular or particle scattering) on the Rrs. The semi-ABOM, similar to GSM, solves the closure relationship between Rrs and IOPs using Levenberg–Marquardt technique in a least square sense. Remote-sensing reflectance (Rrs), as mentioned earlier, is the function of two vectors θ and ϕ. The unknown vector θ = [chl, acdm(λ), bbp(λ)] is simultaneously derived after modification in known vector ϕ = [a∗ ph(λ1)..a∗ ph(λN), S, η] parameterization. Set of equations used in ABOM model is summarized in equation 11 to 15. We have assumed that the absorption due to CDOM dominates over detritus absorption. We also corrected for the CDOM slope bias by introducing empirically derived expression for S (Fig. 3), details are presented in Section II-D. We also accounted for the variability in a∗ph using its dependence on chlorophyll (Bricaud et al., 1995). This whole formulation led to a significant improvement in the retrieval outcome.

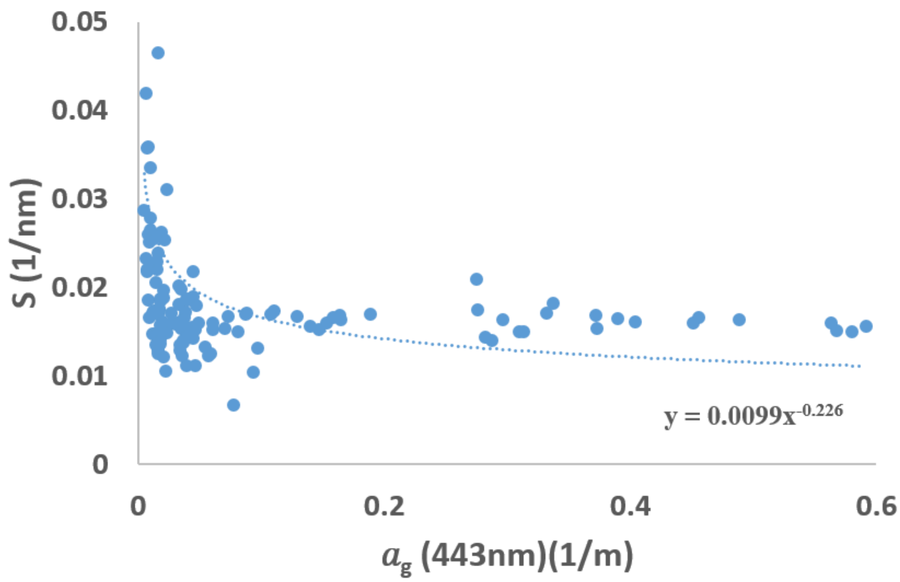


Fig. 3. Relation between CDOM slope "S" (1/nm) and CDOM absorption coefficient ag at 443 nm was established based on the combined data set of NOMAD and Indian coastal data.

rrs(λ) = C1 [$b_w(\lambda)$/ (a+b_b)] + C2 [$b_{bp}(\lambda)$/ (a+b_b)]

C1=0.l13

C2 = 0.197 [1 - 0.636 * exp(-2.552 ($b_{bp}(\lambda)$ / (a+b_b)))] (11)

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_g(\lambda) \quad (12)$$

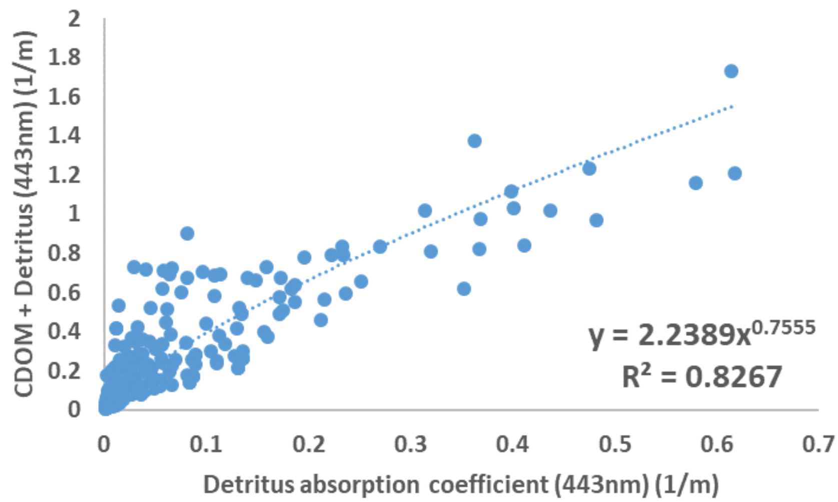
$$a_g(\lambda) = a_g(\lambda_0)\exp(-S(\lambda - \lambda_0)) \quad (13)$$

$$S_g = 0.0099a_g^{-0.226} \quad (14)$$

$$a^*_{ph}(\lambda) = A(\lambda)chl^{-B(\lambda)} \quad (15)$$

In ABOM, if a few changes in parameterizations are carried out then the same becomes ABOM2 as

A relationship between the integrated response of the coloured dissolved organic matter(CDOM) and detritus i.e. a_g+a_d and a_d for global dataset was carried out as shown in the following plot:



$$a_g+a_d = 2.2389a_d^{0.7555} \quad (16)$$

The integrated slope of cdom and detritus for global waters was observed as 0.016±0.0025. [23]

$$S = 0.016 \quad (17)$$

4.3.1 Model for the Slope of CDOM Absorption

The empirical relation for CDOM slope was estimated using the extensively calibrated and enhanced in situ bio-optical NOMAD (NASA Bio-optical Marine algorithm data version 2.0 ALPHA) data set. Based on bathymetric information, all optical data corresponding to locations falling within 50-m depth zone, classically defined as case-2 waters, were extracted from NOMAD. The data points from NOMAD were filtered on the basis of finite values of available optical parameters like water leaving radiance (L_w), surface solar irradiance (Es) etc., with ag available at minimum five wavelengths. Two channels for ag are sufficient to estimate CDOM slope S using [20, eq. (13)]; however, more optical bands were added to make the filtration process robust in order to reduce the data redundancy while retaining its variability. Bio-optical data corresponding to Indian coastal waters collected under various in situ campaigns were also merged with NOMAD and the combined data set with 161 measurements were utilized for model development. Fig. 4 shows the approximate locations of these data points. Slope of CDOM (S) was found to be highly variable ranging from 0.007 to 0.05 nm^{-1} for the values of reference absorption ag (443) ranging from 0.015 to 0.6 m^{-1}. To account for this variability, a power fit was performed as shown in equation (14).

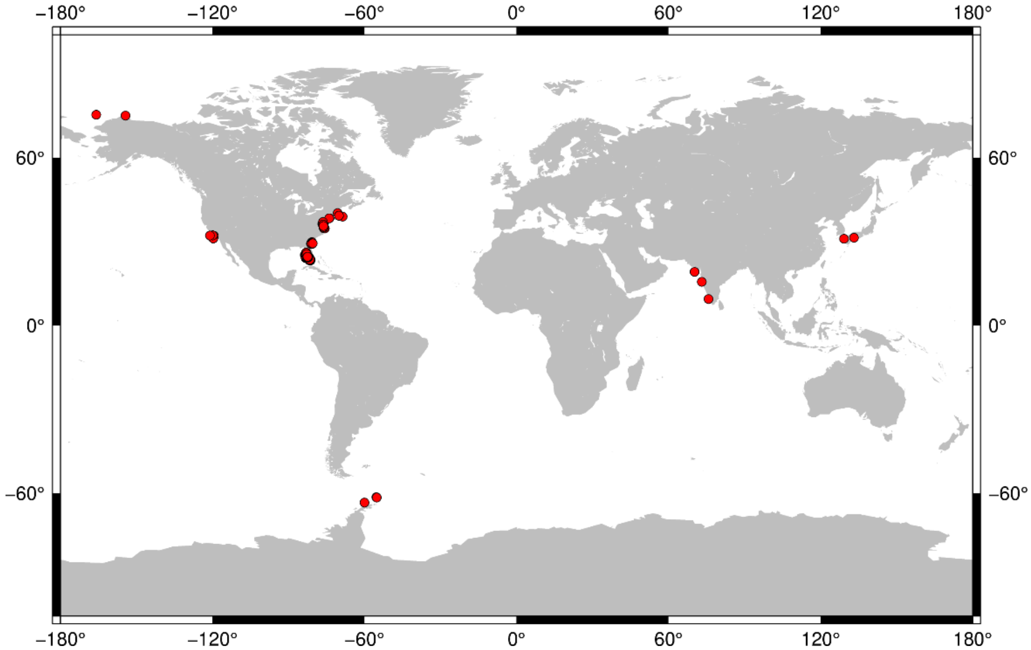


Fig. 4. Set of data points taken from NOMAD and Indian coastal waters.

4.4 Discussion and Validation on ABOM

Water samples from 64 stations were collected during 2014 and 2015 in Chilika lagoon (sampling locations shown in Fig. 1) and in situ chl-a were estimated using spectrophotometer. Comparison of chlorophyll–a concentration derived using Lee–Morel [8], [21], GSM [7], and ABOM model (this letter) in optically complex waters of Chilika Lagoon (see Fig. 5) indicate significant differences among the SA models when compared with in situ measurements. The mean absolute percentage difference (MAPD) of pooled data set for Lee–Morel and GSM was above 150% while ABOM showed significant improvement in reducing the MAPD to 58%. From Table I, it is clear that mean chl-a (10.2 mg/m^3) for ABOM model is very close to mean in situ chl-a (11.05 mg/m^3) unlike to Lee–Morel (27.7 mg/m^3) and GSM (33.1 mg/m^3). In addition to that, a significant improvement in the ABOM model in terms of relative bias (6.92%) was observed over Lee–Morel (188.2%) and GSM (167.8%). Slope S of CDM (colored dissolved and detrital matter combined) used in Lee–Morel is determined dynamically based on an empirical relationship with blue–green ratio.

Table-I Validation statistics

Bio-optical model	**Relative bias(%)**	**Bias at log scale**	**RMSE at log scale**	**Mean chl-a(mg/m^3)**	**Mean insitu chl-a**	**MAPD(%)**

Lee-Morel	188.2	0.38	0.45	27.7	11.05(mg/m^3)	189
GSM	167.8	0.27	0.42	33.1		175
ABOM	6.92	-0.1	0.4	10.2		58

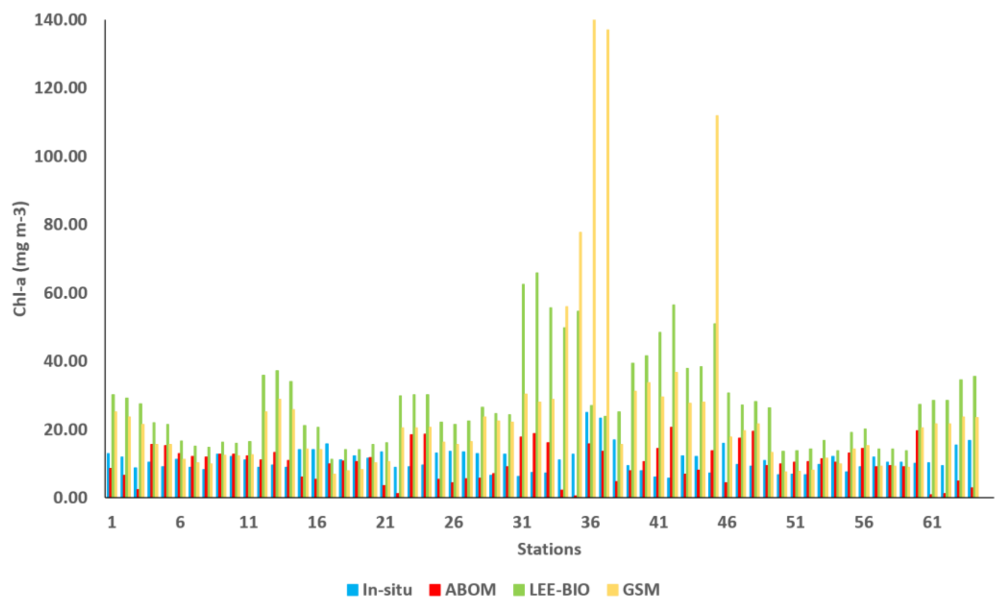


Fig. 5. Validation of chl-a derived from ABOM (this study), GSM and Lee–Morel models with in situ data set.

However, the parametrization causes the slope to be always greater than 0.015 (1/nm). In optically complex waters, the contribution of CDOM and detrital matter to absorption in blue wavelengths is significant and independent. Higher absorption in reference wavelength due to CDOM significantly decreases the slope value (less than 0.01, this study). Therefore, Lee–Morel does not accurately estimate chlorophyll concentration when CDOM is high. In GSM model, the slope value of CDOM absorption is kept constant and high (0.02 nm^{-1}) which also creates a strong bias resulting in overestimation of chlorophyll concentration. The ABOM model accounts for the low magnitude in slope values for higher CDOM absorption in optically complex waters. Although the power function for CDOM slope is able to explain only 24%–25% variability in the data set, incorporation of this equation in ABOM is able to significantly reduce the uncertainty in the estimation of chlorophyll concentration when combined with the model for phytoplankton specific absorption [9]. The model can be further improved by incorporating the contribution by detrital absorption at reference wavelength.

4.5 Discussion and Validation on ABOM2

The performance of the global models was illustrated in Table 2 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 solved using [22] 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 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 (ag), detritus (ad) absorption coefficients and their integrated response at 443nm, have been illustrated in Table 3. 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 (m^{-1}), 0.06 (m^{-1}) and 0.24 (m^{-1}) respectively. LMB and GSM derived integrated responses are 0.21 (m^{-1}) as compared to NOMAD i.e. 0.24 (m^{-1}) while New model derived response is very close to NOMAD i.e. 0.23 (m^{-1}). Further, new model derived individual response i.e. absorption due to CDOM and detritus 0.17 (m^{-1}) and 0.06 (m^{-1}) 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.

The integrated response ad+ag 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 as shown in Figure (6). Also, bio-optical model [22] derived only cdom (ag) 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 coefficients 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 and CDOM absorption coefficient from remote sensing reflectance is novel and can be used globally. Still, there is even much more scope for their further improvements as well.

Table-2 Performance of the global models for deriving CDOM (a_g) and detritus (a_d) absorption coefficients at 443nm with their uncertainties

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

Table-3 Statistics of the performance of the global models for deriving CDOM (ag), detritus (ad) 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 model 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

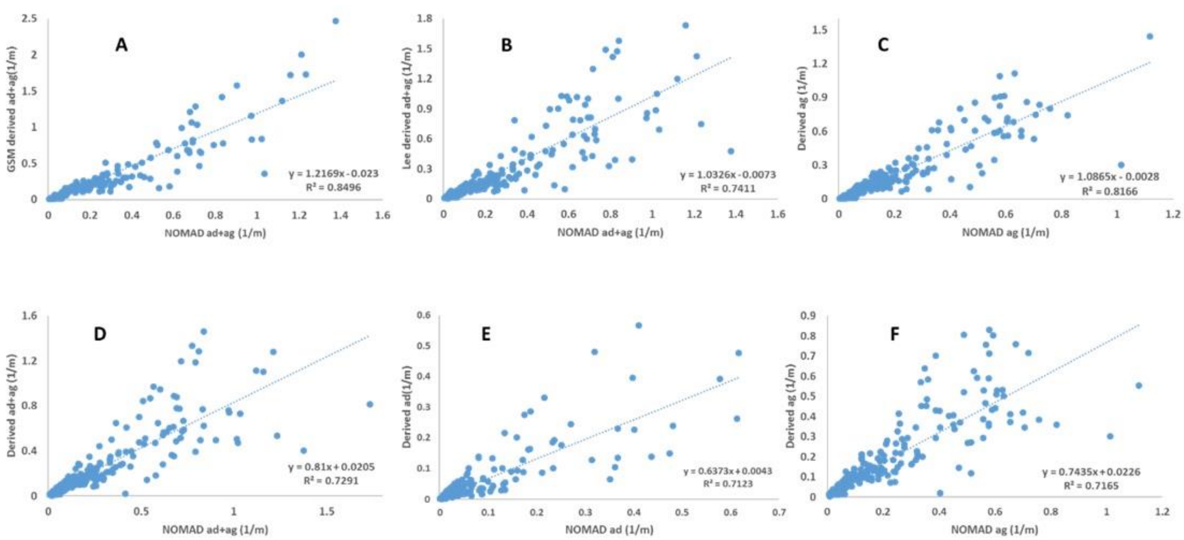


Fig-6 A) GSM derived (ad+ag) at 443 nm versus NOMAD (ad+ag) at 443nm, B) Lee derived (ad+ag) at 443 nm versus NOMAD (ad+ag) at 443nm, C) Gupta et al, 2020 derived ag at 443 nm versus NOMAD ag at 443nm, D), E) and F) new parameterized based model derived ad, ag and (ad+ag) at 443 nm versus NOMAD ad, ag and (ad+ag) at 443nm respectively.

Conclusion

In this study, ABOM with suitable parameterization has been presented to derive chl-a in optically complex waters. In addition, an attempt was made to correct for the CDOM slope bias by introducing empirically derived expression in Fig. 3, using NOMAD data for global waters. This study concludes that ABOM-derived chl-a (mg/m^3) improves significantly with an uncertainty of 58% as compared to GSM (175%) and Lee–Bio (189%) algorithms. Further the study reveals the bio-optical models developed for global oceans needs to be regionally parameterized for optical components in complex waters bodies to accurately estimate the magnitudes of optical constituents.

Similarly, in ABOM2, the study attempted to bring about improvement in the parameterization of Lee 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.

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