Preliminary results of an algorithm to determine the total absorption coefficient of water
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ABSTRACT
An algorithm to determine the spectral total absorption coefficient of water is presented. The algorithm is based on the Gershun’s equation of $a = \mu K_E$. The spectral underwater average cosine, $\mu$ and vertical attenuation coefficient of net irradiance, $K_E$ were obtained from radiative transfer simulations using Hydrolight with large in-situ measured data from the coastal and estuarine waters of Goa. A refined algorithm of spectral $\mu$ as in Ref. [1] is used to determine the spectral underwater average cosine. The spectral $K_E$ was related to the diffuse attenuation coefficient, $K_d$. The algorithms to derive absorption were validated using an independent NOMAD optical data at wavelengths 412, 440, 488, 510, 532, 555, 650 and 676 nm. The performance of the algorithm was evident from the high $R^2$, low bias and low RMSE. The values of $R^2$ at wavelengths 412, 440, 488, 510, 532, 555, 650 and 676 nm were 0.95, 0.95, 0.93, 0.93, 0.88, 0.82, 0.62, and 0.65 respectively. The corresponding bias were -0.0064, 0.0076, 0.0038, 0.0044, 0.0122, 0.0124, 0.0362, and 0.0093 respectively. The algorithms for $\mu$ and $K_E$ provide the spectral weighted average within $Z_{90}$ and have the advantage of deriving the absorption coefficients from the satellite data.

Keywords: Algorithm, inherent optical properties, absorption

1. INTRODUCTION
Inherent optical properties (IOPs) form the basis of radiative transfer equation and helps in understanding the underwater light fields. These IOPs are difficult to measure and model as compared to the apparent optical properties. The IOPs depend only on the constituents in waters and often the constituents are used to characterize the IOPs. IOPs such as absorption, scattering and beam attenuation can be modeled in terms of the constituents and their contributions. Since the apparent optical properties (AOPs) are easier to measure, AOPs are often used to model the IOPs.

There are two types of algorithms to determine the total absorption of water, one that total up the contribution from various components and the other that determine the total absorption, without separating the contributions of the components in water. The contributions to total absorptions are from water itself (pure water), algal particles (chlorophyll and detritus), dissolved material, and non-algal particles. Most of the available semi-analytical and empirical algorithms derive the absorption of these constituents. Since the absorption coefficient like most of the IOPs is additive, the total absorption is then calculated by summing up the absorption coefficients of all the components. There are various algorithms available that uses both the approaches.

One of the earliest method to derive the total absorption coefficient used chlorophyll alone, assuming the co-variations of all other components with chlorophyll. These methods are mostly applicable to Case 1 water types or open ocean and often fail for coastal water due to the complex nature of the variations of optical properties and also as chlorophyll do not correlate with other components at all times in these coastal waters.
Some methods which have gained attention to derive total absorption and claim to be applicable for all water types. These methods include the nonlinear statistical method are those by Garver and Siegel, Maritorena, the constrained linear matrix inversion developed by Hoge and Lyon and modified by Boss and Roesler and the quasi-analytical model (QAA). These models derive absorptions of each components. They have been implemented in SeaDAS software and are widely used for deriving absorption from ocean color satellite data. Few algorithms are also available to determine total absorption coefficient, however they are either available for a single wavelength or applicable within a specific spectral region of blue or green.

The available algorithms for deriving total absorption coefficient had some limitations such as being region and wavelength specific and these prompted us to develop a new, simple, robust and spectral algorithm to derive total spectral absorption. It is based on the relationships derived from the radiative transfer model and can be used to derive absorption coefficient from ocean color satellite data. The algorithm described here determines the spectral total absorption of water, without finding the absorption of components. This algorithm is based on an explicit methods based on rigorous derivations from radiative transfer equation of Gershun that relate the IOP, total absorption to AOPs.

2. METHODOLOGY

2.1 Measurements

The optical properties were measured from the coastal waters and the two estuaries of Goa, namely Mandovi and Zuari during the period 2010-2014 with total of 637 data records. The apparent optical properties were measured using an hyper-spectral radiometer Hyper-OCR (Satlantic, Canada) which provided profiles of downwelling irradiance, upwelling radiance, diffuse attenuation coefficients, surface remote sensing reflectance and surface solar irradiance in the spectral range of 350-800 nm. The surface irradiance data were available from a reference sensor mounted at a clear site on the boat. The surface remote sensing reflectance was measured deploying the instrument in float mode. The IOP profiles were measured using AC-9 (WetLabs, US) which provided spectral absorption and beam attenuation at nine wavelengths 412, 443, 488, 510, 532, 555, 650, 676 and 715 nm. The Hydrolight simulations were carried-out with inputs from AC-9 and the solar surface irradiance from the reference sensor of the radiometer. The simulations were carried-out as given in Ref [1].

2.2 Development

![Figure 1 The approach towards the development of the algorithm](Figure 1 The approach towards the development of the algorithm)
Since the objective was to use the new algorithm for the satellite data, all the depth parameters used for the development and validation are the weighted averages within the first optical depth, $Z_0(\lambda)$. The weighted averages were derived using the methods developed by Gordon\textsuperscript{15} and Sokoltesky\textsuperscript{16} and both matched closely. Since the NOMAD data used for validation were the weighted average data obtained using the method of Gordon\textsuperscript{15}, the same method was adopted to calculate the weighted average for all the measured profile data.

To develop a new algorithm, we opted to use the relationship of Gershun (See equation 5). Though the relationship seem simple, the measurements on optical parameters $\mu(\lambda)$ and $K_E(\lambda)$ were not available. Therefore, both these optical parameters $\mu(\lambda)$ and $K_E(\lambda)$ were first derived using empirical algorithms and then used in the Gershun's equation. The new empirical algorithm derived spectral total absorption at eight wavelengths 412, 440, 488, 510, 532, 555, 650 and 676 nm. The approach is outlined in Figure.1.

The spectral underwater average cosine $\mu(\lambda)$ was derived using a refined algorithm\textsuperscript{1} with larger data set. The new coefficients are given in Table 1. The model to derive $\mu(\lambda)$ is a function of spectral remote sensing, $Rrs(\lambda), Rrs(620)$ and solar zenith angle, $\theta$.

\begin{equation}
\mu(\lambda) = P_0 + P_1 X(\lambda) + P_2 X(\lambda)^2
\end{equation}

\begin{equation}
X(\lambda) = \frac{R_{rs}(\lambda)}{\log[R_{rs}(620)+R_{rs}(\lambda)] \cos(\theta)}
\end{equation}

The vertical attenuation for net irradiance $K_E(\lambda)$ is given as

\begin{equation}
K_E(\lambda) = -\frac{d(\ln[E_d(\lambda) - E_u(\lambda)])}{dx}
\end{equation}

Considering $E_u(\lambda)$ to be relatively negligible compared to $E_d(\lambda)$, $K_d(\lambda)$ is often found to be good match for $K_E(\lambda)$\textsuperscript{17}. Here $K_E(\lambda)$, which is derived from the Hydrolight simulations is related to $K_d(\lambda)$ with a simple linear relation.

\begin{equation}
K_E(\lambda) = K_0 + K_1 K_d(\lambda)
\end{equation}

Where $K_0$ and $K_1$ are the coefficients and their values are given in Table 2

Though the exact equation of Gershun without Raman scattering, is

\begin{equation}
a(\lambda) = \mu(\lambda)K_E(\lambda)
\end{equation}

We have slightly tuned this equation with a bias , $\varepsilon(\lambda)$

\begin{equation}
a(\lambda) = \mu(\lambda)K_E(\lambda) + \varepsilon(\lambda)
\end{equation}

Table 1. Revised coefficients used for deriving spectral underwater average cosine

<table>
<thead>
<tr>
<th>Lambda (nm)</th>
<th>$P_0$</th>
<th>$P_1$</th>
<th>$P_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>412</td>
<td>0.852</td>
<td>109.899</td>
<td>0.651</td>
</tr>
<tr>
<td>440</td>
<td>0.853</td>
<td>119.825</td>
<td>14048.466</td>
</tr>
<tr>
<td>488</td>
<td>0.838</td>
<td>126.575</td>
<td>14510.415</td>
</tr>
<tr>
<td>510</td>
<td>0.839</td>
<td>107.811</td>
<td>9853.532</td>
</tr>
<tr>
<td>532</td>
<td>0.835</td>
<td>98.753</td>
<td>7601.568</td>
</tr>
<tr>
<td>555</td>
<td>0.831</td>
<td>90.895</td>
<td>5893.719</td>
</tr>
<tr>
<td>650</td>
<td>0.836</td>
<td>96.217</td>
<td>6862.377</td>
</tr>
<tr>
<td>676</td>
<td>0.844</td>
<td>92.647</td>
<td>5211.589</td>
</tr>
</tbody>
</table>
Table 2. Coefficients to derive $K_E$ from $K_d$

<table>
<thead>
<tr>
<th>Lambda (nm)</th>
<th>$K_0$</th>
<th>$K_1$</th>
<th>$\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>412</td>
<td>0.867</td>
<td>0.871</td>
<td>-0.570</td>
</tr>
<tr>
<td>440</td>
<td>0.570</td>
<td>0.866</td>
<td>-0.365</td>
</tr>
<tr>
<td>488</td>
<td>0.294</td>
<td>0.773</td>
<td>-0.173</td>
</tr>
<tr>
<td>510</td>
<td>0.244</td>
<td>0.742</td>
<td>-0.151</td>
</tr>
<tr>
<td>532</td>
<td>0.224</td>
<td>0.659</td>
<td>-0.120</td>
</tr>
<tr>
<td>555</td>
<td>0.190</td>
<td>0.554</td>
<td>-0.084</td>
</tr>
<tr>
<td>650</td>
<td>0.485</td>
<td>0.377</td>
<td>-0.032</td>
</tr>
<tr>
<td>676</td>
<td>0.878</td>
<td>0.502</td>
<td>-0.130</td>
</tr>
</tbody>
</table>

2.3 Validation

The absorption coefficients used for the validation excluded the contribution from pure water component, i.e. $a_t(\lambda) = a(\lambda) - a_w(\lambda)$. Validations of the algorithms were carried-out using the NOMAD data\textsuperscript{18}. NOMAD is a publicly available, high quality in situ bio-optical data measured from various waters over the globe and has been used often for the ocean color algorithm developments and also satellite data product validations. (http://seabass.gsfc.nasa.gov/wiki_files/NOMAD/files/nomad_seabass_v2.a_2008200.txt). The error analysis were carried out with statistical parameters such as bias, RMSE (root mean square error), coefficient of determination $R^2$ and regression between model and NOMAD data (Equation 9).

\[
Bias = \left[ \frac{1}{N} \sum_{1}^{N} (a_{Model} - a_{NOMAD}) \right]
\]  

(7)

\[
RMSE_{\log} = \sqrt{\frac{\sum_{1}^{N} [\log(a_{NOMAD}) - \log(a_{Model})]^2}{N - 2}}
\]  

(8)

\[
a_{NOMAD}(\lambda) = m(\lambda)a_{Model}(\lambda) + c(\lambda)
\]  

(9)

3. RESULTS AND DISCUSSION

The results of the simulations using Hydrolight provided optical parameters that closely matched the measured data. The spectral $Z_{50}(\lambda)$ and $Rrs(\lambda)$ compared well with the measured for most of the stations (Fig. 2). This closure assured that the optical parameters derived from the Hydrolight that were not measured such as underwater average cosine $\mu(\lambda)$, scalar irradiance, $E_o(\lambda)$, attenuation coefficient of net irradiance, $K_E(\lambda)$ would match and agree closely with the optical properties of the same environment.
The total absorption coefficient derived from the algorithm matched well with the NOMAD data at all eight wavelengths (Figure 3 and 4). Most of the earlier algorithms have not reported its operation in the longer wavelengths and often the validation and performance measures are restricted to the green region till 555 nm \cite{3,19}.

Figure 2. Comparison of the spectral $Rrs(\lambda)$ (left) and $Z_{90}(\lambda)$ (right) derived from the Hydrolight and measurements.

Figure 3. Comparison of the total absorption (excluding water component) derived from the model and the NOMAD data at 412 nm (left), 532 nm (middle) and 650 nm (right).
Figure 4. Comparison of spectral absorption derived from model and NOMAD data.

Table 3. Error statistics of the absorption model.

<table>
<thead>
<tr>
<th>Lambda (nm)</th>
<th>$R^2$</th>
<th>Bias</th>
<th>RMSE</th>
<th>$c$</th>
<th>$m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>412</td>
<td>0.95</td>
<td>-0.00642</td>
<td>0.187</td>
<td>-0.00637</td>
<td>1.00076</td>
</tr>
<tr>
<td>440</td>
<td>0.95</td>
<td>0.00760</td>
<td>0.161</td>
<td>-0.01047</td>
<td>0.99856</td>
</tr>
<tr>
<td>488</td>
<td>0.93</td>
<td>0.00382</td>
<td>0.187</td>
<td>-0.01341</td>
<td>1.01707</td>
</tr>
<tr>
<td>510</td>
<td>0.93</td>
<td>0.00441</td>
<td>0.190</td>
<td>-0.00905</td>
<td>1.00517</td>
</tr>
<tr>
<td>532</td>
<td>0.88</td>
<td>0.01226</td>
<td>0.351</td>
<td>-0.03077</td>
<td>1.08687</td>
</tr>
<tr>
<td>555</td>
<td>0.82</td>
<td>0.01243</td>
<td>0.441</td>
<td>-0.03607</td>
<td>1.16575</td>
</tr>
<tr>
<td>650</td>
<td>0.62</td>
<td>0.03618</td>
<td>0.282</td>
<td>-0.04158</td>
<td>1.00357</td>
</tr>
<tr>
<td>676</td>
<td>0.65</td>
<td>0.00930</td>
<td>0.263</td>
<td>-0.06451</td>
<td>1.18736</td>
</tr>
</tbody>
</table>

The algorithm performed very well in the blue and green region while its performance was slightly degraded in red region of the spectrum. This could be attributed to the errors in the calibrations of the radiometer, errors in the closures of optical parameters derived from Hydrolight and the measured, measurement errors of AC-9 and the errors in algorithms to derive $\mu(\lambda)$ and $K_d(\lambda)$. This model performed better in the blue region unlike QAA which was reported to over-estimate even in the blue region. The new algorithm to derive $a_t(\lambda)$ can be used to derive absorption coefficient using the optical parameters measured from the radiometer. To derive $a_t(\lambda)$ from the satellite data, it is first required to derive $\mu(\lambda)$ and $K_d(\lambda)$. The selection of the best available algorithms to derive $\mu(\lambda)$, $K_d(\lambda)$ and to correct the atmospheric effects will result in the accurate estimation of absorption coefficient. The evaluations of various algorithms available to derive $K_d(\lambda)$ from the satellite have shown very poor performances of most algorithms to derive $K_d(\lambda)$ at the longer wavelengths. Similarly, the empirical algorithm to determine $\mu(\lambda)$ have to be robust and determine $\mu(\lambda)$ with less errors at all wavelengths. Unlike $K_d(\lambda)$ which can be validated with measurements, $\mu(\lambda)$ has the disadvantage, as the same cannot be measured and validated.
4. CONCLUSION

The algorithm to derive the spectral total absorption coefficient was shown to perform well at all spectral ranges from 412 to 676 nm. This algorithm has the following advantages:

- The algorithm can be used for coastal waters and does not find the absorptions of each component to determine the total absorptions.
- The algorithm given here is simple and can be applied to derive from satellite data with ease.
- This algorithm can derive spectral total absorption at wavelengths in the visible range, from blue to even at longer wavelengths.

Shortcomings of the algorithm

- Presently can be used only at discrete wavelengths.
- The absorption derived at lower wavelengths are better and gradually degrade in performance at longer wavelengths.
- Does not evaluate the absorptions of the components.
- The algorithm does not include the effects of inelastic or Raman processes and the same could also influence the errors, particularly at longer wavelengths. (Gordon). Since the Raman effect is more in the clear waters as compared to coastal and estuarine waters, the contributions due to this to the errors could be marginal.

Improvements and future work:

- The algorithm needs to be compared with the other algorithms to evaluate its performance.
- Presently the algorithm is suited for coastal or Case 2 type waters as the data used has been from the coastal and estuarine waters and the algorithms will have to be refined with wide range of data.
- The algorithm will have to cater to hyper-spectral with closer spectral intervals and wider spectral range. This will help in the various applications such as retrieval of phytoplankton pigments, study of blooms and bio-optical models.
- Require algorithms that will allow determining spectral $K_d(\lambda)$ from satellite data with better accuracy. Earlier evaluations of algorithms to derive $K_d(\lambda)$ does not show any promising algorithms that will allow determining $K_d(\lambda)$ at longer wavelengths with comparable accuracy as to the lower wavelengths.
- Include inelastic scattering such as Raman scattering and fluorescence in the Hydrolight simulations and in the algorithm. Raman scattering could add to the errors in deriving total absorption using Gershun's relation at longer wavelength. Even with the inclusion of Raman scattering correction the absorption will bear a similar form as equation 6 (Gordon 2009).

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6. REFERENCES