Simultaneous atmospheric correction and quantification of suspended particulate matters from orbital and geostationary earth observation sensors

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A B S T R A C T
Earth observation (EO) data are excellent tools for studying the quality and dynamic of estuarine and coastal waters. In this paper we propose a simplified remote sensing method to estimate aerosol reflectance and suspended particulate matter (SPM). We validated this method with in-situ measurements from two different locations: the Poyang Lake in China and the Kenyan Coastal waters. In the validation phase, we used match-up data from orbital ocean color (MERIS) and geostationary (SEVIRI) sensors. Both locations as well as both sensors gave consistent results. The $R^2$ values between derived and measured SPM concentrations were $>0.94$ for MERIS and $>0.7$ for SEVIRI. The RMSE values of derived SPM concentrations were less than 3 and 5 g m$^{-3}$ for MERIS and SEVIRI respectively. Our method derived realistic patterns of SPM dynamics in turbid waters and spatially un-correlated aerosol reflectance maps. The proposed method can be applied to derive either SPM concentrations or its backscattering coefficient.

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1. Introduction

Sediment fluxes in coastal waters play an important role in the quality and dynamics of estuary and coastal environments. Excessive concentrations of suspended particulate matters (SPM) influence the productivity and thermodynamic stability of coastal waters (Muller-Krager et al., 2005). Therefore, reliable information on the spatiotemporal variations of SPM is a key issue in characterizing the quality of marine ecosystem.

Earth observation (EO) data provide rapid and repeated information over large and often inaccessible coastal areas. The primary measurement of EO data over water is the visible light leaving the water column, hereafter called the water leaving reflectance. In estuarine and coastal waters, this water leaving reflectance is strongly affected by different materials, e.g. terrigenous particulate and dissolved materials, re-suspended sediment or highly concentrated phytoplankton bloom. The majority of estuarine and coastal waters can therefore be classified as case 2 waters (Gordon and Morel, 1983). In case 2 waters, the constituents are independent of each other and do not co-vary with chlorophyll-a as in case 1 waters.

Consistent estimates of SPM from EO data necessitate a reliable atmospheric correction procedure. Most of the atmospheric correction procedures fail over case 2 waters. The failure of atmospheric correction might be attributed to the complexity of the recorded reflectance. The standard approach by Gordon and Wang (1994), for example, assumes a zero water leaving reflectance in the near-infrared (NIR). In case 2 waters, this water leaving reflectance has distinctive values at the NIR part of the spectrum (Siegel et al., 2000).

The non-negligible value of water leaving reflectance at the NIR was accounted by many authors. Carder et al. (1999a) introduced the ratio of water leaving reflectance at two NIR bands. The water ratio was either assumed constant (Gould et al., 1999; Ruddick et al., 2000) or estimated from neighboring pixels of case 1 waters (Hu et al., 2000). Assuming a known relationship between the values of water leaving reflectance at two NIR bands is necessary but not sufficient. One still needs information about aerosol type and optical thickness. The ratio of aerosol reflectance at two NIR bands can be related to aerosol optical thickness and type. Ruddick et al. (2000) estimated this aerosol ratio by using visual inspection of the reflectance’s scatter-plot. Hu et al. (2000) determined the values of aerosol ratio over clear water pixels and extrapolated them to adjacent turbid water pixels. Salama et al. (2004) suggested an automated approach to determine the aerosol ratio based on eigenvector decomposition of the NIR bands.

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Coupled approaches are increasingly used to simultaneously retrieve the optical properties of water and atmosphere (Gordon et al., 1997; Chomko et al., 2003). However, most of these algorithms were developed for case 1 waters, i.e. assuming known and spatially homogeneous water leaving reflectance at the NIR. Newly developed algorithms are emerging for case 2 waters (Schroeder et al., 2007; Kuchinke et al., 2009a,b). The spectral optimization method (Kuchinke et al., 2009a) was constrained to 0.1 m\(^{-1}\) as a maximum value of backscattering coefficient of SPM at 0.443 \(\mu\)m. This value of backscattering is equivalent to 12 g m\(^{-3}\) concentration of suspended particles using the specific backscattering coefficient of Albert and Gege (2006). On the other hand, artificial neural network techniques (Schroeder et al., 2007) are usually limited to the range of their training sets. Most of estuarine and coastal waters have high loads of SPM, exceeding 12 g m\(^{-3}\). For instance the Yangtze Estuarine water is extremely turbid with SPM concentration ranging between 80 and 500 g m\(^{-3}\) (Shen et al., in press).

The purpose of this study is to estimate the backscattering coefficient of SPM and aerosol reflectance simultaneously from NIR reflectance. With respect to the introduced assumptions, unique values of SPM backscattering coefficient and aerosol reflectance were found.

2. Methodology

2.1. Top of atmosphere reflectance

The total reflectance at the top of atmosphere (TOA) can be written as the sum of several components (Gordon, 1997):

\[ \rho^T_l = \rho^s_l + \rho^a_l + \rho^d_l + \rho^w_l + T_l \rho^s_w \]  

(1)

where, \(T_l\) is diffuse transmittance of the atmosphere; \(\rho^s_l\) is the sea-surface reflectance; \(\rho^a_l\) is the aerosol reflectance resulting from multiple scattering by aerosol in the absence of air; \(\rho^d_l\) is Rayleigh reflectance resulting from multiple scattering by air molecules in the absence of aerosol; \(\rho^w_l\) is the reflectance from the interaction between air molecules and aerosol; \(\rho^w_l\) is the water leaving reflectance resulting from the interaction between the light and the water column. The calculation of Rayleigh reflectance \(\rho^r\) is well described in terms of geometry and atmospheric pressure (Gordon et al., 1988a). The coupled term \(\rho^w\) can be neglected at the NIR part of the spectrum (Gordon and Castano, 1987). Sea-surface reflectance \(\rho^s_l\) is estimated using the probabilistic formulations of Cox and Munk (1954) and ancillary data on wind field. Gaseous transmittance are calculated from ancillary data on ozone and water vapor concentrations using the transmittance models of Goody (1964) and Malkmus (1967). For viewing angles <60° the diffuse transmittance \(T\) is weakly dependent on aerosol and can be approximated following (Gordon et al., 1983). Basically, Eq. (1) has two unknowns: the aerosol reflectance \(\rho^a_l\) and water leaving reflectance \(\rho^w_l\):

\[ \rho^a_l + T_l \rho^w_l = \rho^r_l - \rho^s_l - T_l \rho^s_w \]  

(2)

Throughout this paper we will call the righthand side of Eq. (2), the corrected-reflectance \(\rho^c\), i.e. \(\rho^c_l = \rho^r_l - \rho^s_l - T_l \rho^s_w\).

2.2. Deriving the water leaving reflectance

The aerosol ratio at two NIR bands \(s\) and \(l\) is:

\[ \varepsilon(s,l) = \frac{\rho^s_l}{\rho^l_l} \]  

(3)

where \(s < l\). Once the value of \(\varepsilon(s,l)\) is estimated, the water leaving reflectance at \(s\) can be derived from Eq. (1):

\[ T(s) \rho^s_w = \rho^s_l - \varepsilon(s,l) \times (\rho^l_l - T(l) \rho^l_w) \]  

(4)

The ratio of water leaving reflectance at two bands \(s\) and \(l\) is (Carter et al., 1999a,b):

\[ \alpha(s,l) = \frac{\rho^s_l}{\rho^l_l} \]  

(5)

The water leaving reflectance at \(l\) can then be derived from the TOA reflectance as:

\[ T(l) \rho^l_w = \frac{\rho^s_l - \varepsilon(s,l) \rho^l_l}{\alpha(s,l) - \varepsilon(s,l)} \]  

(6)

Equation (6) shows that the water leaving reflectance at bands \(s\) and \(l\) can be derived if we have good estimates of the ratios \(\varepsilon(s,l)\) and \(\alpha(s,l)\).

2.3. Semi-analytical water model

Water leaving reflectance is to the first order proportional to the water inherent optical properties (IOPs) Gordon et al. (1988b):

\[ \rho^l_w = 0.54 I_1 Q \frac{b_b(\lambda)}{b_b(\lambda) + a(\lambda)} \]  

(7)

\(I_1 = 0.0949\) is a constant coefficient; \(Q\) is the ratio between up-welling radiance and irradiance (Mobley, 1994). The light field will be assumed isotropic such that \(Q = \pi \ sr\). The bulk backscattering and absorption coefficients of the water column are expressed in \(b_b(\lambda)\) and \(a(\lambda)\) respectively. The constant number 0.54 describes the fraction of transmitted light from below the water surface. At the NIR part of the spectrum the water leaving reflectance column is assumed to be optically governed by the SPM backscattering \(b_b^{\text{SPM}}(\lambda)\) and the water absorption \(a_w(\lambda)\) coefficients:

\[ a(\lambda) = a_w(\lambda) \]  

(8)

\[ b_b(\lambda) = b_b^{\text{SPM}}(\lambda) = b_b^{\text{SPM}}(\lambda) \times C_{\text{SPM}} \]  

(9)

where: \(\lambda \in \text{NIR}\)

where \(b_b^{\text{SPM}}(\lambda)\) and \(C_{\text{SPM}}\) are the specific backscattering coefficient and the concentration of SPM, respectively.

The water ratio (Eq. (5)) can be related to the concentration of SPM via:

\[ C_{\text{SPM}} = \frac{\eta(\lambda) - a(s) \eta(\lambda)}{a(s) - 1} \]  

(10)

where \(\eta(\lambda)\) is the ratio \(a_w(\lambda)/b_b^{\text{SPM}}(\lambda)\). Note that Eq. (10) can also be derived for the backscattering coefficient of SPM at 0.55 \(\mu\)m instead of \(C_{\text{SPM}}\) as follow. The backscattering coefficient of SPM \(b_b^{\text{SPM}}(\lambda)\) can be parameterized as (Kopelevich, 1983; Maritorena et al., 2002):

\[ b_b^{\text{SPM}}(\lambda) = b_b^{\text{SPM}}(0.55) \left(\frac{0.55}{\lambda}\right)^{\gamma} \]  

(11)

where \(\gamma\) is the spectral shape parameter. The value of \(\gamma\) is function of the particle size of SPM and may take the value between 0.3 and 2.5 Lee et al. (1999). Now Eq. (10) can be written for \(b_b^{\text{SPM}}(0.55)\) instead of \(C_{\text{SPM}}\) by changing the ratio \(\eta(\lambda)\) to \(\eta(\lambda) = a_w(\lambda)(0.55/\lambda)^{-\gamma}\).
\[ b_{i}(\text{SPM})(\lambda) = \frac{\eta_{i0} - a_{(s,l)} \eta_{(s)}}{a_{(s,l)} - 1} \] (12)

We will use Eq. (10) for further derivation. To study the effect of SPM on the values of water ratio at the NIR, Eq. (7) was solved for SPM concentrations ranging from 5 to 500 g m\(^{-3}\). The water ratio was estimated for 10 NIR bands ranging from 0.76 to 0.86 \(\mu\)m using the reflectance at 0.87 \(\mu\)m as denominator. Fig. 1 shows that the assumption of constant value of \(a_{(s,l)}\) is acceptable for certain wavelengths and SPM concentrations. For instance, the value of \(a_{(0.858, 0.87)}\) can be considered constant over a wide range of SPM concentrations (Fig. 1-a). The wavelength dependency of \(a_{(s,l)}\) is directly related to the spectral shape of the water leaving reflectance (Fig. 1-b). The water leaving reflectance has a unique peak between 0.8 and 0.82 \(\mu\)m due to the low values of the water absorption coefficient. The value of \(a_{(s,l)}\) will therefore have the highest variation at the spectral range between 0.8 and 0.82 \(\mu\)m (Fig. 1-b).

Equation (10) facilitates the estimation of the water ratio at a shorter NIR band \(i\). If this NIR band \(i\) is available, such that \(i < s < l\), then \(a_{(s,l)}\) can be estimated from \(a_{(s,l)}\) as:

\[ a_{(i,l)} = a_{(s,l)} \left( \frac{\eta_{(l)} - \eta_{(s)}}{\eta_{(l)} - \eta_{(i)}} \right) \] (13)

The aerosol ratio can also be spectrally extrapolated from the pair of bands \(s, l\) to \(i, l\) where \(i < s < l\) (Gordon and Wang, 1994):

\[ \epsilon_{(i,l)} = \epsilon_{(s,l)} \delta_{i} \] (14)

where the exponent \(\delta_{i}\) is the ratio \((l - i)/(l - s)\).

### 2.4. Physical constraints

The task now is to find reliable estimates of \(a_{(s,l)}\) and \(\epsilon_{(s,l)}\) that improve the accuracy of the retrieved water leaving reflectance at the NIR. It is quite important to bound our searching procedure with some physical constraints. The estimated aerosol reflectance at band \(l\) should be positive and less than the corrected-reflectance at this band, i.e. \(r_{c}^{(l)} \leq r_{l}^{(l)}\). The value of the aerosol ratio at band \(s\) and \(l\) should, therefore, satisfy:

\[ 0 \leq \epsilon_{(s,l)} \leq \left( \frac{\rho_{l}^{(l)}}{\rho_{c}^{(s)}} \right)^{-\delta_{i}} \] (15)

Equivalently, water leaving reflectance at band \((l\) or \(s\) should be positive and less than the corrected-reflectance at this band: \(T_{c}^{(s)} \rho_{c}^{(s)} \leq T_{l}^{(s)} \rho_{l}^{(s)}\). Substituting this inequality in Eq. (6) we can find:

\[ \frac{T_{c}^{(s)} \rho_{c}^{(s)}}{T_{l}^{(s)} \rho_{l}^{(s)}} \leq a_{(s,l)} \] (16)

The condition of non-negative concentration \(C_{\text{SPM}} > 0\) of Eq. (10) yields:

\[ a_{(s,l)} < \frac{\eta_{(l)}}{\eta_{(s)}} \text{ if } a_{(s,l)} > 1 \] (17)

\[ a_{(s,l)} > \frac{\eta_{(l)}}{\eta_{(s)}} \text{ if } a_{(s,l)} < 1 \] (18)

Let us note that the reference band \(l\) of the water ratio was selected to be far in the NIR 0.87 \(\mu\)m. This was to achieve a maximum variability in the \(a_{(s,l)}\) w.r.t. SPM concentrations. Hence

Fig. 1. The variation of the water ratio \(a_{(s,l)}\) as a function of SPM concentrations (a) and wavelength (b). The reference \((l)\) band was fixed at 0.87 \(\mu\)m.
the ratio \( \alpha(l, i) \) is always greater than 1 in the NIR (see Fig. 1). The lower and upper bounds on \( \alpha(l, i) \) are therefore:

\[
\frac{T^{(l)}_{\text{pc}}^{(l)}}{T^{(l)}_{\text{pc}}^{(l)}} \leq \alpha(l, i) \leq \frac{\alpha_l(l)}{\alpha_w(l)}
\]

(19)

The above inequality Eq. (19), is valid with respect to the following condition:

\[
i < s < l
\]

(20)

\[\alpha_l(i) < \alpha_w(s) < \alpha_w(l)\]

The bands \( i, s \) and \( l \) should therefore be selected with respect to the associated values of water absorption.

2.5. TOA nonlinear system

The water leaving reflectance at band \( l \) can be calculated using the corrected-reflectance at the band \( i \); in an analogy to Eq. (6):

\[
\frac{T^{(l)}_{\text{pc}}^{(l)}}{T^{(l)}_{\text{pc}}^{(l)}} = \frac{\rho_c(l) - \epsilon_{(l,i)} \rho_c(l)}{\alpha_{(l,i)} - \epsilon_{(l,i)}^2}
\]

(21)

Equation (6) has two unknowns namely the aerosol ratio \( \epsilon_{(s, l)} \) and the water ratio \( \alpha_{(s, l)} \). Equation (21) will add two other unknowns namely \( \alpha_{l(i)} \) and \( \epsilon_{(l,i)} \). The ratios \( \epsilon_{l(s)} \) and \( \epsilon_{l(i)} \) are related through Eq. (14). At the NIR part of the spectrum \( (i < s < l) \), the ratio \( \alpha_{l(i)} \) can be linked to \( \alpha_{l(i)} \) through Eq. (13). This parametrization reduces the number of variables in Eqs. (6) and (21) to two only:

(1) The water ratio \( \alpha_{l(i)} \) which is related to SPM load.
(2) The aerosol ratio \( \epsilon_{l(i)} \) which is related to the aerosol type and optical thickness with \( \lambda \) being \( i \) or \( s \).

These two parameters represent two different media, atmosphere and water, and therefore are physically unrelated. The values of \( \alpha_{l(i)} \) and \( \epsilon_{l(i)} \) are found by minimizing the difference between the water leaving reflectance estimated from Eqs. (6) and (21):

\[
f_1 = \left( T^{(l)}_{\text{pc}}^{(l)} \text{(Eq. 6)} - T^{(l)}_{\text{pc}}^{(l)} \text{(Eq. 21)} \right)^2
\]

(22)

where (Eqs. (6) and (21)) refer to the equations from which the water leaving reflectance was calculated. The cost function (Eq. (22)) is at its minimum when \( f_1 = 0 \). We set \( f_1 = 0 \) in Eq. (22) and rearrange the terms:

\[
A_c \epsilon_{(s, l)} + B_c \epsilon_{(s, l)} + C_c = 0
\]

(23)

Where the coefficients \( A_c, B_c \) and \( C_c \) are given by:

\[
A_c = \rho_{(s, l)}(s) - \alpha_{(s, l)} \epsilon_{(s, l)}(l)
B_c = \alpha_{(s, l)} \epsilon_{(s, l)}(l) - \rho_{(s, l)}(s)
C_c = \alpha_{(s, l)} \epsilon_{(s, l)}(l) - \alpha_{(s, l)} \epsilon_{(s, l)}(l)
\]

(24)

Equation (23) represents the locus of the solution region at which \( f_1 \) attained its minimum. The retrieved parameters from Eq. (23) are, however, interdependent. This dependency can be resolved by introducing another quantity (SPM concentration), which is directly related to the water ratio \( \alpha_{(s, l)} \) and independent of the aerosol ratio \( \epsilon_{(s, l)} \). Derived SPM concentrations from \( \alpha_{(s, l)} \) and \( \epsilon_{(s, l)} \) are in principle totally unrelated to the aerosol ratio. Following this reasoning two values of SPM concentrations can be quantified. The first is Eq. (10) and the second is estimated from Eq. (7):

\[
C_{\text{spm}} = \frac{\eta_{(l)} \rho_{w}^*(l)}{1 - \rho_{w}^*}
\]

(25)

where:

\[
\rho_{w}^* = \frac{\rho_{w}^*}{0.54 l/\omega}
\]

(26)

In analogy to Eq. (10), equation (25) can be written with respect to SPM backscattering coefficient as:

\[
b_{b_{i}^{(p,m)}}(0.55) = \frac{\eta_{(l)} \rho_{w}^*}{1 - \rho_{w}^*}
\]

(27)

We will use Eq. (25) for further derivation. The values of the aerosol and water ratios can be tuned until a minimum difference between the concentrations of Eqs. (25) and (10) is realized. In other words, the following cost function is minimized with respect to \( \alpha_{(s, l)} \) and \( \epsilon_{l(s, l)} \):

\[
f_2 = (C_{\text{spm}} \text{(eq.}(10) - C_{\text{spm}} \text{(eq.}(25)))^2
\]

(28)

where (Eq. (10)) and (Eq. (25)) refer to the equations from which the SPM concentrations were calculated. Setting \( f_2 \) to zero and rearranging the terms, yields:

\[
A_\alpha \alpha_{(s, l)} + B_\alpha \alpha_{(s, l)} + C_\alpha = 0
\]

(29)

where the coefficients \( A_\alpha, B_\alpha \) and \( C_\alpha \) are given by:

\[
A_\alpha = \eta_{(l)}(s)
B_\alpha = -\eta_{(l)}(l) \eta_{(l)}(s)
C_\alpha = \eta_{(l)}(l) \eta_{(l)}(s)
\]

(30)

where \( \rho_{c}(s) \) is the corrected-reflectance normalized to 0.54\( l_{\omega} \)Q, i.e. the same denominator of Eq. (26). Eq. (29) represents the locus of the smallest values of the cost function.

We will solve Eqs. (29) and (23) simultaneously for the two unknowns with respect to the constraints Eqs. (15) and (19).

3. Materials

3.1. Simulated TOA data set

Top of atmosphere (TOA) reflectance of 108 spectra were generated using the radiative transfer model of Vermote et al. (1997) and the semi-analytical model in Eq. (7).

Atmospheric path reflectances were computed for maritime and continental aerosol types at three optical thicknesses: 0.1, 0.25 and 0.5. Atmospheric models were denoted using the first letter of the aerosol type and the value of optical thickness. Example: M0.1 is a maritime aerosol type with 0.1 optical thickness.

Spectra of water leaving reflectance were simulated from varying concentrations of SPM and chlorophyll-\( a \) and absorption of dissolved organic matter. The concentrations of SPM varied from 1 g m\(^{-3}\) to 500 g m\(^{-3}\) while the concentrations of chlorophyll-\( a \) varied from 0.5 mg m\(^{-3}\) to 20 mg m\(^{-3}\). The absorption coefficient of dissolved organic matter at 0.44 \( \mu m \) varied from 0 to 1 m\(^{-1}\).

Specific inherent optical properties (SIOPs) were used (Albert and Gege, 2006) to derive the inherent optical property (IOPs) assuming linear relationships (Bricaud et al., 1995). The zenith angles were 40° and 30° for the sun and the sensor respectively. The azimuthal angle difference was taken as 130°. The values of water vapor and ozone content were set to: \( \text{H}_2\text{O} = 2.93 \text{ cm} \), and \( \text{O}_3 = 0.319 \text{ cm} \).
3.2. In-situ measurements

We organized two in-situ campaigns in two different areas during 2008. The first field campaign was in the Poyang Lake, China. In-situ measurements of chlorophyll-a and SPM concentrations were carried out in 30 sites during the period from 16 to 19 of October 2008. The second field campaign was in the Kenyan coastal waters, offshore the Sabaki River. In-situ measurements of chlorophyll-a and SPM concentrations were carried out in seven sites repeated over seven days from 18 to 25 of October 2008. Table 1 shows statistical summary of measured values of SPM and chlorophyll-a in both locations. We employed the ocean optics protocol (Fargion and Muller, 2000) for estimating SPM and chlorophyll-a from collected water samples. In summary water samples were collected and filtered. The filters were then analyzed for their contents of SPM and chlorophyll-a. Details of the used procedures and collected data during these two field campaigns are reported in Zhou (2009) and Ndungu (2009).

3.3. Earth observation data set

In our work we will apply the developed method on images acquired from two different sensors. The first sensor is the MEdium Resolution Imaging Spectrometer (MERIS) on board of EnviSat. MERIS is an orbital sensor with 15 bands covering the spectral range from 0.4 to 0.95 μm. MERIS has two resolution modes: full and reduced resolution (FR, RR). The nadir pixel size is about 0.3 × 0.3 km² and 1.2 × 1.2 km² for the FR and RR respectively. MERIS is an established ocean color sensor that provides reliable information on water quality parameters in coastal waters and open oceans (Ruddick et al., 2008).

The second sensor is the Spinning Enhanced Visible and Infrared Imager (SEVIRI) on board of the Meteosat Second Generation. SEVIRI is a meteorological geostationary sensor that is positioned above the equator at 3.4°W and scans the complete disk of the Earth every 15 min. SEVIRI operates two channels at visible range of the spectrum. The red band (0.56–0.71 μm) centered around 0.6 μm and the NIR band (0.74–0.88 μm) centered around 0.8 μm. The nadir pixel size of SEVIRI in these two bands is 3 × 3 km² (Schmetz et al., 2002). SEVIRI has promising applications to remote sensing of water quality in regions with dynamic water systems and rapidly changing cloud covers (Neukerms et al., 2008).

Data on atmospheric pressure, ozone total column content and wind speed were also obtained from ancillary data provided by MERIS level-1b products. SEVIRI products on ozone content were used to compute the atmospheric transmittance. Global products on wind field were obtained from IFREMER-CERSAT (2009) and used to compute the sea-surface reflectance.

3.4. In-situ and EO data match-ups

MERIS is used with data collected from the Poyang Lake and SEVIRI is used with data collected from the Kenyan coastal waters. Three RR-MERIS images were concurrent with in-situ measurements in the Poyang Lake. 11 SEVIRI images were concurrent with in-situ measured concentrations of SPM and chlorophyll-a at seven sites. In total, we have 30 match-up sites from three MERIS images over the Poyang Lake and 49 match-up sites from 11 SEVIRI images over the Kenyan coastal waters. Match-up site is a field measurement and an image pixel that have similar sampling time (±1 h) and geographic position.

For demonstration purposes we will also apply the method on MERIS images acquired over three different and optically complex areas: the Yangtze Estuary (China), the Makassar Strait (Indonesia) and the whole disk of SEVIRI covering all African coastal waters. Below is a list specifying the study region, used sensor and date of acquisition.

- **Poyang Lake**: three RR-MERIS images acquired between 16 and 19 of October 2008.
- **Yangtze Estuary**: one FR-MERIS image acquired on 26-07-2008.
- **Makassar Strait**: one RR-MERIS image acquired on 01-07-2004.
- **African coastal waters**: one SEVIRI image acquired 10-02-2009.

4. Results

4.1. Performance

4.1.1. The numerical scheme

Three NIR bands were chosen (i = 0.815 μm, s = 0.835 μm and l = 0.87 μm) such that they satisfied the condition in Eq. (20). Equations (23) and (29) were then applied on the simulated TOA reflectance.

Fig. 2 illustrates the locus of Eq. (23) as ‘LocusW’ and Eq. (29) as ‘LocusA’ with respect to (w.r.t.) the sought variables ξ(l, i) and ξ(s, l). Each figure was bounded to the domain of acceptable solutions represented by Eq. (15) and (19). For all TOA reflectance, the solution curves ‘LocusW’ and ‘LocusA’ intersected at a specific values of aerosol and water ratios. The coordinates of the intersection points were retrieved by solving the system of simultaneous equations ((23) and (29)) for each triplet of corrected-reflectance: \( p(l, i) \), \( p(s, l) \) and \( p(l) \).

The relative error between known c and derive x values is computed as \( 100(1 - x/c) \) and shown in Table 2. Table 2 shows that the relative errors between derived and known quantities are less than 1% for SPM concentration ranging from 5 to 400 g m⁻³. Above 400 g m⁻³ the relative errors reaches large values, up to 28%; especially for C0.1, C0.25 and M0.1 aerosol models.

4.1.2. Sensitivity to random noise

Signal to noise ratio (SNR) is the ratio between the signal received by the sensor to background noise corrupting the signal. At the NIR part of the spectrum the SNR is expected to have small values over water bodies. In consequence, total reflectance at the NIR is more likely to be affected by random noise. The sensitivity of the proposed model to random fluctuations in the data was analyzed as follow. The noise level was set to be 0.5% of the corrected-reflectance at the NIR. 1000 random fluctuations were generated from a normal distribution such that 95% of the fluctuated values were in the range \( x \) (noise level). The proposed algorithm was then applied for each fluctuated triplet of corrected-reflectance. The relative errors between derived and known values were then computed at 95% of confidence. Fig. 3 shows that the accuracy of estimated SPM concentration decreases with increasing aerosol optical thickness. However the values of relative error does not exceed 10% in the SPM range >7 g m⁻³ and <400 g m⁻³.
Fig. 2. The locus of the solution region: ‘LocusW’ (Eq. (23)) and ‘LocusA’ (Eq. (29)). The curves are plotted within the bounds (Eq. (15) and (19)). These curves are for combinations of Continental (a,b,e,f) and Maritime (c,d,g,h) aerosol types with two values of aerosol optical thickness (0.1 and 0.5) and SPM concentrations between $2 \text{ g m}^{-3}$ (a–d) and $50 \text{ g m}^{-3}$ (e–h).
4.2. Validation with in-situ measurements and EO data match-ups

To avoid assuming a certain value of SPM specific backscattering coefficient we derive the $b_{\text{spm}}(0.55)$ instead of $C_{\text{spm}}$ from EO data, i.e. using Eqs. (12) and (27) in the cost function Eq. (28). The spectral exponent of SPM: $y$ was set to 1.7, more discussions on this value will follow in Section 5.

4.2.1. Poyang Lake and MERIS match-ups

We applied our method on three NIR bands of MERIS centered at 0.776, 0.865 and 0.883 μm, respectively. Fig. 4-a shows a linear relationship between derived SPM backscattering coefficients at 0.55 μm and the measured values of SPM concentrations. This linear relationship was already expressed according to Eq. (9). The specific backscattering coefficient $b_{\text{spm}}(0.55)$ of SPM in the Poyang Lake was estimated as follow. We selected three calibration-match-up sites (circles in Fig. 4-a), computed the corresponding values of $b_{\text{spm}}(0.55)$ and then took the average of these values. SPM concentrations were then computed from image-derived values of backscattering coefficients and estimated value of $b_{\text{spm}}(0.55) \approx 0.0321 \, \text{m}^2 \, \text{g}^{-1}$. Fig. 4-b shows measured versus derived concentrations of SPM. The $R^2$ is above 0.94 with root mean of squared-errors being less than 3 g m$^{-3}$. The relative errors between measured and derive values of SPM concentrations does not exceed 21% for all validation sites.

Fig. 5 shows the derived images of aerosol reflectance and SPM backscattering from RR-MERIS image acquired over the Poyang Lake during the field measurement. Remarkably, our method is able to remove the aerosol effects and retain the spatial variability of SPM in the Lake.

4.2.2. Kenyan coast and SEVIRI match-ups

We used the red (0.56–0.71 μm) and near-infrared (0.74–0.88 μm) bands of SEVIRI centered at 0.6 and 0.8 μm respectively. Our method was slightly modified to be applied on SEVIRI’s visible

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Fig. 3. The relative errors % in the retrieved concentrations of SPM at 95% of confidence i.e. mean ± 2 × standard deviation.
bands. Basically, only the cost function Eq. (28) was minimized, i.e. solving the simultaneous equations (6) and (21). Note that the red band of SEVIRI (0.56–0.71 $\mu m$) covers the spectral absorption peak of chlorophyll-a around 0.68 $\mu m$. In the validation process and match-up sites, we accounted for the effects of chlorophyll-a absorption in the red band of SEVIRI using in-situ measured values of chlorophyll-a concentrations and the model of Morel (1991):

$$a(\lambda) = \left[ a_w(\lambda) + 0.06a_{\text{phy}}' (\lambda) C_{\text{phy}}^{0.65} \right] \times \left[ 1 + 0.2 \exp(-0.014(\lambda - 440)) \right]$$

(31)

where $a(\lambda)$ is the total absorption; $a_{\text{phy}}' (\lambda)$ is a statistically derived coefficient, its value was taken from Priour and Sathyendranath (1981); $C_{\text{phy}}$ is the measured concentration of chlorophyll in mg m$^{-3}$. Fig. 6-a shows that the relationship between derived values of $b_{\text{spm}}(0.55)$ and $C_{\text{spm}}$ is linear in a narrow range of SPM concentrations between 20 and 40 g m$^{-3}$. The specific backscattering coefficient was estimated following the same approach in Section (4.2.1): from three calibration-match-up sites (circles in Fig. 6-a), we computed the corresponding values of $b_{\text{spm}}(0.55)$ and then took the average of these values. The estimated value of $b_{\text{spm}}(0.55)$ for SPM in the Kenyan coastal waters was $\approx 0.001612$ m$^2$ g$^{-1}$. We will use this value to estimate the concentrations of SPM in the match-up pixels of SEVIRI. Derived values of SPM concentrations (Fig. 6-b) agree with measured values. The $R^2$ is above 0.7 and the RMSE value is less than 5 g m$^{-3}$. The relative errors in derived SPM concentrations are less than 30%.

4.2.3. Demonstration with EO data

The resulting values of SPM backscattering coefficients and aerosol reflectance are shown in Fig. 7. Remarkably, our method has derived realistic patterns of SPM spatial variability and dynamics. Moreover, the estimated maps of aerosol reflectance and SPM backscattering are spatially independent.

5. Discussion

5.1. Formulation

The approximation of Gordon et al. (1983) was only used to calculate the ratio $T(1)/T(3)$ in the bound Eq. (19). Note that we
formulated the cost functions in such way that they are independent of the diffuse transmittance $T$, i.e. Eqs. (23) and (29) do not contain $T$. Thus using the approximating of Gordon et al. (1983) will slightly affect the lower bound of the water ratio $a_{l (s, l)}$.

We derived two cost functions in our formulations Eqs. (29) and (23). Equation (29) can be regarded as a priori judgement about the likelihood of the resulting water leaving reflectance at band $l$, while Eq. (23) measures the agreement of the SPM derived from two different quantities. Minimizing one of these functions will improve the accuracy of one parameter while the accuracy of the other parameter is deteriorated. This behavior of Eq. (23) and Eq. (29) with respect to the sought variables, i.e. $a_{l (s, l)}$ and $\ell_{l (s, l)}$ was shown in Fig. 2.

5.2. Performance

5.2.1. Simulated data

Fig. 2 shows that the sensitivity of Eqs. (23) and (29) to $a_{l (s, l)}$ is proportional to aerosol optical thickness. On the other hand, the sensitivity of Eq. (23) to $a_{l (s, l)}$ is inversely proportional to SPM concentrations. So we can expect that the performance of our method will be limited to specific range of SPM and better for large values of aerosol optical thickness. Table 2 shows that, for the SPM range between 7 and 400 g m$^{-3}$, the derived values of SPM concentrations are independent of aerosol types and optical thicknesses. The relative errors of derived SPM in this range, are less than 1%. The reduced sensitivity of the water ratio w.r.t increased SPM concentrations resulted in large relative errors (up to 28%) less than 1%. The reduced sensitivity of the water ratio w.r.t increased SPM concentrations is independent of aerosol types and optical thicknesses. Minimizing one of these functions will improve the accuracy of one parameter while the accuracy of the other parameter is deteriorated. This behavior of Eq. (23) and Eq. (29) with respect to the sought variables, i.e. $a_{l (s, l)}$ and $\ell_{l (s, l)}$ was shown in Fig. 2.

5.2.2. Sensitivity to noise

We used 0.5% of the corrected-reflectance to study the sensitivity of our method to random noise. To give the reader a more quantitative feeling of this value let us take the wavelength 0.865 $\mu$m as a reference band. The corrected-reflectance of our simulated data at 0.865 $\mu$m varied from 0.0055 to 0.0918% for SPM concentrations ranging from 5 to 500 g m$^{-3}$ respectively. A noise level of 0.5% for 5 g m$^{-3}$ of SPM would be equal to the noise-equivalent-reflectance of the RR-MERIS NIR (Doerffer, 2008). On the other hand, a noise level of 0.5% for 500 g m$^{-3}$ of SPM would be an order of magnitude larger than the noise-equivalent-reflectance of RR-MERIS. Note that Doerffer (2008) reported the values of noise-equivalent-radiance, i.e. mWm$^{-2}$sr$^{-1}$nm$^{-1}$. We converted the radiance to reflectance using a 40$^\circ$ sun zenith angle and averaged values of solar irradiance Neckel and Labs (1981).

The relative errors in estimated SPM from fluctuated data are less than 10% when the actual range of SPM was between >7 and <400 g m$^{-3}$ and increased with aerosol optical thickness. Note that the performance of our method is deteriorated with increased aerosol optical thickness. This can be explained by the sensitivity of Eqs. (23) and (29) to aerosol optical thickness. This sensitivity, on the one hand, will enhance derived SPM for high values of aerosol optical thickness and, on the other hand, it will deteriorate estimated SPM for noisy data. Large errors are also obtained for low values of SPM concentrations and aerosol optical thicknesses. This time, the sensitivity of Eq. (23) to SPM plays the major role in the accuracy of derived values. These findings were already anticipated in our formulations, i.e. there is a trade-off between Eqs. (23) and (29) and hence the accuracy of derived values w.r.t actual SPM concentrations and aerosol optical thicknesses.

5.3. Validation

5.3.1. Match-ups and generality

We applied our method to EO data using a constant value of $y = 1.7$, i.e. the spectral exponent of SPM backscattering coefficient. The exponent $y$ is related to the particle size of SPM. Any wrongly assumed $y$ will introduce large errors to the derived values of SPM backscattering coefficient at 0.55 $\mu$m. However, the effect of this assumption can be reduced with proper choice of the reference wavelength. For the used MERIS NIR bands (0.776, 0.865, 0.883) this will be 0.865 $\mu$m, i.e. derive $b_{b (spm)}(0.865)$ instead of $b_{b (spm)}(0.55)$. The maximum relative error in assuming $y = 1.7$, while it is 0.3, will not exceed 3% and 17% for wavelengths 0.883 and 0.775 $\mu$m respectively.

The validation results are consistent and show a strong linear relationship between derived SPM backscattering coefficients at 0.55 $\mu$m and measured values of SPM concentrations. However, derived MERIS values of SPM backscattering coefficients are an order of magnitude larger than those derived from SEVIRI. This can be attributed to the improved sensitivity of MERIS on SEVIRI. The low sensitivity of SEVIRI may explain why the sensor could not detect SPM concentrations above 40 g m$^{-3}$.

Three calibration-sites were selected to estimate the value of SPM specific backscattering coefficient. These sites were chosen such that their measured SPM values corresponded to maximum, minimum and median values. This choice was to: (1) limit the calibration set to three points; (2) cover the whole range of measured SPM concentrations. A larger number of calibration points would have improved...
Fig. 7. Derived aerosol reflectance and SPM backscattering at 0.55 μm from SEVIRI acquired on 10-02-2009 (a,b,c), FR-MERIS over the Yangtze Estuary acquired on 26-07-2008 (d,e) and RR-MERIS over the Makassar Strait acquired on 01-07-2004 (f,g). (c) is magnified from (b): the coastal region from Mauritania to Liberia.
the estimated values of $b_i^{\text{spm}}$ and hence SPM concentrations. However we used this, rather rough, estimation of $b_i^{\text{spm}}(0.55)$ to show that our method has derived good estimates of SPM backscattering coefficients.

The relative errors in derived SPM concentration are less than 20% for MERIS and 30% for SEVIRI. The $R^2$ value is larger than 0.94 for MERIS and >0.7 for SEVIRI’s derived SPM concentrations. The RMSE for MERIS and SEVIRI derived values are 2.74 and 4.2 g m$^{-3}$. These RMSE values are within the range of SPM actual variability, about 5 g m$^{-3}$ in both locations (see Table 1).

The proposed method derived spatially un-correlated maps of aerosol reflectance and SPM concentration. For instance, notice how the method retrieved the sediment plume in the south west part of the Poyang Lake in Fig. 5-b. On the other hand, aerosol reflectance Fig. 5-a has spatially homogeneous variability.

The proposed approach is generic in the sense that it derives either the concentration of SPM or its backscattering coefficient.

5.3.2. Demonstration with EO products

The dynamics of the Yangtze’s runoff into the Eastern China Sea is retrieved with a high degree of details (Fig. 7-e). High aerosol reflectance (Fig. 7-d) at the river banks and coastal shorelines are most likely to be results of adjacency effects, sand banks and bottom reflectance, rather than water turbidity. This is because at these near-land regions high water turbidity was also retrieved by our method (Fig. 7-d). In the Makassar Strait, our method is able to derive the spatial heterogeneity of SPM in the coastal areas of Kalamantan (Fig. 7-g). It is worth noting that benthic reflectance of the corals against the Berau Estuary (2 N, 118 E) is interpreted as high concentrations of SPM (Fig. 7-g) and totally removed from the aerosol map in Fig. (7-g). In other words, our method provides fairly accurate prior information on aerosol reflectance, even in shallow areas.

The performance of the proposed method was further tested with a SEVIRI image. Note that in Section (4.2.2) we processed subregions of SEVIRI images covering the Kenyan coastal water. To simplify the process of SEVIRI image, we neglected the effect of chlorophyll-a absorption on SEVIRI’s red band. We emphasize, however, that this assumption was made to demonstrate the “spatial” performance of the method. The absorption of chlorophyll-a should be taken into account as we did in the validation exercise using Eq. (31). Global products on chlorophyll-a are readily available from many sources, e.g. OceanColorWeb (2009) and ChloroGIN (2009). While our method derived, almost, constant values of SPM concentrations in the Atlantic Ocean, the method clearly retrieved the variability of SPM in coastal areas of the Noudadibou Peninsular in Mauritania and the Geba Estuary in Guinea-Bissauas (Fig. 7-c).

Note that we have applied the probabilistic approach of Cox and Munk (1954) on all images used in this work to remove the specular sea-surface reflectance.

Due to the geostationary orbit of SEVIRI, the sunglint effect, i.e. the intense specular reflection of sun light on the sea-surface, is extensively observed every day during several hours in the field-of-view of SEVIRI (Ipe et al. 2003). In this work we define sunglint as being that part of sea-surface reflectance that precludes the retrieval and have values at NIR above 80% of the total reflectance (Montagner et al. 2003). All sunglint contaminated pixels were masked in our work. For example, see the masked pixels in Fig. (7-a,b) located at southwest region of Gulf Guinea.

5.4. Limitations

There are few considerations that should be taken into account when using our proposed method:

(1) Using Eq. (14) and neglecting the coupled term $\rho_a$ at the NIR is applicable for low values of aerosol optical thickness. Therefore the proposed method will be sensitive to the value of aerosol optical thickness.

(2) In water with SPM concentrations $\leq 7$ g m$^{-3}$ half percent of relative fluctuations introduced up to 30% of relative errors.

(3) The approximations in the semi-analytical water model Eq. (7) do not reflect the characteristics of highly turbid waters. The ratio of up-welling radiance to irradiance, i.e. Q factor, under-water surface is usually anisotropic and differs from $\pi$.

6. Conclusions

The spatial variability of the aerosol and water signals at the NIR are characteristic features of turbid estuarine and coastal waters. This variability can be attributed to the different aerosol types that may co-exist in this transaction zone as well as to the distinctive shape of the water leaving reflectance. Considering and quantifying this variability were the objectives of this work. In this paper we proposed an approach to account for the water leaving reflectance at the NIR. The model estimated the values of the water ratio and the aerosol ratio from the TOA reflectance simultaneously. The following conclusions are drawn from the presented results:

(1) The method served as a first step towards a more elaborative atmospheric correction and constituent quantification from orbital ocean color and geostationary sensors.

(2) The method is generic and can be applied to derive SPM concentrations and/or backscattering coefficients.

(3) The proposed method is accurate and invariant to aerosol type and optical thickness and random noise for a wide range of SPM concentrations; between 7 and 400 g m$^{-3}$.

(4) The sensitivity of the sensor plays an important role in the accuracy of the derived products. This is especially so at the NIR part of the spectrum. The sensitivity of SEVIRI is adequate to quantify SPM concentration between 20 and 40 g m$^{-3}$ using the proposed method.

(5) Our method derived realistic patterns of SPM dynamics in turbid waters which are spatially un-correlated to aerosol reflectance.

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A. Used symbols and terminology

Table A.1. Description of the used symbols and terminology in this study.

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>(q(\lambda))</td>
<td>bulk absorption coefficient</td>
<td>(m^{-1})</td>
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<td>(\sigma_{\text{phy}}(\lambda))</td>
<td>statistically derived coefficient</td>
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<td>(a_\text{abs}(\lambda))</td>
<td>absorption coefficient of water molecules</td>
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<td>(b_\lambda)</td>
<td>bulk backscattering coefficient</td>
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<td>specific backscattering coefficient of suspended sediment</td>
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<td>(l_r)</td>
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<td>spectral slope of (b_\text{l}(\lambda))</td>
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<td>(C_{\text{spm}})</td>
<td>concentration of suspended particulate matter</td>
<td>(g m^{-3})</td>
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<td>(C_{\text{phy}})</td>
<td>concentration of chlorophyll-a</td>
<td>(mg m^{-3})</td>
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<td>(Q)</td>
<td>the ratio of up-welling radiance to up-welling irradiance</td>
<td>(sr)</td>
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<td>(\Gamma(\lambda))</td>
<td>diffuse atmospheric transmittance</td>
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<td>the ratio of water leaving reflectance at two wavelengths: (s) and (l)</td>
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<td>(\delta)</td>
<td>Angstrom exponent of aerosol</td>
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<td>(\rho'_{\text{L}})</td>
<td>the ratio (\rho(0.534)/1)</td>
<td>(sr^{-1})</td>
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Term Description

EO Earth observation
FR-MERIS Full resolution MERIS
IOP Inherent optical properties
MERIS Medium resolution imaging Spectrometer
MSG Meteosat second generation
NER Noise-equivalent-radiance
NIR near-infrared
RMSE Root mean of squared error
RR-MERIS Reduced resolution MERIS
SEVIRI Spinning enhanced visible and infrared imager
SIOP Specific inherent optical properties
SNR Signal to noise ratio
SPM Suspended particulate matters
TOA Top of atmosphere

B. Additional tables: measured versus derived values

Table B.1. Measured values of SPM concentration and derived values of \(b_{\text{h}(\text{SPM})(550)}\) from the match up pixels of MERIS. SPM concentrations were derived as \(b_{\text{h}(\text{SPM})(550)})/0.0321\), the relative error is computed between measured and derived SPM concentrations. (*) indicate the used (concentration, \(b_{\text{h}(\text{SPM})(550)}) pair to compute \(b_{\text{h}(\text{SPM})(550)}\).
## References

Albert, A., Gege, P. 2006. Inversion of irradiance and remote sensing reflectance in shallow water between 400 and 800 nm for calculations of water and bottom properties. Applied Optics 45 (10), 2331–2343.


