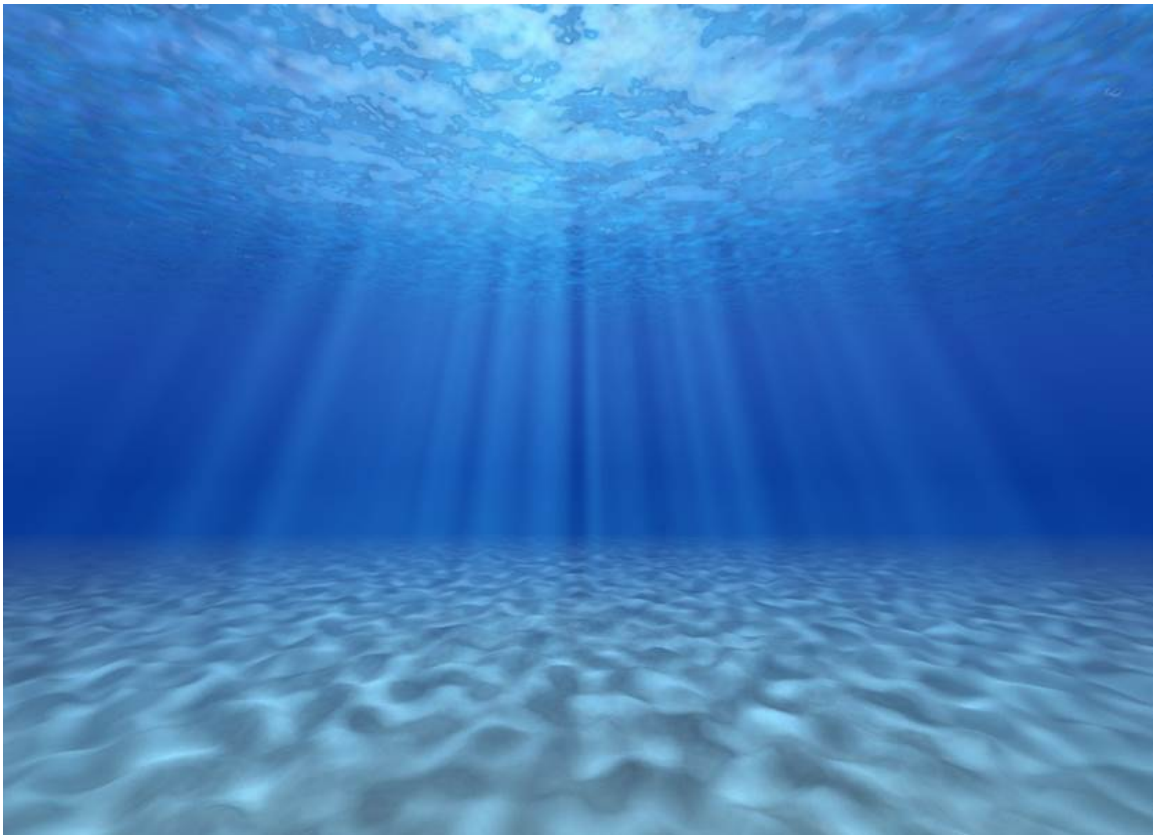
Sentinel-3 OLCI Inherent Optical Properties

Algorithm Theoretical Basis Documents

ATBD



Date: 31 July 2019

EUMETSAT contract: 17/214791

EUMETSAT Ref.: EUM/RSP/REP/20/1160644

Acronyms

ATBD	Algorithm Theoretical Basis Documents
ESA	European Space Agency
IOPs	Inherent Optical Properties
OLCI	Ocean and Land Colour Imager
WCP	Water classification product
OWT	Optical water types
SVD	Single value decomposition

Symbol	definition	Dimension
Geometry, wavelengths, others		
λ	Wavelength	nm
θ_s	Sun Zenith Angle	Degrees
μ_w	Cosine of the angle of refraction of the solar beam just beneath the sea surface	
η	Ratio of molecular scattering to total scattering	
Radiometry and Apparent Optical Properties (AOPs)		
R_{rs}	Remote Sensing Reflectance (above water)	sr^{-1}
r_{rs}	Remote Sensing Reflectance (bellow water)	sr^{-1}
K_d	Attenuation coefficient for downwelling irradiance	m^{-1}
Inherent Optical Properties (IOPs)		
$a(\lambda)$	Total absorption coefficient	m^{-1}
$a_w(\lambda)$	Water absorption coefficient	m^{-1}
$a_{nw}(\lambda)$	Non water absorption coefficient	m^{-1}
$a_{phy}(\lambda)$	Phytoplankton absorption coefficient	m^{-1}
$a^*_{phy}(\lambda)$	Phytoplankton specific absorption coefficient	$m^2\ mg^{-1}$
$a_{cdm}(\lambda)$	Colored Dissolved Matter absorption coefficient	m^{-1}
$a_{CDOM}(\lambda)$	Colored Dissolved Organic Matter absorption coefficient	m^{-1}
$b_b(\lambda)$	Total backscattering coefficient	m^{-1}
$b_{bp}(\lambda)$	Water backscattering coefficient	m^{-1}
$b_w(\lambda)$	Particulate backscattering coefficient	m^{-1}
S	CDOM spectral slope	m^{-1}
Y	Particle backscattering slope	m^{-1}

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1 INTRODUCTION

1.1 Purpose and Scope

This Algorithm Theoretical Basis Document (ATBD) is written for the Level-2 product of aquatic Inherent Optical Properties from the Ocean and Land Colour Instrument (OLCI) on board of the European Commission Earth Observation Sentinel-3 satellite. The purpose of this document is to describe the final algorithm (the "two-step algorithm") which has been selected, among others after an evaluation procedure, to estimate different Inherent Optical Properties (IOPs) from OLCI observations.

1.2 Algorithm identification

The two-step algorithm is identified under reference "EUM/RSP/REP/20/1160644" in the Sentinel-3 OLCI documentation. In this document, it will be referred to as a "two-step semi-analytical algorithm", 2SAA.

2 ALGORITHM OVERVIEW

2.1 Objectives

The objective is to derive several bio optical products from the spectrum of OLCI remote sensing reflectance, $R_{rs}(\lambda)$. The following products can be derived from 2SAA (bands Oa2 412.5nm and Oa3 442.5nm are abbreviated as 412 and 443nm):

- The diffuse attenuation coefficient for downward irradiance, $K_d(\lambda)$, (in m^{-1}) at 400, 412, 443, 490, 510, 560, 620, and 665 nm.
- The non-water absorption coefficients, a_{nw} and particulate backscattering coefficient, b_{bp}, (in m^{-1}) at 400, 412, 443, 490, 510, 560, 620, and 665 nm.
- The absorption by phytoplankton, a_{phy}, and colored detrital matter, a_{cdm} at 400, 412, 443, 490, 510, 560, 620, and 665 nm (all in m^{-1}).
- The absorption by colored dissolved organic matter, $a_{cdom}(443)$ (in m^{-1})

The selected products recommended for operational generation are the following:

- The non-water absorption coefficient, a_{nw} (443), and particulate backscattering coefficient, b_{bp} (443)
- The absorption coefficient by colored detrital matter, a_{cdm} (443)
- The absorption coefficient by phytoplankton, a_{phy} (443)
- The absorption coefficient by colored dissolved organic matter, a_{cdom} (443)

- The spectral slope of $b_{bp}(\lambda)$, *Y*
- The vertical diffuse attenuation coefficient for downward irradiance at 490 nm, K_d (490)
- Optical Water Class (OWC)

Another set of parameters will be provided as measurements of uncertainty:

- The percentage of error during the R_{rs} reconstruction
- The percentage of uncertainty based of the given water class (fixed)
- A flag addressing the possible failures during the inversion

For users requiring all IOP products in all OLCI spectral bands, a SNAP plugin will be delivered for processing of these products from operational OLCI Level-2 products:

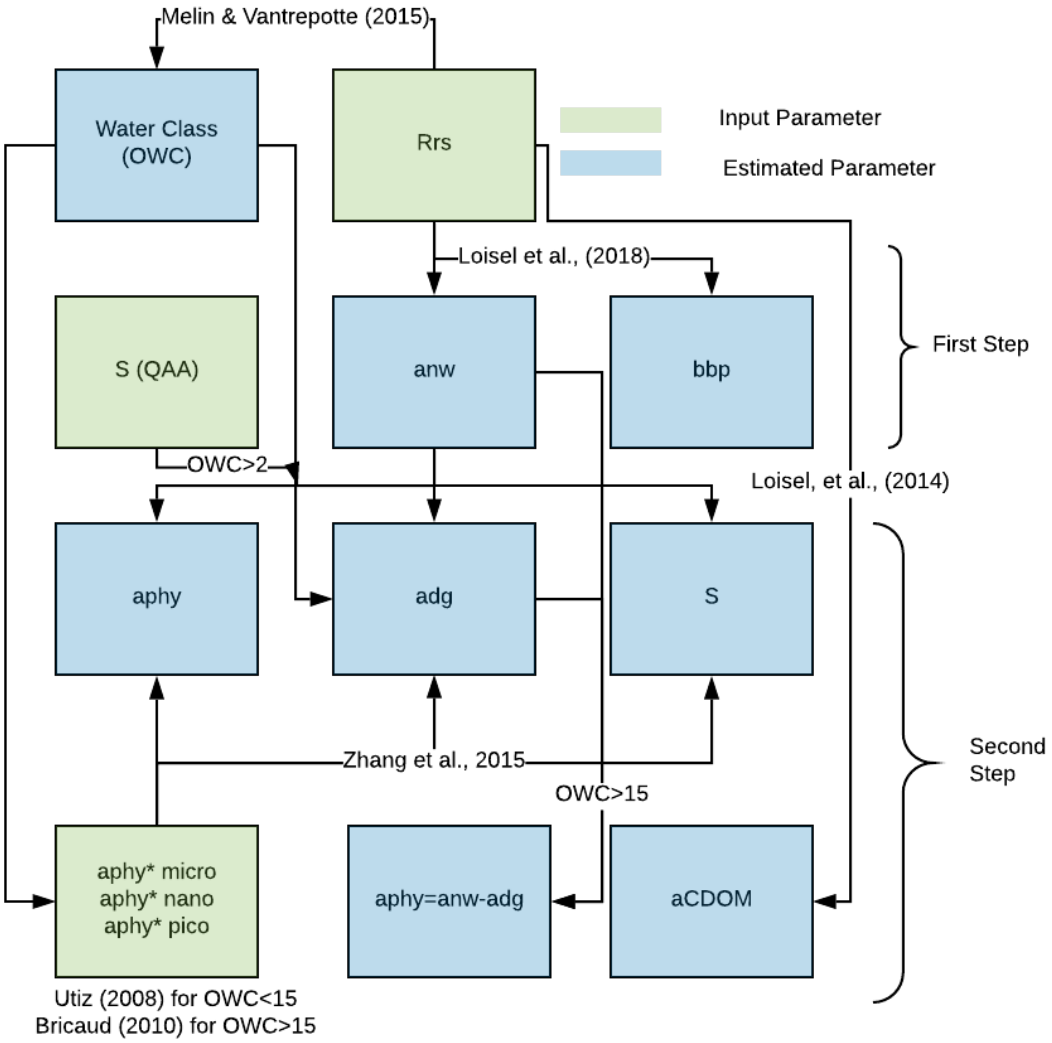
- The non-water absorption coefficient and particulate backscattering coefficient at 400, 412, 443, 490, 510, 560, 620, and 665 nm.
- The vertical diffuse attenuation coefficient for downward irradiance at 490 nm.
- The absorption coefficient by phytoplankton and colored detrital matter at 400, 412, 443, 490, 510, 560, 620, and 665 nm.
- The absorption by colored dissolved organic matter at 443 nm.

3 ALGORITHM DESCRIPTION

3.1 Implementation workflow

The general workflow of the algorithm can be divided in two steps. First, a_{nw} and b_{bp} will be estimated in the first step from the Loisel et al. (2018) algorithm. Then, a_{cdm} and a_{phy} will be estimated in the second step mainly based on the algorithm of Zhang et al., (2015) which has been slightly modified using optical water classes (OWC) (Melin and Vantrepotte, 2015). The original version of the Zhang et al. (2015) algorithm requires the spectral values of a^*_{phy} for three phytoplankton size classes (pico, nano, micro-phytoplankton), and automatically calculate the spectral shape of a_{cdm}, S_{cdm}. Two different a^*_{phy} references spectra are used in 2SAA. If the class belongs to 15 or higher (clear waters) the algorithm uses the a^*_{phy} provided by Bricaud et al. (2010), otherwise the algorithm uses the original a^*_{phy} from Uitz et al. (2008), as it is used in Zhang et al. (2015).This step is necessary to increase the precision in extremely clear waters. The estimation of S_{cdm} was also done based on OWC. If the pixel belongs to an optically complex waters (class 1 and 2), the algorithm uses the full Zhang et al. (2015) optimization techniques, otherwise the formulation of Lee et al (2009) to estimate S_{cdm} is used.

Note that 2SSA only addresses the total phytoplankton absorption, so the a_{phy} for each size class is not discussed here since it was not tested. Lastly the algorithm also retrieve a_{phy} in two different ways. If the class is strictly under 15, Zhang et al. (2015) optimization is used, otherwise a_{phy} is estimated by subtracting a_{cdm} from a_{nw}.



3.2 Estimation of the total absorption and backscattering coefficients

The proposed algorithm is the "LS2" semi analytical algorithm developed by Loisel et al. (2018). It is the last version of the original LS1 algorithm, proposed in Loisel & Stramski (2000). The LS2 model was developed on the basis of radiative transfer simulations to enable the estimation of two IOPs, the total absorption, $a(\lambda)$, and backscattering, $b_b(\lambda)$, coefficients within the surface ocean, from the Remote Sensing Reflectance, $R_{rs}(\lambda)$ (sr^{-1}), and the average attenuation coefficient for downwelling irradiance, $< K_d >_1$ (m^{-1}). It also includes the

correction by Raman scattering by water molecules, which can be significant for clear waters.

The algorithm can be written as:

$$\frac{b_b}{< K_d >_1} = f(R_{rs})$$

$$\frac{< K_d >_1}{a} = g(R_{rs})$$

where the functions f and g depend on the ratio of molecular scattering to total scattering, η, and sun zenith angle, θ_s, or equivalently μ_w(cos(arcsin(sin(θ_s)/1.34))). η is calculated as in Loisel et al. (2018) which requires the chlorophyll-a concentration.

The first equation can be rewritten as:

$$b_b =< K_d >_1 [b_{b1}(\eta, \mu_w)R_{rs} + b_{b2}(\eta, \mu_w)R_{rs}^2 + b_{b3}(\eta, \mu_w)R_{rs}^3]$$

Where the coefficients b_{b1}, b_{b2} and b_{b3} vary as a function of η and μ_w.

In the same way:

$$a =< K_d >_1 / [a_1(\eta, \mu_w) + a_2(\eta, \mu_w)R_{rs}^1 + a_3(\eta, \mu_w)R_{rs}^2 + a_4(\eta, \mu_w)R_{rs}^3]$$

Where the coefficients b_{b1}, b_{b2} and b_{b3} vary as a function of η and μ_w. Specific values of the coefficients a_i and b_{bi} are provided in a look-up-table and an interpolation procedure is applied to calculate these coefficients for intermediate values of η and μ_w that are not included in the look-up table.

The last parameter needed for LS2 inversion is the diffuse attenuation coefficient for downwelling radiance ($< K_d >_1$). The algorithm of Jamet et al. (2012) is based on a neural network approach which allows the estimation of $< K_d >_1$ at any wavelength between 412 and 670 nm from $R_{rs}(\lambda)$. For the LS2, a modified version of Jamet et al. (2012) was implemented, to improve the retrieval accuracy in very oligotrophic and turbid waters. In this case, the model calculates the ratio between R_{rs} at 490 and 555 nm and if it is lower or equal to 0.85, the neural networks use all R_{rs} values between 443 and 670 nm as input parameters. In this case, the neural network has two hidden layers with five neurons for each layer. On the other hand, if the R_{rs} is higher than 0.85, the neural network ignores the red part of the spectrum. In this case, the neural network has two hidden layers with four neurons for each layer. This difference for clear waters is due to the low signal and high signal-to-noise ratio when compared to other bands. For both cases, $< K_d >_1$ is estimated for all OLCI bands, and in each case, the algorithm architecture combines a minimal error with a minimal number of neurons. The neural network additionally inputs the solar geometry to allow for more accurate $< K_d >_1$ retrieval.

The non-water absorption coefficient, $a_{nw}(\lambda)$, and particulate backscattering, $b_{bp}(\lambda)$, coefficients are estimated from $a(\lambda)$ and $b_b(\lambda)$ for which the pure sea water absorption and backscattering coefficients have been removed. The $a_w(\lambda)$ and $b_{bw}(\lambda)$ values are estimated from Mason et al. (2016) and Zhang et al. (2009), respectively. The implementation of the Temperature and Salinity dependence of $b_{bw}(\lambda)$ is done following Werdell et al. (2013).

The calculation of *Y* is done through a linear regression analysis between $\text{Log}(b_{bp}(\lambda))$ and $\text{Log}(\lambda)$. For that purpose, only the $b_{bp}(\lambda)$ values at 443, 490, 510 and 560 nm are used.

3.3 Water classification approach

The optical water classes (OWC) considered are based on the work of Melin & Vantrepotte (2015) where they applied a classification method of waters with a broad range of bio optical properties. Sixteen OWC were initially defined by these authors in their initial paper, an additional 17th optical class has then been added in order to take into account the ultra-oligotrophic waters of the oceanic gyres. These OWC were defined by Mélin and Vantrepotte (2015) considering a training data set of normalized R_{rs} spectra (Figure 1).

The classification then consists in calculating the class membership of a given R_{rs} spectrum to each of the 17 OWC which is defined statistically by its average spectrum, μ (normalized and log transformed reflectance data), and a covariance matrix, $\sum$.

$$r_n = \frac{R_{rs}}{\int_{\lambda 1}^{\lambda 2} R_{rs}\, d\lambda}$$

Then, the classification method calculates the distance between the log value of the normalized input spectrum (x = $\log(r_n)$) and the given class ic using the squared Mahalanobis distance Δ_{ic}^2:

$$\Delta_{ic}^2(x) = (x - \mu_{ic})^T \sum_{ic}^{-1} (x - \mu_{ic})$$

where T indicates the matrix transpose. As a first approximation, this distance was used to quantify the proximity between an unknown R_{rs} spectra x and the R_{rs} data sets corresponding to the different optical classes defined in Mélin and Vantrepotte (2015), μ_{ic}. It has to be compared to a theoretical threshold (Δ_T^2) provided from the Chi-square distribution which represents a given percentage of the data distribution for a degree of freedom corresponding to the dimension d (i.e. the number of wavelengths considered for testing the correspondence

between satellite R_{rs} spectra and those associated with the referenced optical classes (Vantrepotte et al. (2012)).

Note that an accurate estimation of the class membership probability associated with an unknown spectrum (like through the fuzzy logic approach described in Moore et al., 2001, Mélin and Vantrepotte 2015) would provide more precise information, particularly useful in deriving class based inversion algorithms using OWCs.

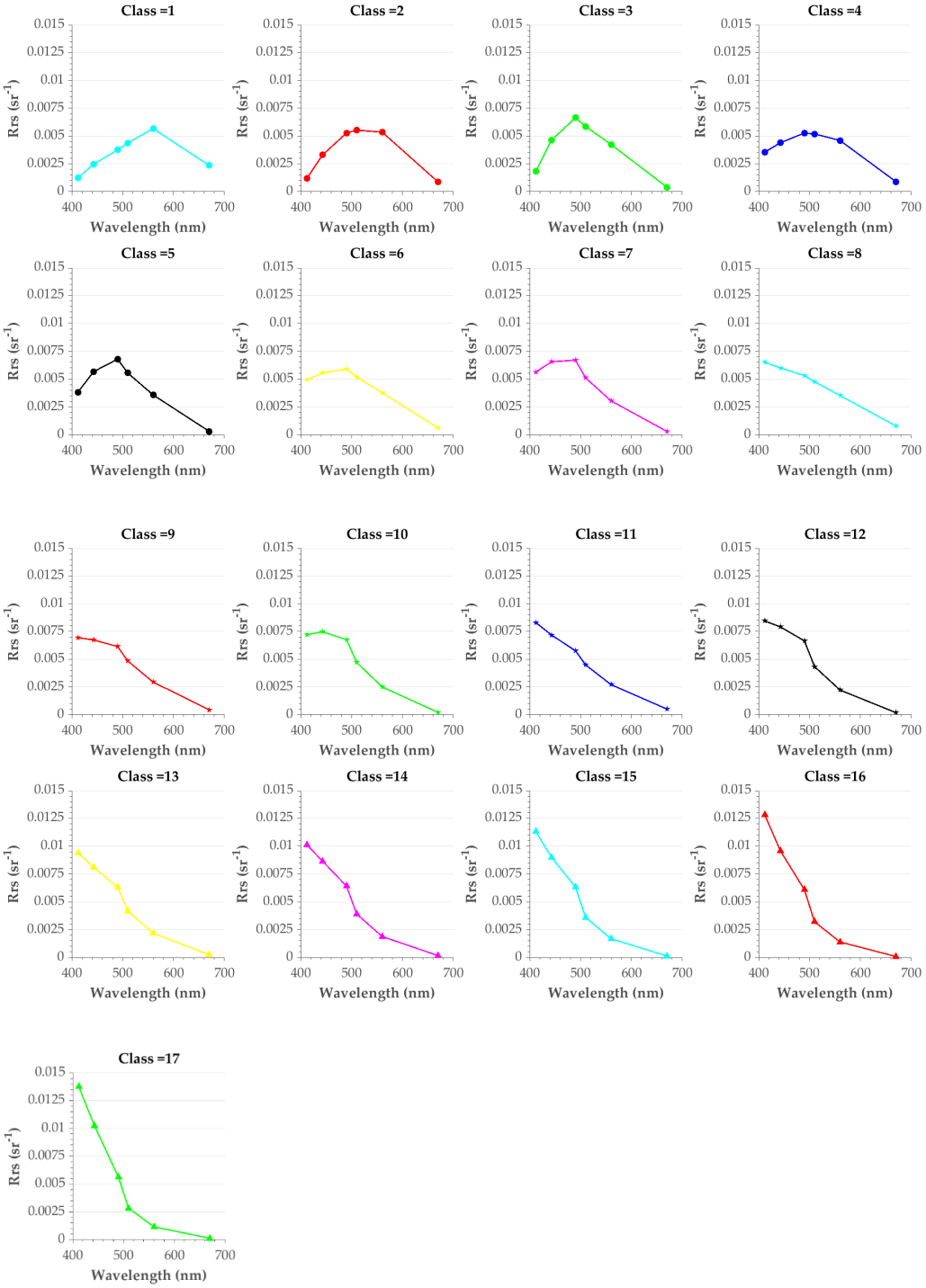


Figure 1: Illustration of the mean spectrum associated with the 17 OWT considered in the frame of this study (16 from Mélin and Vantrepotte, 2015 + 1 OWT for gyre area). Unclassified spectra are flagged as class -1.

3.4 Estimation of the absorption by phytoplankton and colored dissolved organic matter

The step 2 inversion is based on the model of Zhang et al. (2015) in which $a_{nw}(\lambda)$ is fractioned into $a_{phy}(\lambda)$ and $a_{cdm}(\lambda)$, where specific absorption a^*_{phy} is further decomposed in three size classes: micro, nano and picoplankton. For each phytoplankton size class, the specific absorption spectrum is assumed from Uitz et al. (2008). For a_{cdm} the authors assumed the specific absorption spectra normalized at 400 nm as wavelength-dependent exponential $a^*_{cdm} = e^{(-S(\lambda-400))}$. Consequently,

$$a(\lambda) = \sum_{i=1}^{M} m_i a_i^*(\lambda)$$

where M is the number of constituents, $a_i^*(\lambda)$ is the specific absorption of constituent i at λ (eigenvector), and m_i is its specific contribution (eigenvalue). The eigenvectors were constructed to avoid either singularity or ill-condition, which requires that for any given a_i^* the difference to the other constituents (a_j^*) is beyond a certain threshold. For this algorithm, the threshold $S_{i,j}$ was set at 0.1 and is calculated as follows:

$$S_{i,j} = \frac{2}{BN} \sum_{k=1}^{BN} \left| \frac{a_i^*(\lambda_k) - a_j^*(\lambda_k)}{a_i^*(\lambda_k) + a_j^*(\lambda_k)} \right|$$

where BN stands for band number. The authors used a non-negative optimization scheme to obtain the absorption fractions, and this process can be done in two different ways based on which OWC the R_{rs} spectrum belongs to. First, the $a_{cdm}(\lambda)$ slope (S) is estimated from the a_{nw} as originally done in Zhang et al. (2015) for OWC 1 and 2. For OWC between 3 and 17, S is directly calculated using a similar equation as developed in Lee et al. (2009) which has been slightly adapted for 2SAA :

$$S_{cdm} = 0.019 + \left(\frac{0.002}{0.6 + r_{rs}(443)/r_{rs}(560)} \right)$$

where r_{rs} is the remote sensing reflectance bellow water which is linked to R_{rs} as follows: $r_{rs} = R_{rs}/(0.52+1.7R_{rs})$.

In the second part of the algorithm, a single value decomposition (SVD) is used to optimize the eigenvalues and extract the corresponding fractions. The algorithm uses the proposed eigenvectors (specific absorption spectra) to extract chlorophyll-a for each size class and a_{cdm} at reference wavelength. From the chorophyll-a and the specific absorptions spectrum, the model can reconstruct a_{phy}. A distinct characteristic of Zhang et al. (2015) model is the use of a non-negative optimization, in which all the solutions are feasible. The model

can use R_{rs} at any number of wavelengths as input during the optimization, and will give the full spectrum as output. For this optimization, the bands 412, 443, 490 and 510 proved to be the most accurate. Lastly the algorithm reconstructs a_{phy} in two different ways. If the class is 14 or bellow, the Zhang et al. (2015) optimization is used, and the a_{phy} is the sum of a_{phy} of each size class, otherwise a_{phy} is estimated by subtracting a_{cdm} from a_{nw}. This procedure is required because of the low values of a_{phy} in very oligotrophic waters (Bricaud et al. 2010), typically in gyres, and the higher sensitivity to noise in the inversion of of a_{phy} compared to a_{cdm}.

3.5 Estimation of the colored dissolved organic matter

The last output generated in the proposed model is $a_{cdom}(443)$, based on the algorithm described in Loisel et al. (2014). The algorithm assumes that $K_d(443)$ is mainly driven by the absorption coefficient. So, for wavelengths in which the absorption by CDOM is dominant, we can describe K_d as follows:

$$K_d(443) = K_w(443) + f\big(a_{cdom}(443)\big) + \Delta_p(443)$$

where $K_w(443)$ is the diffuse attenuation coefficient for a pure sea water body, $f\big(a_{CDOM}(443)\big)$ is a function that only depends on the absorption coefficient by CDOM at 443 nm, and $\Delta_p(443)$ is the residual term accounting for impact of scattering and absorption of particulate matters on the $K_d(443)$ values.

The effect of particulate scattering and absorption on $K_d(443)$ can be partially assessed using an appropriated wavelength, at which colored dissolved organic matter has a negligible or limited effect due to the dominating impact of pure sea water and particulate IOPs. In this case, the wavelength chosen is 560nm. As such, based on the equation previously described, a fit was constructed between the attenuation dominated by the effect of CDOM (X) and the a_{CDOM} at 443 nm. For this algorithm, a linear fit performed on the IOCCG in situ data set was the most adequate, and it can be defined as:

$$a_{CDOM}(443) = 10^{[a1\ log10(X)+b1]}$$

where a1 and b1 are equal to 0.9902 and -0.0522, respectively, $X = Y - (\Delta_p(443) - \Delta_p(560))$ and $Y = \big(K_d(443) - K_w(443)\big) - (K_d(560) - \big(K_w(560)\big)$

The term X is retrieved by dividing the equation in two parts, the contribution from K_d and K_w (term Y), and the contribution from Δ_p. The calculation of the term Y is done using a neural network approach based on Loisel et al. 2018 and Jamet et al. 2012, meanwhile the term $\Delta_p(443) - \Delta_p(560)$ is calculated as follows:

$$\Delta_p(443) - \Delta_p(560) = 10^{[a2\ log_{10}(Y)+b2]}$$

where a2 and b2 are equal to 0.906 and -0.5259 respectively, and Y is the term estimated by the neural network.

4 CRITERIA APPLIED TO CONSIDER A PIXEL VALID

During the implementation of the algorithm, different criteria were used to consider the pixel valid or not. For the first step of the inversion (LS2), the following criteria are used, otherwise the pixel is set as flagged, and no output is given for a_{nw} and b_{bp}:

- The input R_{rs} at 443, 490, 510 and 560 nm need to be positive.
- Retrieved K_d need to be positive for all wavelengths.

For the Y product, the value of R^2 and the Significance Level based on the value of R and the degrees of freedom will be provided to the user as a parameter of uncertainty.

For the second step of the algorithm, the criteria are specific to the Zhang et al. (2015) algorithm. The optimization is done using a non-negative linear optimization, in which only positive values for $a_{cdm}(443)$ and Chlorophyll-a are accepted. Another criteria used during the optimization is the tolerance between the input a_{nw} and the reconstructed a_{nw}, which was set at 1.10^{-4}.

Lastly, a final set of criteria is used for all the retrieved parameters. The R_{rs} is reconstructed following Werdell et al. (2013) and the thresholds are set as such:

- -0.05<b_{bp}<1
- -0.05<a_{cdm}<10
- -0.05<a_{phy}<5
- ΔR_{rs}<33%

where ΔR_{rs} is calculated as follows:

$$\Delta R_{rs} = \frac{100\%}{N_\lambda} = \sum_{i=1}^{N_\lambda} \frac{\left|\hat{R}_{rs}(\lambda_i) - R_{rs}(\lambda_i)\right|}{R_{rs}(\lambda_i)}$$

where $\hat{R}_{rs}(\lambda_i)$ is the reconstructed R_{rs} at the wavelength i, and $R_{rs}(\lambda_i)$ is the measured R_{rs} at wavelength i. The value of ΔR_{rs} is provided as a standard product, allowing the end-user to have a certain confidence in the inversion process.

A table with all the flags used in 2SAA can be seen bellow:

Table 1 Specific flags for each parameter described in this section.

Flag name	Flag condition	Flag output
R_{rs} failure	ΔR_{rs}>33%	1
b_{bp} Failure	-0.05>b_{bp}>1	2
a_{cdm} Failure	-0.05>a_{cdm}>10	4
a_{phy} Failure	-0.05>a_{phy}>5	8
K_d Failure	K_d<0	16

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