SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM DEFINITION

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OLCI Level 2

Algorithm Theoretical Basis Document

Ocean Colour Products in Case 1 waters

("Clear Waters Ocean Colour Products" or "CWOC")

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1. INTRODUCTION

1.1 Purpose and scope

This Algorithm Theoretical Basis document (ATBD) is written for the Ocean and Land Colour Imager (OLCI) of the Earth Observation Mission Sentinel-3 of the European Space Agency (ESA).

The purpose of this document is to lay out algorithms for the OLCI ocean colour products in Case 1 waters. As much as possible, basic principles of the algorithm and the description of their various segments will refer to publications in the peer-reviewed scientific literature. When such literature exists, minimum information will be provided here for the sake of clarity, and the reader will be referred to the relevant literature for further information.

1.2 Acronyms

ATBD Algorithm Theoretical Basis Document

CDOM Colored Dissolved Organic Matter

ENVISAT Environmental Satellite
ESA European Space Agency

LOV Laboratoire d'Océanographie de Villefranche
MERIS Medium Resolution Imaging Spectrometer
NASA National Aeronautics & Space Administration

nLw Normalized Water-leaving radiance

NOMAD NASA bio-Optical Marine Algorithm Data set

OC Ocean Color

OLCI Ocean and Land Color Imager

PnB Plumes and Blooms (Bio-optics time series in the Santa Barbara Channel)

SeaWiFS Sea-viewing Wide Field-of-view Sensor Sentinel-3 Third series of "sentinel" (ESA satellites)

TOA Top of Atmosphere

UV Ultra Violet

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1.3 Symbols

Symbol	definition	Dimension / units
	demidon	Differision / drifts
Geometry, wavele	engths, others	
λ	Wavelength	nm
hetas	Sun zenith angle (μ s = $\cos(\theta$ s))	degrees
$ heta_{\! ext{V}}$	Satellite viewing angle ($\mu v = \cos(\theta v)$)	degrees
$arDelta \phi$	Azimuth difference between the sun-pixel and pixel-sensor half vertical planes	degrees
Chl	Chlorophyll concentration	mg m ⁻³
Radiometry and A	Apparent Optical properties (AOPs)	
$F_0(\lambda)$	Mean extraterrestrial spectral irradiance	$\mathrm{W}\;\mathrm{m}^{-2}\;\mathrm{nm}^{-1}$
$L(\lambda, \theta_s, \theta_v, \Delta\phi)$	Radiance	${ m W m}^{-2} { m nm}^{-1} { m sr}^{-1}$
$E_d(z)$	Downward irradiance at depth z	$\mathrm{W}~\mathrm{m}^{-2}~\mathrm{nm}^{-1}$
$E_{u}(z)$	Upward irradiance at depth z	W m ⁻² nm ⁻¹
$E_{d}(0^{+})$	Downward irradiance just above the sea surface	W m ⁻² nm ⁻¹
$R(\lambda, 0^{-})$	Diffuse reflectance at null depth, or irradiance ratio (E $_{u}$ / E $_{d}$)	dimensionless
	(upward and downward irradiances, respectively)	
$K_{d}(\lambda)$	Diffuse attenuation coefficient for the downward plane irradiance	m ⁻¹
$K_{w}(\lambda)$	Contribution of seawater to $K_d(\lambda)$	m^{-1}
f	Ratio of R(0 ⁻) to (b _b /a); subscript 0 when $\theta_S = 0$	dimensionless
f'	Ratio of R(0 ⁻) to ($b_b/(a+b_b)$); subscript 0 when $\theta_s = 0$	dimensionless
μ_d	Average cosine of the downward irradiance	dimensionless
$Q(\lambda,\theta s,\theta v,\Delta\phi)$	Factor describing the bidirectional character of $R(\lambda, 0)$ $Q = E_u / L_u$. Subscript 0 when $\theta_s = \theta_v = 0$,	sr
$ ho_{_{ m W}}(\lambda)$	Water-leaving reflectance (i.e., π L _w / E _d (0 ⁺))	dimensionless
$[\rho_{\mathrm{w}}]_{\mathrm{N}}(\lambda)$	Normalised water-leaving reflectance (i.e., the reflectance if	
	there were no atmosphere, and for $\theta_S = \theta_V = 0$)	
dimensionless		
Inherent optical p	properties (IOPs)	
$a(\lambda)$	Total absorption coefficient	m^{-1}
$a_w(\lambda)$	Water absorption coefficient	m^{-1}
$a_{ph}(\lambda)$ or $a_f(\lambda)$	Phytoplankton absorption coefficient	m^{-1}
$a_g(\lambda)$ or $a_{cdom}(\lambda)$	CDOM absorption coefficient	m^{-1}

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$a_{cdm}(\lambda)$	Coloured detrital material absorption coefficient	m ⁻¹
$b_b(\lambda)$	Total backscattering coefficient	m^{-1}
$b_{\rm bw}(\lambda)$	Water backscattering coefficient	m ⁻¹
$b_{bp}(\lambda)$	Particulate backscattering coefficient	m^{-1}

Air-water interface

 $\mathfrak{R}(\theta)$ Geometrical factor, accounting for all refraction and reflection dimensionless effects at the air-sea interface (Morel and Gentili, 1996)

$$\Re(\theta') = \left[\frac{(1-\overline{\rho})}{(1-\overline{r}\,R)} \frac{(1-\rho_F(\theta'))}{n^2}\right] \text{(subscript 0 when } \theta = 0)$$

where n is the refractive index of water dimensionless $\rho F(\theta)$ is the Fresnel reflection coefficient for incident angle θ dimensionless $\overline{\rho}$ is the mean reflection coefficient for the downward dimensionless irradiance at the sea surface

r is the average reflection for upwelling irradiance at the dimensionless water-air interface

 θ is the refracted viewing angle ($\theta = \sin^{-1}(n.\sin(\theta v))$) degrees

Others

 $t_d(\lambda, \theta_s)$ Upward diffuse atmospheric transmittance (pixel-to-sensor) dimensionless

 $t_s(\lambda, \theta_s)$ Downward global atmospheric transmittance $(E_d(0^+) / F_0 \mu_s)$ dimensionless

1.4 Algorithm identification

This algorithm is identified under reference "SD-03-C10" in the Sentinel-3 OLCI documentation.

In this document, it will be referred to as "CWOC", standing for "Clear-Water Ocean Colour Products".

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2. ALGORITHM OVERVIEW

2.1 Objectives

The objective is to derive several ocean colour products from the spectrum of the normalised water-leaving reflectances.

The following products are to be derived here:

- The chlorophyll concentration, Chl, expressed in units of mg (Chl) m⁻³.
- The diffuse attenuation coefficient for downward irradiance at 490 nm, K_d(490), expressed in units of m⁻¹.
- The total absorption and backscattering coefficients, a and bb, expressed in units of m⁻¹.
- The CDOM absorption coefficient, expressed in units of m⁻¹.

The proposed algorithms are from Morel et al. (2006; 2007a) (see also the latest version of the MERIS ATBD 2.9 for the chlorophyll concentration), and from Maritorena et al. (2002).

Note: the products presented here are all derived from various combinations of the fully normalized water-leaving reflectances. The latter are actually the main ocean colour product above Case 1 waters. There is no need to describe them in this document, however; they are simply the output of the atmospheric correction algorithm, for which a specific ATBD exists [SD-03-CO7].

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3. ALGORITHM DESCRIPTION

3.1 Theoretical Description

3.1.1 The chlorophyll concentration, Chl

The proposed algorithm is the "OC4Me" maximum-band-ratio (MBR) semi-analytical algorithm developed by Morel et al. (2007a). (*cf.* O'Reilly *et al.*, 1998 for a more general description of such algorithms)

It is the latest version of the MERIS pigment index algorithm, which is fully described in the MERIS ATBD 2.9¹ and in Morel et al. (2007a). A brief reminder is provided here:

OC4Me is a polynomial based on the use of a semi-analytical model, itself based on the analysis of AOPs measured *in situ* over the past decades in various oceanic regions (Morel 1988; Morel and Maritorena, 2001).

It is expressed as:

1
$$q [C k] = l \sum_{x=0}^{n} A_{i} (1_{1} Q_{i,j})^{x}$$
 (1)

where $\rho_{i,j}$ is the ratio of the irradiance reflectance, R, at band i (λ_i) to the irradiance reflectance at band j (λ_j). The value of this ratio is the maximum found among the 3 ratios formed with the following bands: 560 nm for λ_j , and 443 or 490 or 510 nm for λ_i . In Eq. (1), n is equal to 4.

Figures 1 and 2 show how the algorithm behaves.

The "A" coefficients to be used are (Morel et al., 2007a):

A_0	A_1	A_2	A_3	A_4
0.4502748	-3.259491	3.522731	-3.359422	0.949586

Because this algorithm uses R and the MERIS atmospheric correction provides directional reflectances, $\rho_{w'}$ a conversion is needed as follows:

$$R = \frac{\rho_w Q}{\pi \Re}$$
 (2)

The Q factor is from Morel et al., 2002 (it is chlorophyll-dependent so an iterative procedure is needed similarly as in Morel and Gentili, 1996).

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The \Re geometrical factor merges all reflection / refraction effects at the air-sea interface. It is defined as (Morel and Gentili, 1996):

$$\Re(\theta') = \left[\frac{(1 - \overline{\rho})}{(1 - \overline{r}R)} \frac{(1 - \rho_F(\theta'))}{n^2} \right] \text{ (subscript 0 when } \theta = 0)$$
 (3)

where

n is the refractive index of water

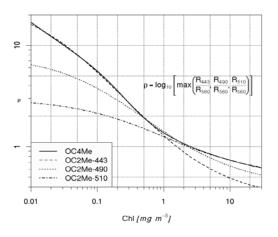
 $\rho F(\theta)$ is the Fresnel reflection coefficient for incident angle θ

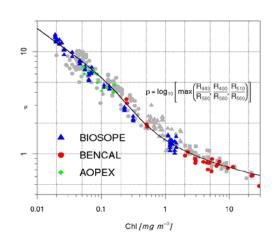
 $\bar{\rho}$ is the mean reflection coefficient for the downward irradiance at the sea surface

 \dot{r} is the average reflection for upward irradiance at the water-air interface

 θ is the refracted viewing angle ($\theta = \sin^{-1}(n \sin(\theta v))$)

In Eq. (3), the dependence of $\overline{\rho}$ and R on θ_s are neglected. This dependence was recently shown significant for low sun elevations by Wang (2006). It is here proposed to include this effect, which can be done easily by adding one more dimension to the R lookup tables currently in use.





 $\rho_{2,5}$, $\rho_{3,5}$, $\rho_{4,5}$ of reflectances at 443, 490, and 510 nm maximum band ratio technique, represented by the (indices 2, 3, and 4) to the reflectance at 560 nm (indice curve reproduced from Fig. 6, is compared to recent 5), as a function of the Chlorophyll concentration. The measurements of irradiance reflectance, made at sea corresponding algorithms making use of only 2 during the following cruises: Bencal (Benguela current, wavelengths are denoted OC2Me-443, OC2Me-490, and 2002), Biosope, (South-East Pacific, 2004), Aopex, OC2Me-510. The envelope of these three curves (Western Mediterranean Sea, 2004)." (maximum band ratio technique) forms the currently used MERIS algorithm, denoted OC4Me. The ρ is the log_{10} of the maximum of the 3 ($\rho_{2,5}$, $\rho_{3,5}$, $\rho_{4,5}$) ratios

Figure 1: Adapted from Fig. 6 of Morel 2007: Ratios Figure 2: Adapted from Fig. 7 of Morel 2007: "The

Recommendation: use the OC4Me algorithm, and include a θ_s -dependence in the \Re lookup table.

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3.1.2 The diffuse attenuation coefficient at 490 nm, $K_d(490)$

The diffuse attenuation coefficient for the downward plane irradiance at wavelength λ and at a given depth z is defined as:

$$K_d(\lambda) = -\left[1/E_d(z, \lambda)\right] \left[dE_d(z, \lambda)/dz\right] \quad \text{or} \quad K_d(\lambda) = -\left[d\left[lnE_d(z, \lambda)\right]/dz\right] \quad (3)$$

Many realisations of this coefficient are possible, as a function of the depth range over which it is computed. It can be a local coefficient around a given small depth interval between any depths z_1 and z_2 :

$$K_d(\lambda) = -\frac{1 \left[E_d(zg\lambda) / E_d(z_2, \lambda) \right]}{z_2 - z_1}$$
(5)

It can be computed for the upper layer defined from below the surface (0-) to a given depth z:

$$K_{d} = -\frac{1 \left[\frac{dE_{d}(z)}{E_{d}(0^{-})} \right]}{z}$$
 (6)

It can also be an E_d -weighted average value computed over a certain depth z, e.g., the 1% light level (Kirk, 2003):

$$K_{d,a}(\lambda) = \frac{\int_{0}^{z} K_{d}(z,\lambda)E_{d}(z,\lambda)d}{\int_{0}^{z} E_{d}(z,\lambda)dz}$$
(7)

Practically speaking, the K_d 's found in *in situ* data bases are essentially of the second category. The reason is simply that measuring properly $E_d(z)$ at sea requires that the irradiance sensor is placed at a depth where the irradiance fluctuations due to surface waves are small enough (or even absent). This depth can be as large as ~30 meters in clear waters. Then this $E_d(z)$ measurement is combined with the downward irradiance measured above the surface after it is multiplied by the transmission across the air-sea interface, which provides $E_d(0^-)$, in order to get K_d as per $E_d(6)$ above.

It is proposed here to use the "OK2-560" algorithm proposed by Morel et al. (2007a). It is based on the 490-560 reflectance ratio (see Fig. 3) and has the form:

$$K_{d}(4) = 9K_{w}(4) + 91 \sum_{x=0}^{n} A_{x}(1 + \rho_{0}, s_{0}) g^{x}_{60}$$
(8)

where $K_w(490)$ is 0.0166 m⁻¹, $\rho_{490,560}$ is the ratio of the irradiance reflectances at 490 and 560 nm, and the n+1=5 coefficients A_x have the values :

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A_0	A_1	A_2	A_3	A_4
-0,82789	-1,64219	0,90261	-1,62685	0,088504

Conversion from directional reflectances to irradiance reflectances is as per Eq. (2).

Recommendation: use the OK2-560 algorithm to determine $K_d(490)$.

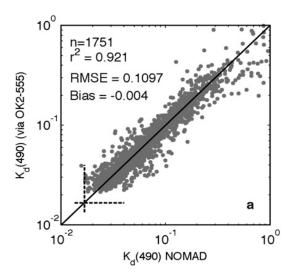


Figure 3: reproduced from Morel et al. (2007a): validation of the OK2-555 algorithm against the NOMAD in situ data set (Werdell and Bailey, 2005)

3.1.3 The total absorption and backscattering coefficients (a and bb)

Many algorithms have been proposed to derive inherent optical properties (IOPs), particularly the total absorption coefficient (a_t) and the total backscattering coefficients (b_b) , from various AOPs (very often from R_{rs} or from R and K_d). It is out of scope here to enter into these details, and the reader is referred to the comprehensive review by Gordon (2002) and to the IOCCG report N°5 (IOCCG, 2006).

In particular, the results of the inter-comparison presented in the IOCCG report don't reveal one algorithm as performing significantly better than the others (whatever their degree of complexity).

Therefore, it is proposed here to use a simple approach, as proposed by Morel et al. (2006); see their Eq. (10) to (13). This approach combines two equations (Gordon, 1989; Gordon et al., 1975; Morel and Gentili, 2004):

$$K_{d}(\lambda) = 1.0395 \left[a(\lambda) + b_{b}(\lambda) \right] / \mu_{d}$$
(9)

and

$$R(\lambda) = f' b_b(\lambda) / [a(\lambda) + b_b(\lambda)]$$
(10)

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which leads to

$$a(\lambda) = 0.962 \text{ K}_{d}(\lambda) \,\mu_{d}(\lambda, \,\theta_{s}, \,\text{Chl}) \,x \left[1 - R(\lambda) \,/\, f'(\lambda, \,\theta_{s}, \,\text{Chl})\right] \tag{11}$$

$$b_b(\lambda) = 0.962 \text{ K}_d(\lambda) \,\mu_d(\lambda, \,\theta_s, \,\text{Chl}) \,x \left[R(\lambda) \,/\, f'(\lambda, \,\theta_s, \,\text{Chl}) \right] \tag{12}$$

where the dependence of f' and μd on the sun zenith angle and Chl is explicitly introduced. These two parameters are taken from pre-computed lookup tables, following Morel et al. (2002).

To operate Eqs (11) and (12) $K_d(555)$ is derived from an algorithm similar to the OK2-560 but adapted to λ =555 nm and R(555) is derived from $\rho_w(555)$ through Eq. (2).

Because Chl is needed to operate Eqs 11 and 12, this algorithm would be applied after the Chl algorithm.

It must be stressed, however, that the nominal application of such a method needs independent K_d and R estimates, which is the case when using *in situ* data. When applying the same method in the remote sensing context, the sole quantity available directly is ρ_W , whereas K_d is derived from a reflectance ratio (Eq. 8). It is no longer a quantity independent from R. The performance of the algorithm is, therefore, expected to be affected in this case (this is a general statement valid for any type of IOP inversion algorithm using the remote sensing signal).

This scheme has been tested in order to assess its performance as compared to other methods and as compared to *in situ* data. The synthetic and the *in situ* data bases previously used by the IOCCG working group on IOP algorithms (IOCCG, 2006) have been used here, as well as backscattering measurements from the BOUSSOLE site (Antoine et al., 2006), the "Plumes and Blooms" site (Kostadinov et al., 2007), and the NOMAD V2 data set (Werdell and Bailey, 2005). The results are provided in Figs. 4 to 7 below.

Figure 4 shows that the proposed algorithm is working well when applied to synthetic data.

More importantly, Figure 5 still shows good performances when the same algorithm is applied to independent *in situ* data (only for absorption). Total absorption tends to be underestimated by the algorithm; this needs to be confirmed or invalidated through additional validation exercises (using, e.g., NOMAD). It is, therefore, proposed to use Eqs 11 and 12 to derive total absorption at 443 nm.

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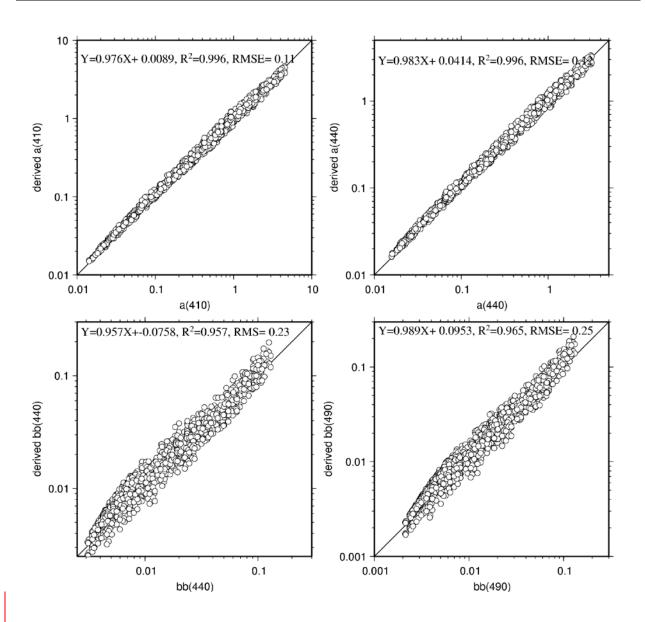


Figure 4: Validation of the proposed IOP algorithm against the synthetic data set of IOCCG (IOCCG, 2006). The four panels are for total absorption and total backscattering at two wavelengths. The parameters of a linear regression on the log-transformed data are provided in each panel. Here K_d and R are taken from the synthetic data set so they are independent quantities

Figure 6 shows good results for the derivation of b_{bp} in the green.

It is, therefore, proposed to derive the total backscattering coefficient in the 560 nm green band. This coefficient is usually produced at 443 nm, the accuracy of which being likely affected by the presence of the large phytoplankton absorption in mesoto eutrophic Case 1 waters. In oligotrophic waters, the respective contributions of particles and seawater to the total backscattering is largely unbalanced to the advantage of seawater (the backscattering coefficient of seawater at 443 nm is 2.45 10-

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³ m⁻¹). The signal to be retrieved (b_{bp}) is therefore small and the uncertainty on its derivation is large.

These two disadvantages are largely suppressed at 560 nm. Atmospheric correction errors are also much lower in the green than they are in the blue.

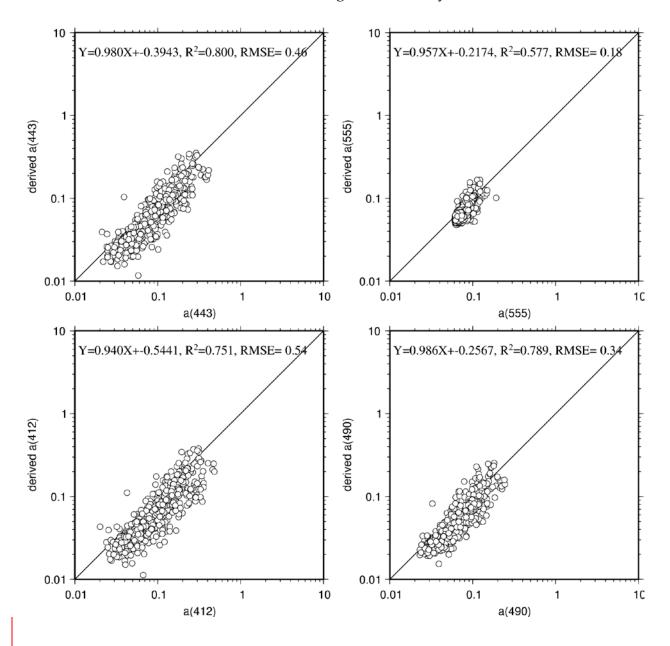


Figure 5: Validation of the proposed IOP algorithm against the *in situ* data set of IOCCG (IOCCG, 2006). The four panels are for total absorption at four wavelengths (no backscattering measurements in the IOCCG data set). Here, K_d has been derived from Chl before entering into the algorithm (no K_d data within the IOCCG *in situ* data base). The parameters of a linear regression on the log-transformed data are provided in each panel. **Note: data from the** Chesapeake bay and its vicinity (experiment name: "LMER-TIES"), suspected of having been collected in Case 2 waters, have been removed from the data base.

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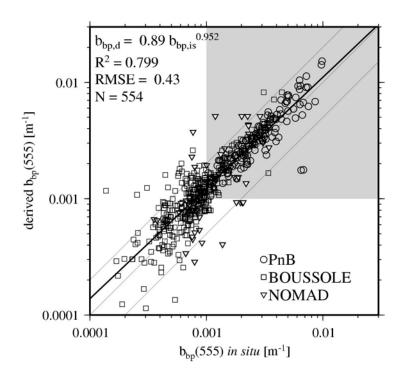


Figure 6: Validation of the proposed algorithm for the particulate backscattering coefficient, against *in situ* data from the BOUSSOLE site (Antoine et al., 2006; hydroscat-II instrument), the Plumes and Blooms site (Kostadinov et al., 2007; hydroscat-VI instrument), and the NOMAD v2 data set (Werdell and Bailey, 2005; various instrument). The parameters of a linear regression on the log-transformed data are provided. The shaded area corresponds to the usual range over which inversion methods are validated, clearly showing that validation for clear waters was missing up to now.

In clear waters, getting accurate particulate backscattering coefficients, b_{bp} , requires accurate determination of the backscattering by seawater itself, b_{bw} . A recent analysis by Twardowski et al (2007) provided a refined computation for b_{bw} (used to produce the results shown in Fig. 6 here). Their recommendations should be followed, which means that the water temperature (SST) and salinity (SSS) should be known to determine b_{bw} . Sufficiently accurate climatologies exist for these two parameters so there is no need to determine their actual values to compute b_{bw} when processing OLCI data (for instance a 1psu difference in SSS for SST=20°C ends up with a 1 10^{-5} m⁻¹ difference in b_{bw} at 555 nm). More realistic values could be incorporated, however, and at least for SST, when reprocessing the data (e.g., weekly global products for SST such as the ones provided by the GHRSST project).

Recommendation: use the Morel et al. (2006) approach (Eqs. 11 & 12 here) to derive total absorption and total backscattering coefficients. Follow Twardowski et al. (2007)

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to determine b_{bw} (to get b_{bp}) and Morel et al. (2007b) to determine a_w (to get a_t – a_{wv} i.e., the sum a_p + a_{cdom}). Data sources for SST and SSS to be discussed / selected during algorithm implementation.

3.1.4 Can the CDOM absorption coefficient (ag) be derivable?

The uncertainty on absorption by CDOM is known to be a major problem in the derivation of the chlorophyll concentration, for instance. An accurate determination of a_g would be, therefore, a significant advance in the retrieval of OC products in Case 1 waters. A better separation of the influence of CDOM and phytoplankton in the absorption budget is also important to improve the modelling of primary production. Deriving a_g is, however, far from easy, because the deconvolution of the effects of Chl and CDOM is largely impeded by their intermingled influences in the blue part of the e.m. spectrum. Non-algal particles also intervene.

Once the total absorption coefficient is known (see above), it is feasible in theory to decompose it into several components and the associated "partial-coefficients" corresponding to various optically-significant quantities. This is feasible by virtue of the additive character of IOPs, so that one can write:

$$a(\lambda) = a_{w}(\lambda) + a_{\phi}(\lambda) + a_{nap}(\lambda) + a_{g}(\lambda)$$
 (13)

where $a_w(\lambda)$ is the absorption coefficient of sea water, $a_\phi(\lambda)$ is the absorption coefficient of phytoplankton, $a_{nap}(\lambda)$ is the absorption coefficient of non-algal particles, and $a_g(\lambda)$ is the absorption coefficient of coloured dissolved organic matter (also called gelbstoff, hence the "g" subscript). The sum of $a_\phi(\lambda)$ plus $a_{nap}(\lambda)$ is denoted $a_p(\lambda)$, standing for the absorption coefficient of all particles.

The error budget that could be derived from each component depends on the wavelength, because the relative importance of the different components is varying dramatically with wavelength.

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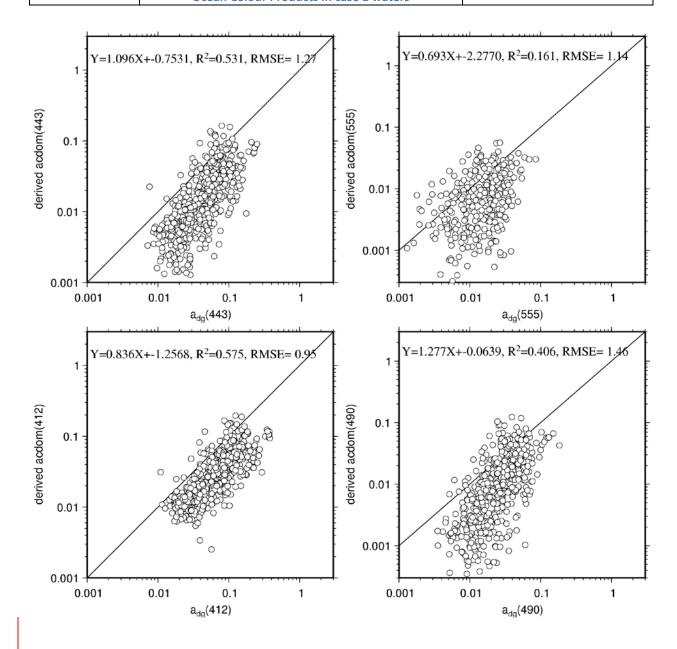


Figure 7: Validation of the proposed a_g algorithm against the *in situ* data set of IOCCG (IOCCG, 2006). The four panels are for CDOM absorption at four wavelengths. Here, a_p has been derived from Chl following Bricaud et al. (1998). The parameters of a linear regression on the log-transformed data are provided in each panel.

Roughly speaking, it is illusory to derive $a_g(\lambda)$ with an acceptable accuracy for λ >500 nm, and it is best to derive $a_{\varphi}(\lambda)$ in the vicinity of phytoplankton absorption peaks.

Here, the feasibility to derive $a_g(412)$ from a(412) has been examined, because (1) a_g increases exponentially in the blue, (2) water absorption is small at 412 nm, and (3)

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the particle absorption is not at its maximum (in other words, the relative contribution of a_g to the total absorption budget is larger). The operation to perform is:

$$a_{g}(\lambda) = a(\lambda) - [a_{W}(\lambda) + a_{p}(\lambda)]$$
(14)

The difficulty is the unavailability of a direct estimate of $a_p(\lambda)$. The use of an empirical relationship between $a_p(412)$ and Chl has been tested, following Bricaud et al. (1998). By doing so, it is assumed that the uncertainty on the Chl-derived particle absorption is still low enough for $a_g(412)$ to be derived meaningfully.

This approach has been tested on the IOCCG *in situ* data set and the results are presented in Fig. 7. An acceptable accuracy is only obtained at 412 nm. It seems, therefore, possible to derive the absorption coefficient of the coloured dissolved organic matter through this technique.

A much thorough validation is still needed, however, to definitely conclude on the appropriateness of this approach.

A data base of CDOM absorption measurements should be assembled for that purpose. It will rely in particular on data presently collected at BOUSSOLE, and on any other available data sets (e.g., NOMAD), provided that their quality is appropriate.

Recommendation: combine the total absorption, a_t , as derived from the Kd-R inversion algorithm (Morel et al., 2006: Eqs. 11 & 12 here), the Chl-derived a_p from Bricaud et al. (1998) and a_w derived as per Morel et al. (2007b) to determine $a_{cdom}(412) = a_t(412) - a_w(412) - a_p(412)$.

3.1.5 Alternative approach: the GSM algorithm

The algorithms proposed above are independent one from each other, so that the various products are separately determined from the water-leaving reflectance spectrum derived after atmospheric correction. This solution has one advantage, which is precisely to have independent estimates of each parameter, i.e., the possible error on one of them doesn't transfer as an error on the others. This solution also has some disadvantages, among which is the impossibility to derive an error estimate on each determination of the geophysical parameters. In other words, there is no possible pixel-by-pixel uncertainty estimate. The nature of these algorithms only allows an overall uncertainty to be assessed (in general though the comparison with in situ data).

Another approach is therefore proposed here, which consists of a simultaneous determination of the inherent optical properties and derived parameters (chlorophyll

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via its absorption coefficient in the blue, the particulate backscattering coefficient at 443 nm, and the absorption by coloured detrital matter at 443 nm), and which is able to provide a pixel-by-pixel uncertainty estimate. This is the so-called "GSM" semi-analytical algorithm (for "Garver, Siegel and Maritorena"; Garver and Siegel, 1997; Maritorena et al., 2002; Maritorena and Siegel, 2005). The inputs to this model are the spectral normalized water-leaving radiances ($L_{\rm wN}(\lambda)$) (i.e., the full spectrum is used from 412 nm to the red).

The GSM model is briefly described below (essentially taken from IOCCG, 2006). It is based on the quadratic relationship between the remote-sensing reflectance (R_{rs}) and the absorption and backscattering coefficients (Gordon et al., 1988):

$$R_{\rm rs}(\lambda) = \frac{t^2}{n_{\rm W}^2} \sum_{t=1}^2 g_t \left(\frac{b_{\rm b}(\lambda)}{b_{\rm b}(\lambda) + a(\lambda)} \right)^t,$$

where g1(= 0.0949) and g2(= 0.0794) are geometrical factors. The absorption coefficient, a(λ), is decomposed into $a_w(\lambda)$ (seawater), $a_{ph}(\lambda)$ (phytoplankton), and $a_{dg}(\lambda)$ (coloured detrital and dissolved material, CDM). Similarly $b_b(\lambda)$, is partitioned into backscattering by seawater, $b_{bw}(\lambda)$, and by suspended particulates, $b_{bp}(\lambda)$. The non-water absorption and scattering terms are parameterized as a known shape with an unknown magnitude:

$$\begin{aligned} a_{\rm ph}(\lambda) &= Ca_{\rm ph}^*(\lambda), \\ a_{\rm dg}(\lambda) &= a_{\rm dg}(\lambda) \exp(-S(\lambda - \lambda_0)), \\ b_{\rm bp}(\lambda) &= b_{\rm bp}(\lambda_0) \left(\frac{\lambda_0}{\lambda}\right)^Y, \end{aligned}$$

where $a_{ph}^*(\lambda)$ is the chlorophyll-a specific absorption coefficient, S is the spectral slope for CDM absorption (Bricaud et al., 1981, 1998), Y is the power law exponent for b_{bp} , and λ_0 is a scaling wavelength (443 nm). S, Y and $a_{ph}^*(\lambda)$ are set to constant values.

For $a_{ph}(\lambda)$, $a_{dg}(\lambda)$, and $b_{bp}(\lambda)$, the unknown magnitudes are the chlorophyll-a concentration (Chl), the detritus/gelbstoff absorption coefficient, $a_{dg}(443)$, and the particulate backscatter coefficient, $b_{bp}(443)$, respectively.

GSM validation results are shown in Fig. 8 with MERIS, SeaWiFS, and MODIS (in situ data from NOMAD data set for the 1997-2003 time period and additional data from the SeaBASS archive for the 2003-2007 period).

0.10

0.01

0.10

1.00

In situ CHL [mg m⁻³]

10.00

100.00

0.001

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0.0001

0.0001

0.0010

In situ BBP [m⁻¹]

0.0100

0.1000

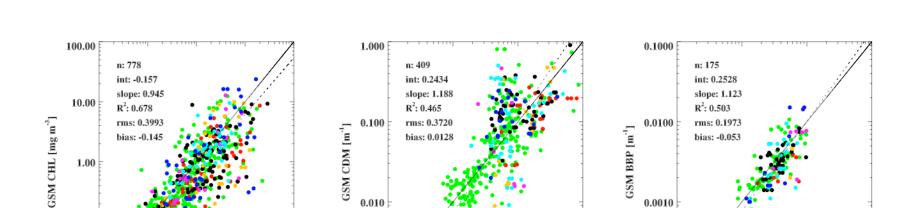


Figure 8: Adapted from Fig. 11 of Maritorena et al. 2009. Matchups statistics for the three GSM merged products, Chl (left), CDM (centre) and b_{bp} (right). The colour of each matchup point indicates which satellite data sources were used for that point (green: SeaWiFS only, red: AQUA only, yellow: MERIS only, light blue: AQUA+MERIS, purple: SeaWiFS+MERIS, black: SeaWiFS+AQUA, dark blue: SeaWiFS+AQUA+MERIS).

In situ CDM [m⁻¹]

0.010

0.100

1.000

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3.2 Error estimates

3.2.1 Semi-empirical algorithm

For the semi-empirical algorithms proposed in section 3.1, there is no possible pixel-by-pixel uncertainty (error) estimate. An average uncertainty can be derived from the comparison with in situ data, typically providing the slope and intercept of a regression, and the associated coefficient of regression and root mean square error.

Numbers are not provided here because they depend on the data base that is used for this assessment.

Such an approach can be global or regionalized to some extent (see Dwell et al., 2009).

This will have to be discussed among the Sentinel-3 group and an agreement found on which data base has to be used to produce such numbers.

The reader is referred also to the MERIS ATBD 2.9 for some discussions about the uncertainties inherent to such algorithms (Morel and Antoine, 2007).

Another approach could be tested, however, where some kind of quality indicator could be derived on a pixel-by-pixel basis. The approach would rely on the fact that the ratio of reflectances at 490 and 560 nm is one of the parameters that is retrieved with the best accuracy. This is illustrated on Fig. 9, from the results of an intercomparison of atmospheric correction algorithms performed under the auspices of the IOCCG (chair M. Wang). It is clear from this figure that the ratio of reflectances at 490 to 560 nm is better retrieved than the reflectances themselves, and that the uncertainty in this ratio is often within 5%. The same results, i.e., the band at 490 nm being better retrieved than others, are also obtained from validation with respect to in situ data bases (e.g., Antoine et al., 2008).

The logic would be to re-compute the various reflectances from this band ratio using a semi-analytical reflectance model (e.g., Morel and Maritorena, 2001), and to derive an average relative difference between this reconstructed reflectance spectrum and the spectrum available after atmospheric correction of the satellite measurements.

Large values of this average difference may result from a variety of situations, including in particular large errors in atmospheric corrections or inappropriateness of the semi-analytical reflectance model. The combination of this quality indicator with other science flags may also provide some insight about the behaviour of the algorithms in varied situations.

This approach has not been tested up to now. It could be tested using existing MERIS data.

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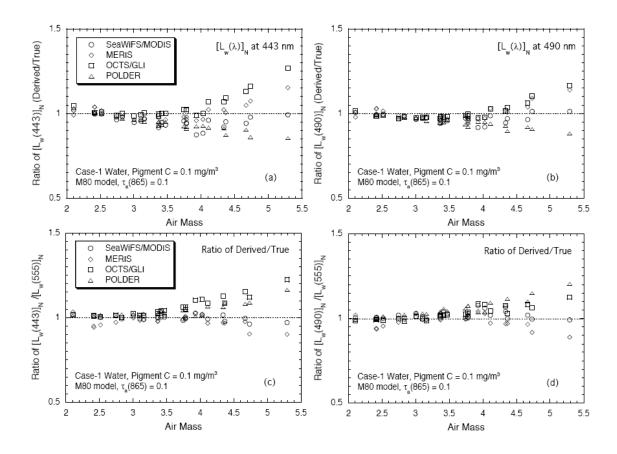


Figure 9: (from Wang et al., in preparation, IOCCG report #10): Ratio values (derived/true) of various ocean colour parameters as a function of the air mass from atmospheric correction algorithms of SeaWiFS/MODIS, MERIS, OCTS/GLI, and POLDER for (a) $[L_w(\lambda)]_N$ at 443 nm, (b) $[L_w(\lambda)]_N$ at 490 nm, (c) ratio $[L_w(443)]_N/[L_w(555)]_N$, and (d) ratio $[L_w(490)]_N/[L_w(555)]_N$. These results are for the M80 aerosols with aerosol optical thickness of 0.1 at 865 nm and for open ocean (Case-1) water with pigment concentration of 0.1 mg/m³. Air mass is for the sun-pixel plus pixel-satellite paths).

3.2.2 GSM algorithm

Concerning the GSM algorithm, error estimates can be provided on a pixel-by-pixel basis (from Maritorena et al., Remote Sensing of Environment, submitted). This paper presents the outcomes of the ESA GlobColour project to what concern error estimates based on the use of the GSM (or even GSM-like) algorithms.

For any "semi-analytical" inversion technique, a minimisation is done between a "reference spectrum model" and the observed model by iterating on values of free-parameters. The invaluable advantage is that, providing error estimates on inputs and appropriated minimisation technique, the fitting procedure provides, mathematically, the range of uncertainties of inversion and, by this, the three IOP presented above, as well as their uncertainties.

This potential for providing error bars has been extensively explored during GlobColour and some consolidated results are presented below.

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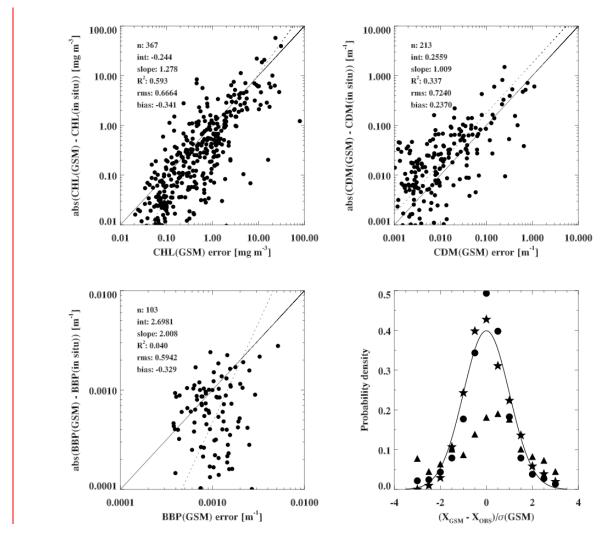


Figure 10: Adapted from Fig. 9 of Maritorena et al. 2009. Comparisons of the predicted and actual uncertainties using the NOMAD data set (upper left: Chl; upper right: CDM; lower left: b_{bp} . If the predicted uncertainties are accurate, about 2/3 of the data points should be below the 1:1 line. The centred variables (retrieval/error; lower right panel) show a normal distribution for CHL (circles) and b_{bp} (stars) while the CDM (triangles) distribution departs from normal (curve).

The requested qualification of inputs (as well as model uncertainties) has been done through GlobColour and propagation of error through Levenberg-Marquardt minimisation procedure has allowed production of reliable error bars at least for Chla and for b_{bp} . For CDM the propagation of uncertainties has proven to be less reliable and points toward a requested adaptation of the reference reflectance spectrum.

Fig. 10 shows the results for all three parameters (see the three first panels) of the retrieved error estimates wrt to actual error obtained through matchup analysis. Scatter plots for which (visually) two third of the actual error is under the 1/1 line of error estimates, indicate a satisfactory estimates of the error (as assumed to follow a normal probability function). The three normalised distribution function have been reported on the fourth panel (bottom right) and theoretically should be comparable

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to the normalised centred density probability function which is also sketched. Good correlation between this theoretical shape and the ones obtained for Chla and b_{bp} (while CDM deserves some attention) indicates that this approach is the one to be followed for the implementation of the OLCI L2 processing.

3.3 Summary of recommendations

3.3.1 Products

The list of products is:

- Pigment index (Chl) (OC4Me algorithm)
- K_d(490) (OK2-560 algorithm)
- b_{bp}(560) (Morel et al., 2006 algorithm)
- a_{cdom}(412) (Morel et al., 2006 algorithm)
- a_{phy}(443) (GSM algorithm)
- b_{bp}(443) (GSM algorithm)
- a_{cdm}(443) (GSM algorithm)

The marine reflectances in all visible bands ($\rho_w(\lambda)$) are obviously part of the product list as well (it is just not clear whether they are considered as the final products of the atmospheric correction, and so to be listed in the CWAC ATBD, or as the first basic ocean colour product, to be listed in this ATBD).

"Pigment index" (Chl): use the OC4Me algorithm, and include a θ_s -dependence in the \mathfrak{R} lookup table. Derive Chl also from the GSM algorithm (Garver and Siegel, 1997; Maritorena et al., 2002; Maritorena and Siegel, 2005).

 K_d (490): use the OK2-560 algorithm (Morel et al. 2007a).

IOPs:

At λ = 560 nm only: use the Morel et al. (2006) approach (Eqs. 11 & 12 here) to derive the total backscattering coefficient (b_b). Follow Twardowski et al. (2007) to determine b_{bw} (see appendix) so that b_{bp} is obtained as b_b - b_{bw}. Data sources for SST and SSS to be discussed / selected during algorithm implementation.

At λ = 412 nm only: combine the total absorption, a_t , as derived from the Kd-R inversion algorithm (Morel et al., 2006: Eqs. 11 & 12 here), the Chl-derived a_p from Bricaud et al. (1998) and a_w derived as per Morel et al. (2007b) to determine

$$a_{cdom} = a_t - a_w - a_p.$$

In parallel, use the GSM (Garver and Siegel, 1997; Maritorena et al., 2002; Maritorena and Siegel, 2005) to get a_{ph} , b_{bp} and a_{cdm} , at λ = 443 nm.

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3.3.2 Pixel-by-pixel error estimates

Semi-empirical algorithms: both the Chl and the $K_d(490)$ algorithms proposed here rely on the Morel and Maritorena (2001) semi-analytical model (MM01). Therefore, they follow this global average algorithm. The approach described here (section 3.2.1) will provide an indication about how far from the average model each pixel is. Would the water optical properties behave exactly as in MM01 (as a function of Chl) and the atmospheric correction error be null, the reconstructed reflectance spectra should be equal to the one derived from the TOA signal after atmospheric correction. Therefore, the average difference proposed in section 3.2.1 will conceal the effects of atmospheric correction errors and deviation of optical properties from the MM01 model.

GSM algorithm: proceed as described in section 3.2.2 of this ATBD.

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4. ASSUMPTIONS AND LIMITATIONS

4.1 Assumptions

Pixel-by-pixel error estimates of the water leaving reflectance (each marine band) are available as input.

4.2 Constraints, limitations

The algorithms proposed here are valid above Case 1 waters, which means that they cannot provide reliable results when applied over Case 2 waters that would not have been identified as such (in particular turbid Case 2 waters).

The same comment is valid for any other "non-nominal" conditions of applications, including but not being limited to, coccolithophorid blooms, residual, non-identified, sun glint, non-corrected adjacency effects, cloud shadows and unidentified thin clouds.

For the chlorophyll concentration, the reader is referred more specifically to Morel (2007a) and the MERIS ATBD 2.9 for a detailed discussion of the assumptions and limitations related to the OC4Me algorithm.

For the K_d algorithm, the reader is referred more specifically to Morel et al. (2007a) for a detailed discussion about the OK2-560 algorithm.

A possible limitation of the GSM algorithm lies in the range of variability of the data bases used for its optimization. It is known that GSM isn't totally optimized for clear oceanic waters. This is under study and an improved version optimized for a larger range of trophic states is under development.

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SENTINEL-3 OPTICAL PRODUCTS AND ALGORITHM DEFINITION

OLCI Level 2 Algorithm Theoretical Basis Document
Ocean Colour Products in case 1 waters

Ref: S3-L2-SD-03- C10-LOV-ATBD

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6. Appendix: bbw computation

Computation of b_{bw} as per Twardowski et al. (2007) (Eqs. 1-3 and Table 1) and references therein:

Parameters:

 $k = Boltzmann constant, 1.38054 10^{-23} J K^{-1}$

 δ = 0.051 (depolarization ratio).

SST is sea-surface temperature, in °C

SSS is sea-surface salinity, in psu

 λ is the wavelength in nm.

Equations:

$$n_wat = 1.3247 + 3.3 \cdot 10^3 \lambda^{-2} - 3.2 \cdot 10^7 \lambda^{-4} - 2.5 \cdot 10^{-6} \text{ SST}^2$$

 $isothermal_compress = (5.062271 - 0.03179 SST + 0.000407 SST^2) 10^{-10}$

comp1 =
$$(-0.000156 \lambda + 1.5989) 10^{-10}$$

$$comp2 = (1.61857 - 0.005785 SST) 10^{-10}$$

n_pressure_derivative = $(comp1 comp2) / 1.5014 10^{-1}$

$$\beta_{\rm w}(90) = \frac{2\,\pi^2\,\,\mathrm{k}\,\,(\mathrm{SST} + 273)\,\,\mathrm{n}\,\,\mathrm{wat}^2}{(\lambda\,10^{-9})^4\,\,\mathrm{isothermal}\,\,\mathrm{compress}}\,\mathrm{n}\,\,\mathrm{pressure}\,\,\mathrm{derivative}^2\,\frac{\left(6+6\,\delta\right)}{\left(6-7\,\delta\right)}$$

$$b_{wat} = [\ 16\ \pi\ /\ 3\]\ \beta_w(90)\ [\ (1/2)\ ((2+\delta)\ /\ (1+\delta))\]$$

$$b_w = b_{wat} (1 + 0.3 (SSS / 37))$$

$$b_{bw} = b_w / 2$$

Values of b_{bw} for two bands and two SST-SSS configurations, for verification:

	$\lambda = 442 \text{ nm}$	$\lambda = 555 \text{ nm}$
SST = 20°C, $SSS = 38$ psu	0.004586 m ⁻¹	0.00178731 m ⁻¹
SST = 30°C, SSS = 36 psu	0.00443253 m ⁻¹	0.00172748 m ⁻¹