Algorithm Theoretical Basis Document

ATBD 2.8

CASE 2 ANOMALOUS SCATTERING AND GELBSTOFF WATERS FLAGS

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Case II Anomalous Scattering and Gelbstoff Waters Flag

2. Algorithm Overview

These flags determine those waters which meet Case II criteria, but whose scattering is not sufficient to cause significant water-leaving radiance in the near infra red.

a) Gelbstoff dominated waters.

In waters dominated by gelbstoff, but with low sediment loads, conventional two-band ratio methods for pigment or chlorophyll do not work. Aiken *et al.* (1995) have demonstrated that the radiance or reflectance ratios are determined by IOPs, principally by the absorption coefficients. It is known from a number of studies that the absorbency of gelbstoff exponentially decreases with increasing wavelength, and the coefficient of decrease is broadly similar over a number of water types. This fact can be used to compare retrievals of apparent chlorophyll using a number of bands in the blue spectral region.

b) Anomalous scattering waters.

The second test determines whether the scattering is consistent with the chlorophyll determined by the hyperbolic chlorophyll retrieval of Aiken *et al.*, 1995. The retrieval uses the 490nm and 560nm wavebands, and is described as the H(490,560). This test will flag waters where the scattering is higher than normal and will produce anomalous chlorophyll retrievals. These waters although rare may produce effects such as rings of apparently high chlorophyll around coccolithophore blooms.

3. Algorithm Description

3.1 Theoretical Description

3.1.1 Physics of the Problem

Gelbstoff, yellow substance or coloured dissolved organic material (CDOM) of terrestrial or biogenic origin absorbs UV and blue light strongly, with an exponential decrease to longer wavelengths. When high concentrations of gelbstoff are present, simple two band ratio retrieval algorithms give abnormally high chlorophyll (pigment) values, since the absorption of co-existing gelbstoff can not be distinguished from chlorophyll. However the spectral signature of gelbstoff is different from that of chlorophyll and accessory pigments. Chlorophyll absorbs strongly at 442.5nm (band 2) and the co-varying carotenoids at 490 and 510 nm (bands 3,4). Gelbstoff shows an exponential decrease in absorption with wavelength. Thus the extent of the anomalous over-estimate diminishes for the 490nm and 510nm, two band ratio algorithms. In waters with low gelbstoff, estimates of pigment based absorption at these three wavelengths will be broadly similar; a test which examines the discrepancy of chlorophyll estimation will indicate high gelbstoff concentrations.

By definition the scattering in Case I waters results from chlorophyll, detrital and bacterial particles. This scattering is in proportion of the chlorophyll concentration (Gordon and Morel, 1983), although not directly attributable to the phytoplankton. Where the scattering is abnormally high, these waters are termed Case II waters; most such waters are flagged by ATBD 2.5, however there are some occasional transitional waters where the scattering can be high enough to affect the Case II chlorophyll retrieval, but not affect $\rho_w(705)$.

3.1.2 Mathematical Description of Algorithm

3.1.2.1 Case II(y) Detection

Using the hyperbolic fit described by Aiken et al (1995) three estimates of chlorophyll are generated. These estimates are based on a reflectance ratio fit (See attached appendix) :

$$H(\lambda_1,\lambda_2) = \left[\frac{\rho w(\lambda_1) / \rho w(\lambda_2) - A_1}{A_2 - A_3 \times \rho w(\lambda_1) / \rho w(\lambda_2)} \right]^N$$

where $\rho_w(\lambda)$ is the reflectance, and A_i , N are constants obtained from empirical fits of in-situ data.

For each pixel the estimates *H(442.5,560), H(490,560), H(510,560)* are generated. Where $\rho_w(\lambda)$ is zero, the estimate is set at the asymptotic limit of the retrieval (Moore *et al.*, in press). The test does not use the estimate from 412:560, since $\rho_w(412)$ will be zero in high chlorophyll waters. Two tests are applied according to the chlorophyll value retrieved by *H(490,560)*. Test 1 is applied where *H(490,560)* is less than 5mg.m^{-3}, and test 2 at higher levels.

1: $(H(443,555) >= B_1 \times H(490,560))$

2: $(H(490,560) >= B_2 \times H(510,560))$

(B_1,B_2 are constants which are given in the parameters table below).

If the test is satisfied then the pixel is assumed to be gelbstoff contaminated. See Figure 2.2

If this test is passed the Case II anomalous scattering detection test is performed.

3.1.2.2 Case II Anomalous Scattering Detection

An estimate of chlorophyll is calculated from H(490,560), this chlorophyll is used to estimate a' and b' using the a'(Chl), and b'(Chl) lookup tables. $\rho'_W(560)$ is then estimated using the $\rho'_W(\lambda, a'(Chl), b'(Chl), \theta_v, \theta_s, \Delta\phi)$ lookup table (see ATBD 2.6 for the definition of the lookup tables). The pixel is flagged if :

$$\rho_W(560) > 1.2 \times \rho^*_W(560)$$

The threshold of 1.2 approximates the Case I *vs.* case II definition; however it may need further refinement. Since the algorithm uses IOPs corrected for angular properties, any such refinement will be in terms of quantities already derived with the algorithm.

3.2 Sensitivity Tests

Test data for the algorithm were generated according to the Reference Model (Document PO-TN-MEL-GS-0016), with the exception of the sediment IOPs which were as described in ATBD 2.6. The test set consisted of 5000 randomly generated points with additions of CDOM and sediment to Case I data. The baseline Case I water consisted of a log random scale of chlorophyll ranging from 0.01 to 100.0 mg.m^{-3} (arithmetic mean 10 mg.m^{-3}). To this case I data CDOM and sediment was added with a probability of 0.5. The data consisted of 25% Case I, 25% Case II.y, 25% Case II.S and 25% both Case II.S and Case II.y. The Case II.y data consisted of log random CDOM ranging from 0 to 9 m^{-1}

at 440nm, arithmetic mean 0.7 m^{-1}. The Case II.S data consisted of log random sediment ranging from 0 to 100 $g.m^{-2}$, arithmetic mean 7.8 $g.m^{-2}$.

Figure 2 shows the distribution of the model data for Case II.y (a) and Case II.S (b). The modelled chlorophyll is the model input, and the retrieved chlorophyll is the output of the H(490,555) retrieval. As expected the CDOM addition results in a systematic overestimation of chlorophyll by this ratio model (Figure 2.a). The result from the Case II.S data is less clear cut, with overestimation at low to moderate chlorophyll, and underestimation at high chlorophyll (Figure 2.b).

Figure 3 shows the comparison of the chlorophyll retrieved using two ratios, 442.5:560 and 490:560. The Case II.y simulation (Figure 3.a) shows a clear separation of in the retrievals with the 442.5:560 retrieval producing higher retrievals than the 490:560 ration. No such systematic effect is shown in the Case II.S data (Figure 3.b).

Figure 4 shows the result of the flag algorithm in the same format as Figure 2. Figure 4.a shows the result of the turbid water flag (ATBD 2.5). This flag identified: 67.4% of the Case II.S data; 66.0% of the data that was both Case II.S and Case II.y; 3.9 % of the Case II.y data; and 6.9% of the Case I data. Both the Case I and Case II.y data corresponded to high chlorophyll data.

The Case II.y flag (Figure 4.b) identified : 30.8% of the Case II.S data; 31.6% of the data that was both Case II.S and Case II.y; 66.1 % of the Case II.y data; and none of the Case I data. The anomalous scattering flag (Figure 4.c) identified : 30.8% of the Case II.S data; 15.1% of the data that was both Case II.S and Case II.y; and none of the Case II.y or Case I data.

The combined result of the flagging is shown in figure 4.d. There are some misidentified values. The majority of these are Case II.y values (29.9%) with a low percentage of Case II.S values (2%). These consist of low chlorophyll high gelbstoff values.

Overall the Case II.S (Combined anomalous scattering and turbid water flag) worked well, but the Case II.y showed disappointing results with a significant proportion of data that the flag failed to determine. From the modelled data, this is an identifiable sub-population of values and the test will be expanded to include detection of these values.

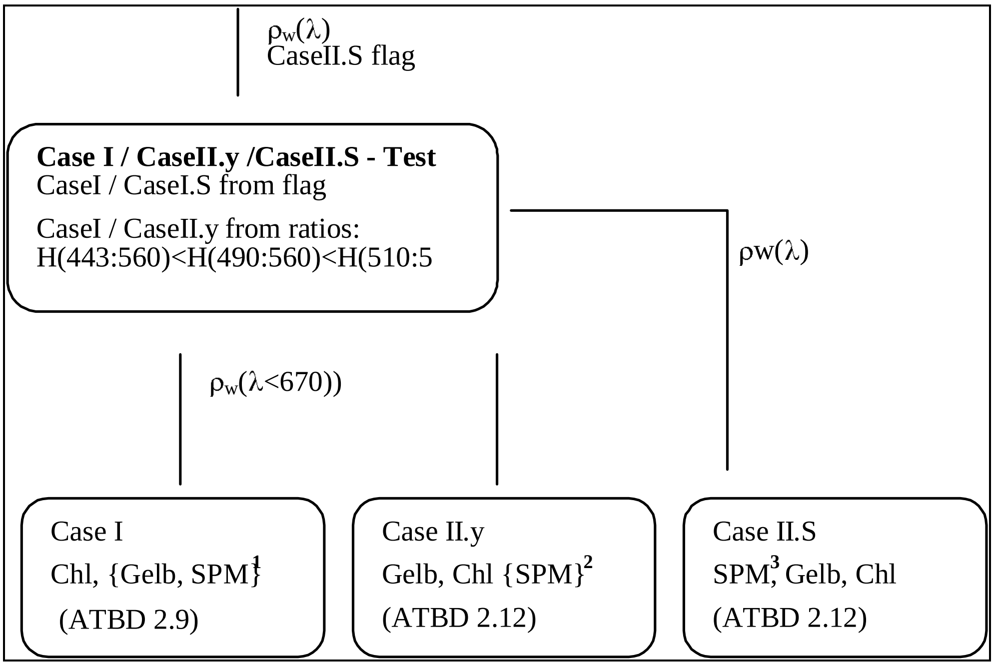


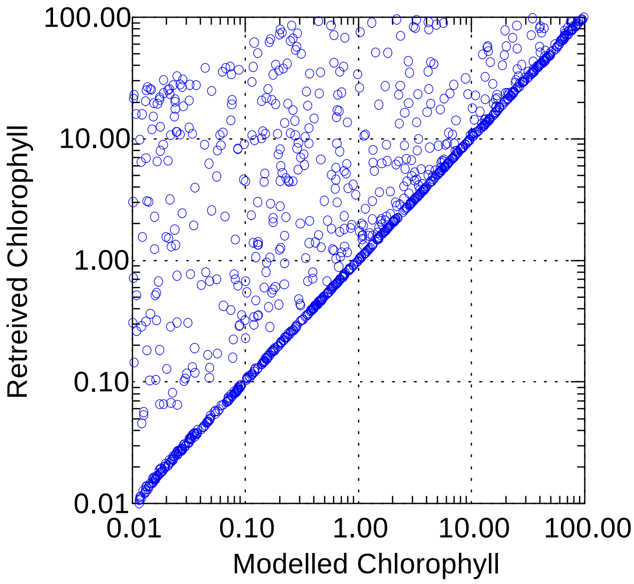
Figure 1 In Water Component of Processing Chain (Bold indicates PML contribution).

1 By definition gelbstoff and SPM are low, but biogenic CDOM and particulates may be retrieved.

2 By default SPM is low (<1.5 mg.m^{-3}) since the Case II.S test pre selects data for this.

3 SPM would equate to coccolith concentration in oceanic and shelf sea waters, and SPM could be equated to alternative units *i.e.* number m^{-3}

a)



b)

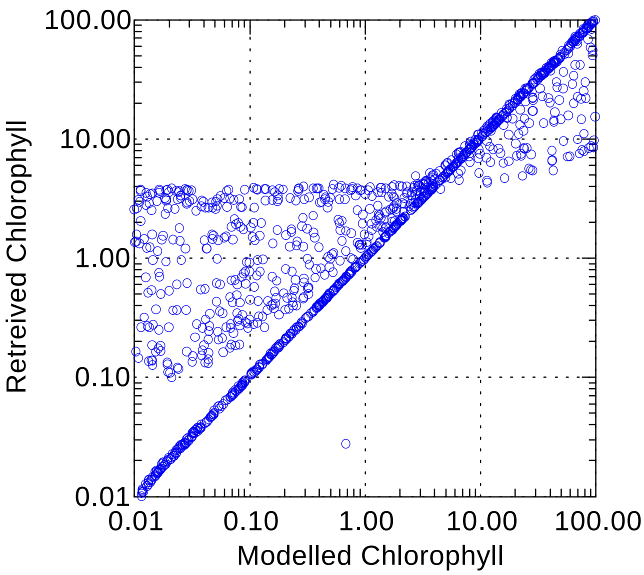
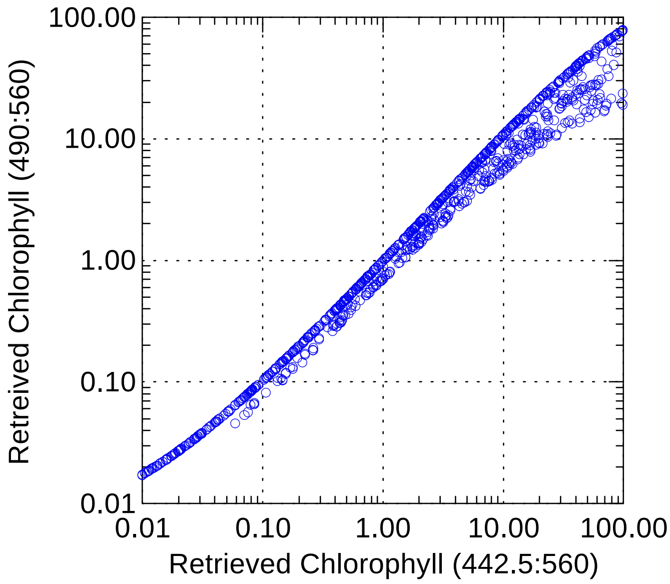


Figure 2 (a) Case I data plotted with Case II.y points (b) Case I data plotted with Case II.S date. The flags are those generated by the model. The retrieved chlorophyll is from the H(490:560) algorithm.

a)



b)

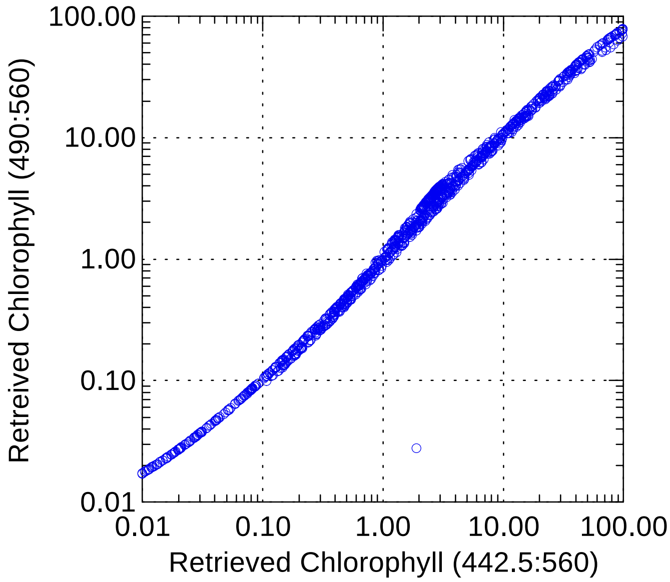


Figure 3 (a) Hyperbolic retrievals for 443:55 vs. 490:555 for Case I and Case II.y. (b) Hyperbolic retrievals for 443:55 vs. 490:555 for Case I and Case II.S. These correspond to the data plotted above.

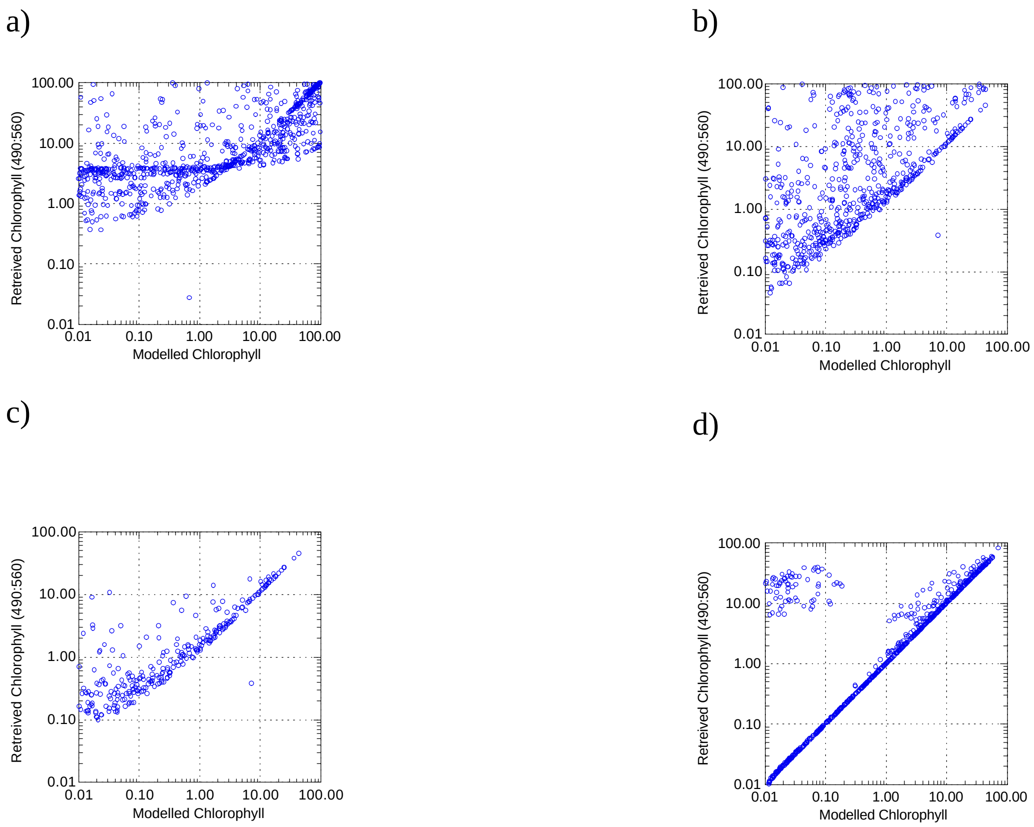


Figure 4. The results of the flagging a) the bright pixel flag – ATBD 2.5, b) the Case II.y flag c) the anomalous scattering flag, and d) the data not flagged.

3.2.1 Parameter Description

Symbol	Descriptive Name	I/O	Range/Reference/Remarks
$\rho'_W(\lambda,\theta)$	Atmospherically corrected water reflectance	i	From atmospheric correction.
A_1, A_2, A_3, N	Hyperbolic fit constants	I	From Database (See Below)
B_1, B_2 [0.8,0.8]	Test constants	i	From Database (See Table)
CaseII(y)	Case II yellow substance water flag	o	
CaseII_F	Case II anomalous scattering water flag	o	
θ_v, θ_s, $\Delta\phi$	Viewing Angles	i	From Geometry

Ratio	A_1	A_2	A_3	N
442.5:560	19.80	6.123	11.00	1.297
490.0:560	6.798	2.838	3.709	1.477
510.0:560	2.765	0.981	1.350	1.699

3.2.2 Error Budget Estimates

TBD

3.2.3 Practical Considerations

The constants (B_1,B_2) need to be calculated for the MERIS bands

3.3 Practical Considerations

3.3.1 Calibration and Validation

The method will be validated using aircraft imagery and the SeaWiFS / OCTS sensor when they become available.

3.3.2 Quality Control and Diagnostics.

The scattering flag threshold needs further diagnostics

3.3.3 Exception Handling

None required - simple pass / fail algorithm.

3.3.4 Output Product

Two binary flags, per pixel: Case 2 (Y), Case 2 (Anomalous scattering)

4. Assumptions and Limitations

The main limitation of the Case 2 (Y) flagging algorithm lies in the optical ambiguity between absorption in water, as caused by yellow substance, and absorption in the atmosphere caused by absorbing aerosols. In fact, when the atmospheric correction algorithm (ATBD 2.7) is applied, yellow substance causes the false detection of absorbing aerosols; the resulting atmosphere-corrected reflectance does not allow the detection of yellow substance.

SUMMARY SHEET

Product Name:	Case II Anomalous Scattering and Gelbstoff Water Flag
Product Code:	
Product Level:	MERIS Level 2 products

Product Parameters:

Coverage	Coastal Waters, not flagged Case 2(S)
Packaging	Level 2 annotation flags
Units	Boolean
Range	Boolean
Sampling	by pixel
Resolution	RR, FR
Accuracy	TBD
Geo.-Location Requirements	View Angles
Format	Single bit
Appended Data	N/A
Frequency Of Generation	As Geophysical Products
Size of Product	2 bits /pixel

Additional Information

Identification of Bands	442.5, 490, 510, 560
Assumptions on MERIS input Data	Atmospherically Corrected water-leaving reflectance

Identification of Ancillary and Auxiliary Data

ρ'_w (λ, a', b', θ_s, θ_v, $\Delta\phi$)	LUT of reflectance *vs.* IOP (see ATBD 2.5)
a'(λ, Chl), b'(λ, Chl)	LUT of IOP *vs.* geo-chemical variables (*idem*)

Assumptions on Ancillary and Auxiliary Data

LUTs are computed according to the Reference Model

References:

Aiken, J., Moore, G.F., Trees, C.C., Hooker, S.B. and Clark, D.K., 1995, The SeaWiFS CZCS-Type Pigment Algorithm. *NASA Tech. Memo. 104566, Vol.29*, S.B. Hooker, E.R. Firestone, Eds., NASA Goddard Space Flight Center, Greenbelt, Maryland, 34 pp.

Gordon, H.R. & Morel, A.Y. 1983. Remote Assessment of Ocean Colour for Interpretation of Satellite Visible Imagery. Lecture Notes on Coastal and Estuarine Studies: Springer-Verlag, Berlin. 4, pp. 114.