A SENSITIVITY ANALYSIS OF ANALYTICAL INVERSION METHODS TO DERIVE CHLOROPHYLL FROM MERIS SPECTRA IN CASE-II WATERS

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ABSTRACT

This paper reports on a sensitivity analysis of various analytical algorithms that use spectral information of MERIS to retrieve CHL, TSM, and CDOM. Investigated are Matrix Inversion Methods (MIM), Ratio Matrix Inversion (RMI), Levenberg Marquardt methods (LM), and a new method called Ratio Levenberg Marquardt Method. Through forward and inverse modeling the sensitivity of those algorithms is assessed for typical sources of error that might influence the outcome of analytical MERIS algorithms. Errors investigated in this study are white and blue reflectance offsets (mostly introduced by atmospheric correction), reflectance scaling errors (introduced by the underwater light field distribution and bi-directional aspects) and variations in the specific inherent optical properties used in the inverse modeling. It is found that the algorithms greatly benefit from initial estimation by simple but robust algorithms. A wrong choice of SIOP-set causes the largest errors in concentration retrieval for all methods.

INTRODUCTION

The retrieval of chlorophyll concentrations (CHL) from reflectance spectra of case-II waters has presented problems due to a number of reasons. Well known are the difficulties in atmospheric correction, due to the turbidity of these waters and the variable aerosol loading in coastal areas. Also the bad discrimination of CHL at higher concentrations of CDOM and/or TSM poses challenges to algorithm design. In the past numerous analytical algorithms have been published that were developed to achieve the most accurate CHL values for specific waters and for specific band-settings.
However, for the interpretation of MERIS observations, it is more interesting to have an algorithm that gives reliable values for CHL, even when the atmospheric composition and the inherent optical properties of the coastal waters are not perfectly well known.

In this paper we present the first results of a study on the stability of some of these analytical algorithms for a suite of error sources. The errors are based on knowledge of the Dutch-Belgian coastal waters of the North Sea. The study is done with a fixed band setting, based on the European Ocean Color instrument MERIS. Selected MERIS bands for this study were the spectral bands at 412.5, 442.5, 490, 510, 560, 665 and 705 nm. The 681.25 and 620 nm bands were omitted because fluorescence and cyanophycocyanin absorption are not incorporated in the forward and inverse model. The 754 nm band was omitted because the water leaving radiance in this band will be very low.

MATERIAL AND METHODS

Specific Inherent Optical Properties (SIOP)

For this study it is assumed that the optical active constituents groups are: 1) TSM: Total Suspended Matter; 2) TCHL: Total Chlorophyll and 3) CDOM: Chromophoric Dissolved Organic Matter. In most cases this is a workable assumption, especially because the optical properties of these groups can be determined relatively easy and unambiguously. If red tides or e.g. cyanobacterial blooms are present, this assumption no longer holds.
It is assumed that the inherent optical properties (IOPs): a and b_b (respectively absorption and backscattering) are linear functions of the constituents' concentration which allows defining Specific Inherent Optical Properties (SIOP). So a and b_b of natural water are expressed in terms of the constituents of the water as follows:

$$a = a_w + a^*_{TCHL} \cdot TCHL + a^*_{TSM} \cdot TSM + a^*_{CDOM} \cdot CDOM \qquad (1)$$

$$b_b = b_{b,w} + Bb^*_{TSM} \cdot TSM \qquad (2)$$

The test dataset comprised of 4 datasets of mean inherent specific optical properties collected in Dutch and Belgian Coastal waters. In three campaigns (see Table 1) 39 samples were analysed for concentrations of TCHL, TSM and CDOM, above water measured spectra of subsurface irradiance reflectance ($R0^-$) and IOPs (Peters et al., 2001). The set of measurements in Belgian coastal waters was split in a high TSM and a low TSM set. Of the four resulting sets cruise-mean SIOPs were calculated and used for the sensitivity study. These average SIOP, together with the used MERIS bands are shown in Fig. 1a-d.

The laboratory analysis of the samples was done as follows: TCHL (chlorophyll-a plus phaeopigment) was determined spectrophotometrically after pigments extraction using hot ethanol (80%, 75^{o}C). TSM was determined by filtering samples over Whatman GF/F filters and drying the filters at 80^{o}C. Ignition loss was determined by ashing the filters with TSM at 550°C. The filters were flushed with tap water to remove salt. The absorption of CDOM was determined (after filtration through a Whatman GF/F filter) from optical density measurements in a 5-cm cuvette. CDOM concentrations are expressed as the absorption at 440 nm. Total absorption (a) and beam attenuation (c) were measured in a 5 cm cuvette using a double-beam spectrophotometer. All spectra were measured between 350 and 750 nm, at 1-nm intervals. Absorption spectra of TSM and bleached TSM were determined using the filter pad method with Whatman GF/F filters. (see e.g. Peters et al., 2001). The concentrations are plotted in Fig. 2.

The optical model

Bio-optical models describe the relationship between the amount of upwelling light just below the water surface (here expressed as subsurface irradiance reflectance) and the optical properties of water and its optical active constituents. Analytical model inversion schemes benefit from simplified models. Therefore, in a number of studies of turbid inland and coastal waters, use has been made of a version of the Gordon (1975) reflectance model to predict the subsurface irradiance reflectance $R(0^{-})$:

$$R(0^{-}) = f \cdot \frac{b_b}{a + b_b} \tag{3}$$

f may vary due to solar and viewing geometry; in the forward model f is set at 0.38. Numerous studies have shown that the model can give good matches between observed and modelled spectra as long as the model is correctly parameterised (e.g. f the backscatter to scatter ratio) and the measured reflectance is accurately calculated (bottlenecks: sky reflection, Q-factor). Peters et al., (2000) presented good matches for several North Sea spectra.

The set of equations 1, 2 and 3 provides an explicit relationship between the SIOP, the concentrations of the water constituents and $R(0^{-})$. All backscattering is lumped as total particulate backscattering. Since phytoplankton backscattering is decoupled from phytoplankton absorption unrealistic simulations may occur at high TCHL concentrations and (very) low TSM values.

TYPES OF ANALYTICAL ALGORITHMS TESTED

This study features the sensitivity analysis of 4 types of inversion schemes of water reflectance spectra. All four solve the over-determined system of seven spectral bands and a maximum of three concentrations.

1. Matrix Inversion (***MIM***: Hoge and Lyon., 1996)
2. Levenberg Marquardt (***LM***)
3. Ratio Matrix Inversion (***RMI***: Peters et al., 2001). Note that RMI is non-linear in TSM, which means that in addition to the matrix inversion itself a predictor-corrector method is used to estimate TSM.
4. In addition a new inversion scheme was attempted, called Ratio Levenberg Marquardt (***RLM***). ***RMI*** and ***RLM*** use as input a vector of band-ratios derived from the input vector (each possible ratio (permutation) exists precisely once in the ratio vector).

Some analytical algorithms like LM require or benefit from a robust and reasonably exact initial estimation of the water quality parameters. Note that ***MIM***, ***LM*** and ***RMI*** can also be used as 3, 2 or 1-parameter algorithms which also require initial estimations of the non-retrieved parameters. Below we present some simple algorithms that are based on reflectance values in a limited window of the R(0-) spectrum (1-band or 2-bands); the ***Initial*** algorithms.

Initial CHL

There is a long history of CHL-estimation using band ratios. Input bands for case-2 waters are usually centered on the CHL-absorption maximum around 667 nm and around 705 nm (reference band). A useful algorithm was published by Gons (1999) based on the following assumptions: 1) At 700 nm and further in the infrared the only two factors that influence R(0-) are a_w and b_b; therefore observations beyond 700 nm can be used to estimate b_b directly from R(0-). 2) At 676 nm R(0-) is influenced by a_w, a_{TCHL} and b_b. For this study we redefine[1] the Gons algorithm for CHL-a to:

$$TCHL = \left(\frac{R(0^-)_{704}}{R(0^-)_{665}} \left(a_{w,704} + b_b \right) - a_{w665} - b_b \right) / \left(a^*_{TCHL,665} \right) \tag{4}$$

For application with MERIS we take the 704 nm band to determine b_b according to:

$$b_b = \left(\frac{R(0^-)_{704}}{f} a_{w,704} \right) / \left(1 - \frac{R(0^-)_{704}}{f} \right) \tag{5}$$

Note that for this simulation study it is sufficient to fix *f*; for application with satellite data *f* needs to be calculated as function of the solar and viewing geometry. The TCHL-specific pigments absorption at 665 nm was determined as the mean value from the three described cruises in Dutch-Belgian national waters: $a^*_{TCHL,665}$=0.0115 which is significantly lower than the inland waters value derived by Gons (0.0176). Note that ratio algorithms are relatively insensitive to errors in b_b, which means that with $a_{w,704} = 0.658$ and f=0.38, b_b can be approximated as:

$$b_b = 2.3 R(0^-)_{704} \tag{6}$$

Initial CDOM

It is difficult to define robust CDOM algorithms because the CDOM influence on the spectrum is (in almost all regions of the spectrum) masked by the influence of other constituents. Here we developed an algorithm based on the following assumptions: 1) CDOM can best be calculated from a band ratio; 2) the exact band choice is less important; 3) b_b is spectrally neutral and equation (6) can be used to estimate b_b and 4) the sum of a_w; a_{TCHL} and a_{TSM} is treated as an empirical constant. A ratio of two spectral bands based on equations 1, 2 and 6 leads to:

$$CDOM = \left(c_{443} - R \cdot c_{561} + 2.3 \cdot R(0^-)_{704} - R \cdot 2.3 \cdot R(0^-)_{704} \right) / \left(R \cdot a^*_{CDOM,561} - a^*_{CDOM,443} \right) \tag{7}$$

With $R = \frac{R(0^-)_{561}}{R(0^-)_{443}}$ and

$$c_\lambda = a_{w,\lambda} + TCHL \cdot a^*_{TCHL,\lambda} + TSM \cdot a^*_{TSM,\lambda} \tag{8}$$

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[1] dropping the empirical constant p (see Gons, 1999); normalizing pigment absorption using TCHL instead of CHL-*a*; using the 665 nm band instead of 672 nm and the 704 band instead of e.g. the 754 nm band

Where λ is 561 and 443. From SIOP analysis it was found that $c_{443} \cong 2 \cdot c_{561}$ and from regression analysis (based on spectra simulated using random concentrations and 4 random SIOP sets) it was found that $c_{561} \cong 0.1196$.

Initial TSM

For initial North Sea TSM estimations a one-band inversion of the Gordon model is very suitable (van der Woerd et al., 2000). The MERIS band around 704 nm is the most suitable for TSM estimations since the relationship R(0-) vs. TSM at this wavelength is linear and does not saturate at higher concentrations. For the parameterization either global/regional mean or location-specific SIOPs can be used. The TSM algorithm needs initial estimates of CHL and CDOM, although the sensitivity to errors in both parameters is low.

SET-UP OF THE SENSITIVITY ANALYSIS

In the sensitivity analysis the influence of a number of error-types on the concentration retrieval was tested. For each test 1000 sets of concentrations were generated at random from a uniform distribution in the concentration ranges: TSM: 1-50 g m^{-3}, TCHL: 1-40 mg m^{-3}, CDOM 0.1 – 1.5 m^{-1}. Using a random choice from the set of 4 cruise-mean SIOP-sets (see figure 1) 1000 input spectra were simulated (see equations 1-3). Then the spectra were increasingly deteriorated in 5 steps using one of the following errors:

1) Scaling error: implemented as f_{inverse} = (0.34 ; 0.36 ; 0.38; 0.40; 0.42)
2) White error: implemented as R(0-,λ) = R(0-,λ) + (0; 0.00125; 0.0025; 0.00375; 0.005)
3) Blue error: implemented as R(0-,λ) = R(0-,λ) – X.$\lambda^{-1.5}$ (X = 0..4)
4) SIOP error: in order to test the general sensitivity to SIOP errors the spectra were inverted using a mean SIOP-set based on the four input-sets.

Finally, the 1-nm spectra were convolved with the MERIS band characteristics to yield simulated MERIS observations.

The influence of these 4 error-types on concentration retrieval was tested separately and in a ‘worst case’ analysis all lumped together. For each algorithm and each step the linear correlation was calculated (expressed as r^2) between the initial (random) concentrations and the retrieved concentrations. Finally the correlation coefficients of each 5 steps were averaged, giving an indication of the sensitivity of the algorithm under investigation for each error type, specified for both TSM and CHL. Note that the correlation coefficient is thus not a direct measure of the accuracy, like e.g. the root-mean-square error in the retrieved concentrations.

RESULTS AND DISCUSSION

Table 2 shows the results of all tested algorithms (MIM, RMI, LM, RLM). InitTSM is the result of the 1-band-704 algorithm fed with the initCHL and initCDOM estimations. Next InitCDOM estimations were improved by feeding initTSM and initCHL into the RLM1CDOM algorithm. InitCDOM estimations are only improved by other algorithms in case of SIOP errors. RMI appeared to be unstable at TSM<5, hence the lower r^2 values in a number of tests. Ratio based methods give good results for TCHL and CDOM. The LM method also gave very stable TCHL retrieval. The adapted Gons-TCHL algorithm (initCHL) was parameterized with a mean $a^*_{TCHL,665}$ which explains the lower starting value (r^2 0.84). In the worst-case analysis this algorithm performs best. Some conclusions from this analysis are:

1) The initialization algorithms perform very good on themselves and result in overall high correlations in the analytical algorithms.
2) Initial CDOM gave the worst initial estimation (r^2 0.4 – 0.5) and was improved by an additional step consisting of the RLM1CDOM algorithm. It was however sufficient to initialize the 1band-704 TSM algorithm.
3) Matrix inversion methods for TCHL estimations appeared to be sensitive in cases of white and SIOP errors. RMI results are affected by instabilities in low-TSM concentration retrieval.
4) Ratio LM is very useful for CDOM estimations.
5) Although further testing is required, the least-sensitive algorithm under all conditions seems to be a combination of initTSM, initTCHL or LM1CHL and MIM1cdom in a non-iterative scheme.

Most important is that all analytical methods are sensitive to errors in SIOP-choice. The closer the SIOP that is used for inversion is to the actual SIOP set, the better. Methods should be investigated to estimate SIOPs from the images themselves.

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APPENDIX: FIGURES AND TABLES

Table 1: Logistical information of in-situ sampling campaigns

Vessel	Date	#Samples	Location description
Mitra	May 8+9, 2000	8	Noordwijk Transect, The Netherlands. Lat: 52° 05' - 52° 18' N; Lon: 4 °15' - 4 °18' E
Navicula	May 22+23, 2000	12	Marsdiep, The Netherlands Fixed location Lat: 52.58 N; Lon: 4.46 E
Belgica	April 17, 18+19, 2000	19	Belgian coastal waters Lat: 51° 09' - 51° 30' N; Lon: 2 °36' - 3 °19' E

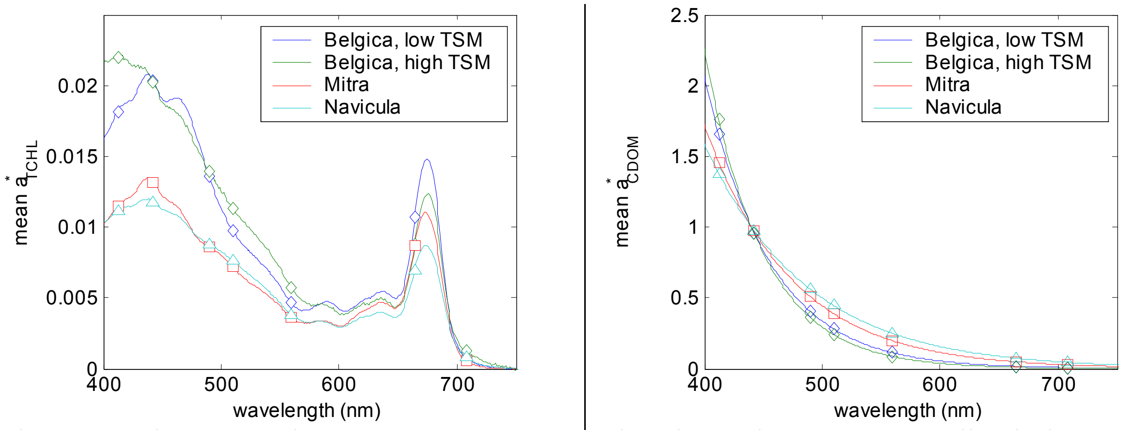

Fig. 1a: Cruise mean a*$_{TCHL}$

Fig. 1b: Cruise mean normalized a*$_{CDOM}$

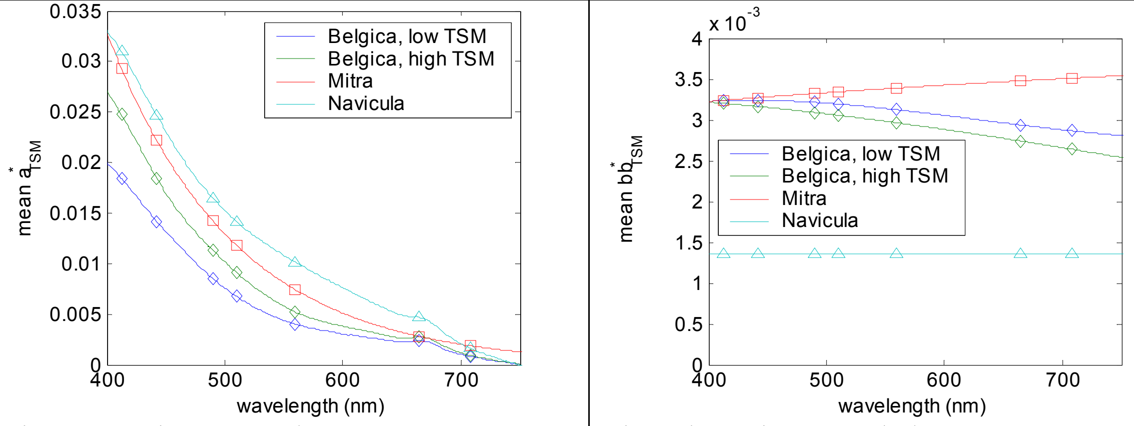

Fig. 1c: Cruise mean a*$_{TSM}$

Fig. 1d: Cruise mean b_b*$_{TSM}$

Figure 1: Cruise mean values of a*$_{TCHL}$, a*$_{CDOM}$, a*$_{TSM}$, b*$_{TSM}$. A total of 39 samples were taken in 2000 at 3 locations: 1) in Belgian coastal waters (Belgica); 2) a transect from "Noordwijk" into the North Sea (Mitra) and 3) the "Marsdiep" (Navicula).

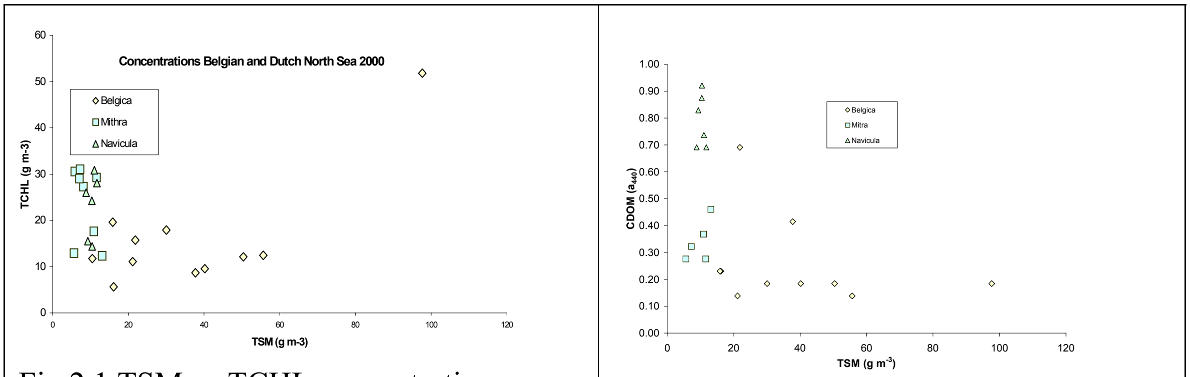

Fig 2.1 TSM vs TCHL concentrations

Fig 2.2 TSM versus CDOM concentrations

Figure 2: Scatter plots of TSM versus TCHL concentrations (Fig 2.1) and TSM versus CDOM concentrations (Fig 2.2).

__Table 2: Results of the sensitivity analysis for TCHL, TSM and CDOM__

			No-error		**Scaling error**		**White error**		**Blue error**		**SIOP-error**		**All-errors**	
inversion method	**retrieved parame**	**Acronym in text**	**TCHL**	**TSM**	**TCHL**	**TSM**	**TCHL**	**TSM**	**TCHL**	**TSM**	**TCHL**	**TSM**	**TCHL**	**TSM**
Matrix inversion	all three	MIM3	1.00	1.00	1.00	1.00	0.92	1.00	0.98	1.00	0.70	0.82	0.73	0.80
	TSM, TCHL	MIM2	0.93	1.00	0.90	1.00	0.62	0.99	0.93	1.00	0.62	0.81	0.26	0.77
	TCHL	MIM1CHL	0.86		0.85		0.65		0.86		0.44		0.38	
	TSM	MIM1TSM		1.00		1.00		0.99		1.00		0.84		0.84
Ratio-Matrix inversion	all three	RMI3	1.00	0.99	1.00	0.99	0.96	0.72	0.97	0.78	0.84	0.46	0.76	0.34
	TSM, TCHL	RMI2	1.00		1.00		0.86		0.99		0.93		0.76	
	TCHL	RMI1CHL	0.97		0.96		0.64		0.95		0.67		0.26	
	TSM	RMI1TSM		0.92		0.89		0.87		0.91		0.35		0.33
Levenberg-Marquardt	all three	LM3	1.00	1.00	1.00	1.00	0.88	1.00	1.00	1.00	0.78	0.84	0.59	0.84
	TSM, TCHL	LM2	0.97	1.00	0.97	1.00	0.96	1.00	0.97	1.00	0.82	0.84	0.78	0.84
	TCHL	LM1CHL	0.97		0.97		0.98		0.97		0.87		0.83	
	TSM	LM1TSM		0.99		0.99		0.99		0.99		0.83		0.83
Ratio-Levenberg-Marquardt	all three	RLM3	1.00	1.00	1.00	1.00	0.39	0.79	1.00	1.00	0.90	0.63	0.35	0.41
	TSM, TCHL	RLM2	1.00		1.00		0.93		1.00		0.83		0.74	
	TCHL	RLM1CHL	0.98		0.98		0.97		0.98		0.83		0.78	
	TSM	RLM1TSM		1.00		1.00		0.99		1.00		0.91		0.86
Initial estimate	TSM	InitTSM		1.00		1.00		1.00		1.00		0.84		0.84
	TCHL	InitCHL	0.84		0.86		0.86		0.85		0.86		0.85	