

VALIDATION OF MERIS WATER PRODUCTS IN THE SOUTHERN NORTH SEA: 2002-2008

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ABSTRACT

This paper describes the validation of MERIS water products for the Southern North Sea for the period July 2002 to September 2008. During this period, 39 match-ups were obtained for the parameters water-leaving reflectance spectra, chlorophyll *a* concentration and total suspended matter concentration, of which 12 are in optimal conditions. Previous validation results reported for 2002-5 are updated to 2008. Conclusions are largely reinforced since the MERIS processor has not changed. In particular it is recommended to improve estimation of the spectral slope of aerosol reflectance in turbid waters. Some image artifacts are noted including noisy low chlorophyll data. Inherent optical property data is analysed and compared to the assumptions used for derivation of the MERIS products. Turbidity has been added to the *in situ* parameter set, strengthening quality control of water sample analysis.

1. INTRODUCTION

Since launch on 1st March 2002, the Medium Resolution Imaging Spectrometer (MERIS) has successfully acquired images all around the Earth until the time of writing (September 2008). During this period, a number of cruise measurements were made at the time of MERIS overpasses for acquisition of match-up data. The previous MERIS validation reports ([1,2,3]) describe the 2002-5 match-up data, focusing on the validation of the water-leaving reflectance spectra ($\rho_w(\lambda)$) and the visual inspection of the images of algal pigment index 2 (Algal2 or Chl2) and total suspended matter (TSM). The previous matchup analysis has been brought up to date here with inclusion of *in situ* data collected for 2006-8. In addition to this matchup analysis, new data is presented for specific inherent optical properties in this region and is compared to the scattering/TSM and phytoplankton/chlorophyll *a* relationships used as basis for the MERIS product retrieval algorithm.

In addition to the validation with *in situ* data reported here, a cross validation between MERIS and MODIS chlorophyll *a* products has been carried out and a comparison between MERIS data and data from a

SmartBuoy operated by CEFAS is in progress. Both will be reported separately.

Satellite imagery has been downloaded from the MERCY website or, since June 2006, from the near-real time Rolling Archive of the European Space Agency. All data presented here has been processed as in [3] with the MEGS processor version 7.4 (“2nd Reprocessing”) or the equivalent processor MERIS/5.0x.

2. OVERVIEW OF MEASUREMENTS

Validation measurements have been made during a series of seaborne cruises in Belgian, Dutch, French and UK coastal waters and in open sea on transects in Spanish, Portuguese, French and Irish waters from the oceanographic Research Vessels Belgica (51m), Zeeleeuw (56m) and Tuimelaar (7m). Table 1 summarizes these cruises and the corresponding MERIS imagery.

Table 1. Summary of MERIS Validation cruises undertaken in 2006-8 and corresponding MERIS match-up possibilities. See [3] for details of cruises in 2002-5.

Month	Days at sea	Potentially optimal match-up images	Sub-optimal match-ups images
SUBTOTAL 2002-5	92	14	6-7
Apr 2006	5	0	0
May 2006	1	1	0
Jun 2006	13	4	1
Jul 2006	3	3	0
Sep 2006	5	2	1
SUBTOTAL 2006	27	10	2
Apr 2007	5	0	0
Jun 2007	9	3	1
Jul 2007	6	0	0
Sep 2007	3	0	0
SUBTOTAL 2007	23	3	1
Apr 2008	4	0	1
Jun 2008	9	0	0
Jul 2008	7	0	0
Aug 2008	2	1	0
Sep 2008	4	1	0
SUBTOTAL 2008	26	2	1
TOTAL	168	29	10-11

In this context only “match-up” MERIS imagery acquired within one hour, or preferably 30 minutes, of seaborne measurements has been considered in order to minimize uncertainties associated with temporal variability of marine and atmospheric properties. The “best” match-up stations after filtering with MERIS PCD and High_Glint flags are described in section 4.1.

3. MEASUREMENT METHODS

At each station measurements of seaborne water-leaving reflectance, Algal2 and total suspended matter are made, following measurements methods based on the MERIS validation protocols [4], summarised briefly here and described in more detail in [3].

3.1 Water-leaving reflectance

Water-leaving reflectance is measured using two different above water methods: a three-sensor TriOS system (2002-8) and a handheld SIMBADA radiometer/sunphotometer (2002-4). The TriOS system is used to make measurements above-water of upwelling radiance, sky radiance and downwelling irradiance as outlined in Method 1 of [5] and detailed in Web Appendices 1 and 2 of [6].

3.1.1 TriOS system data processing, quality control and measurement uncertainty

The data processing of the TriOS measurements is described in Web Appendix 1 of [6], see http://www.aslo.org/lo/toc/vol_51/issue_2/1167a1.pdf, which includes details of scans rejected because of high inclination, large temporal fluctuations (spikes) and possible instrument malfunctioning. For the present study the stations considered as optimal matchups all fulfill the clear, sunny skies conditions given in [6] as $L_{sky} / E_d^+(750nm) < 0.05$ and the sea state condition of wind speed < 10 m/s necessary for optimal above-water measurements. For some of these stations the standard deviation of the 5 scans used for reflectance measurement exceeded 10% of the mean reflectance for some wavelengths in the red and near infrared (NIR). These stations are not rejected in the present study, but the temporal variability over the 5 scans is presented as separate lines in spectral plots.

The measurement uncertainty for these TriOS measurements is described and evaluated in detail in Web Appendix 2 of [6], see http://www.aslo.org/lo/toc/vol_51/issue_2/1167a2.pdf for near infrared wavelengths and in [3] for the full wavelength range 400-900nm.

In addition to these *a priori* estimates of measurement uncertainty, *a posteriori* estimates can be made for each reflectance spectrum based on the similarity spectrum

for the NIR water-leaving reflectance as described in [7]. For the spectra presented here this method yielded estimates of water-leaving reflectance error in the NIR ranging from 0.0001 to 0.001.

3.1.2. SIMBADA system

The handheld SIMBADA radiometer/sunphotometer system deduces water-leaving reflectance from above-water measurements of upwelling radiance, viewing at the Brewster angle through a polarized filter, and direct sun radiance, from which downwelling irradiance is calculated. This corresponds to Method 3 of [5] and is described in detail in [8]. The SIMBADA system is only used in 2002-2004 and only for clear sun and low cloud ($< 2/8$) conditions. For stations where both TriOS and SIMBADA systems were used reflectance measurements are generally within about 5% for the range 412-620nm giving confidence in the methods which differ significantly in treatment of air-sea interface reflection.

3.2 Algal pigment index Chl2 (Algal2)

The algal pigment index Chl2 is validated as defined in the MERIS validation protocols [4] by High performance liquid chromatography (HPLC) measurements of the chlorophyll-a concentration (chl.2.hplc). Water samples taken in surface water (0.5m depth) are filtered on-board with GF/F filters, which are then frozen in liquid nitrogen and stored long-term at -80°C . Pigments are extracted in 90% acetone with the use of a cell-homogenizer, followed by centrifugation [9]. The chlorophyll pigments are separated with reversed phase HPLC.

3.3 Total suspended matter (TSM)

Total suspended matter, TSM, is validated as defined in the MERIS validation protocols by the gravimetric method. Water samples taken in surface water (0.5m depth) are filtered on-board with pre-weighed pre-ashed GF/F filters and rinsed with milli-Q water (including the filter rim). After the cruise the filters are dried and weighed for determination of dry weight. Full details of the method are found in [10].

3.4 Turbidity

Turbidity has been measured on all water samples for the period 2007-8. Before filtration of a water sample a 10ml subsample is taken and placed in the cuvette of a Hach 2100P ISO turbidimeter. A second subsample is analysed after all filtrations have been completed. Although not currently a MERIS water quality product, the turbidity data can be used in the future to develop a new turbidity product for MERIS and other ocean colour sensors. Such a product will be similar in concept to the TSM product and strongly correlated, but will be easier to validate in regions where facilities for TSM analysis do not exist. Moreover comparison of turbidity

data with the *in situ* TSM data allows a quality check of the TSM data (and particulate scattering or backscattering data), highlighting suspect or extreme data.

Measurement of turbidity before filtration allows filtration volume to be optimally set, ensuring that enough matter is collected for accurate measurement but not so much that the filter clogs. Comparison of the turbidity data before and after filtration provides a quality check on mixing of the water sample during the subsampling and filtration operations.

Finally it is noted that turbidity measurement has a much lower detection limit than TSM measurement, which is highly uncertain in clear waters. Surprisingly, turbidity has not yet been included in the parameter set in MERIS validation protocols.

3.5 Phytoplankton absorption

Phytoplankton absorption is measured using the Transmittance-Reflectance method [11] as detailed in [12]. Seawater was filtered onto 25 mm glass fibre filters (Whatman GF/F). The absorbance spectra of particles $OD_{part}(\lambda)$ retained on each filter was determined by measuring the transmittance and reflectance of each filter between 400 and 750 nm with dual beam spectrophotometers equipped with an integrating sphere. The absorbance spectrum of non-algal particles retained on the filter $OD_{NAP}(\lambda)$ was measured after particle bleaching with NaOCl (0.13% active chlorine) [13]. Pathlength amplification was corrected using the algorithm proposed by [14]. Absorbance values at each wavelength were converted into absorption coefficients by:

$$a_{part/NAP}(\lambda) = 2.303 * OD_{part/NAP}(\lambda) / X \quad (1)$$

where X is the ratio of filtered volume to the filter clearance area. The absorption spectra $a_{part/NAP}(\lambda)$ were then corrected for scattering in the near infrared [15]. The $a_{NAP}(\lambda)$ spectra were corrected with an exponential function [15]. The phytoplankton absorption coefficient $a_{\phi}(\text{m}^{-1})$ was obtained from

$$a_{\phi}(\lambda) = a_{part}(\lambda) - a_{NAP}(\lambda) \quad (2)$$

3.6 Particulate scattering

At all stations total non-water absorption $a(\lambda)$ and beam attenuation $c(\lambda)$ coefficients were measured with an AC-9 profiler (WetLabs, Inc). The instrument measures at the following 9 bands: 412, 440, 488, 510, 555, 630, 650, 676 and 715 nm.

The AC-9 was placed vertically in the wet lab of the ship. Surface water was passed through the AC-9 tubes from the bottom to the top by gravity, immediately after collection [16]. Data were recorded during 2 minutes,

and then the median was taken over 0.5-minute noise-free data. Temperature and salinity corrections were performed on the raw data [17]. Absorption was corrected also for residual scattering applying the proportional method developed by [18].

The particle scattering coefficient $b_p(\lambda)$ is obtained from

$$b_p(\lambda) = c(\lambda) - a(\lambda) \quad (3)$$

A pure water calibration was performed daily using freshly produced Milli-Q water, to check for deviations from the annual WetLabs calibration [19].

4. RESULTS

4.1. Match-up stations

Between 2002 and 2008, there are in total 39 “potentially optimal” match-ups (29 match-up images). These are listed in Table 2 for 2006-8 (16 stations, 15 images) and in [3] for the period 2002-5 (23 stations, 14 images). These have optimal sea-state condition, clear sky and less than ~1hr time difference to MERIS overpass (or less than 2 hours in the case of clear Case 1 waters). Figure 1 shows the locations of these match-up stations.

Table 2. Match-up stations for 2006-8 (see [3] for information on the 2002-5 matchups). The stations in red bold face are accepted for subsequent analysis while the stations in italic font were excluded by match-up selection criteria (see text). Pending indicates that processing is in progress.

Date	Stations	Time diff. (mins)	Flags	Remark
20060531	ZB5	11	H_Glint	
20060601	ZB7	16		
20060606	BB3	4	H_Glint	
20060609	BB10	10	H_Glint	
20060629	I30	1		Pending
20060707	I30	2	H_Glint	
20060712	I30	1	H_Glint	
20060713	I30	3		
20060920	MH2E	3		Pending
20060921	MH5	5		
20070618	CZ1	3		
	CZ2	103		Clear waters
20070619	CZ3	5		Pending
20070620	CZ5	7		Pending
20080804	I80T4	5	H_Glint	
20080909	O820A	2		Pending

The majority of the match-ups are classified as turbid case 2 water. Of the 39 match-ups, 15 stations (11 images) were affected by high glint, indicated as H_Glint in the “Flags” column, and 4 stations (2 images, both from 2002-5) have negative MERIS reflectance in the blue indicated as PCD1_13 in the Flags column. 1 image (2 stations) from 2002 has geolocation error and 1 station (1 image from 2005) was influenced

significantly by heavy ship rolling. Data processing is still in progress for a further 5 stations (5 images).

reflectance is found for the clear blue waters of CZ1-A 20070618 and CZ2-A 20070618.

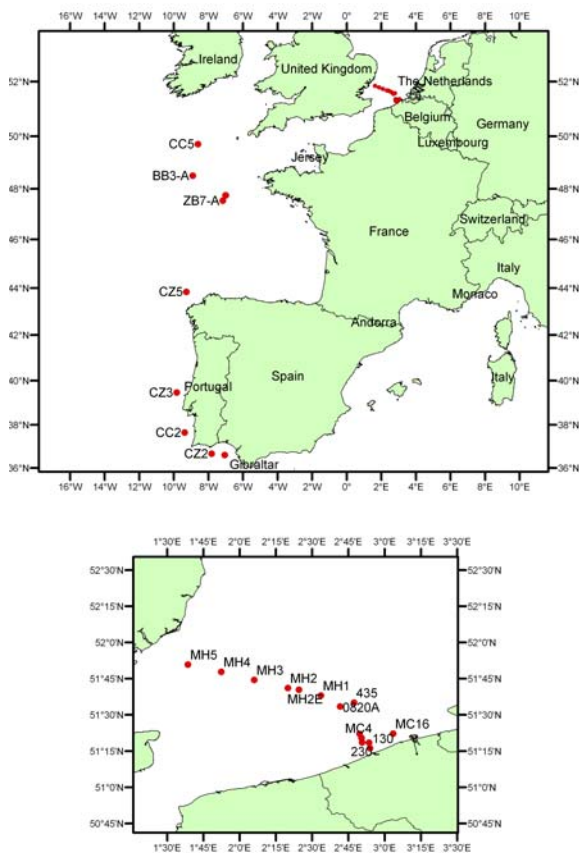


Figure 1. Locations of all match-up stations in 2002-8: all stations (top) and southern North Sea stations (bottom).

After exclusion of these 27 stations, indicated in italic font above, finally the 12 “best” match-ups remain as indicated in red bold face in Table 2 and [3].

4.2. Water-leaving reflectance spectra

Figure 2 shows the satellite-seaborne comparison for these 12 best match-ups. In general, water-leaving reflectance spectra match well between MERIS (continuous black curves) and seaborne (dashed red or blue curves) measurements, indicating that the turbid atmospheric correction works reasonably. However, a larger difference at blue bands especially at 412nm can be seen for several stations such as MC5A 20030422, MC16A 20030616, CC2A 20050531 and ZB7-A 20060601. For station 130-B 20060713 a significant difference is found throughout the spectrum, which may be related to spatial heterogeneity at this nearshore station. Excellent agreement of water-leaving

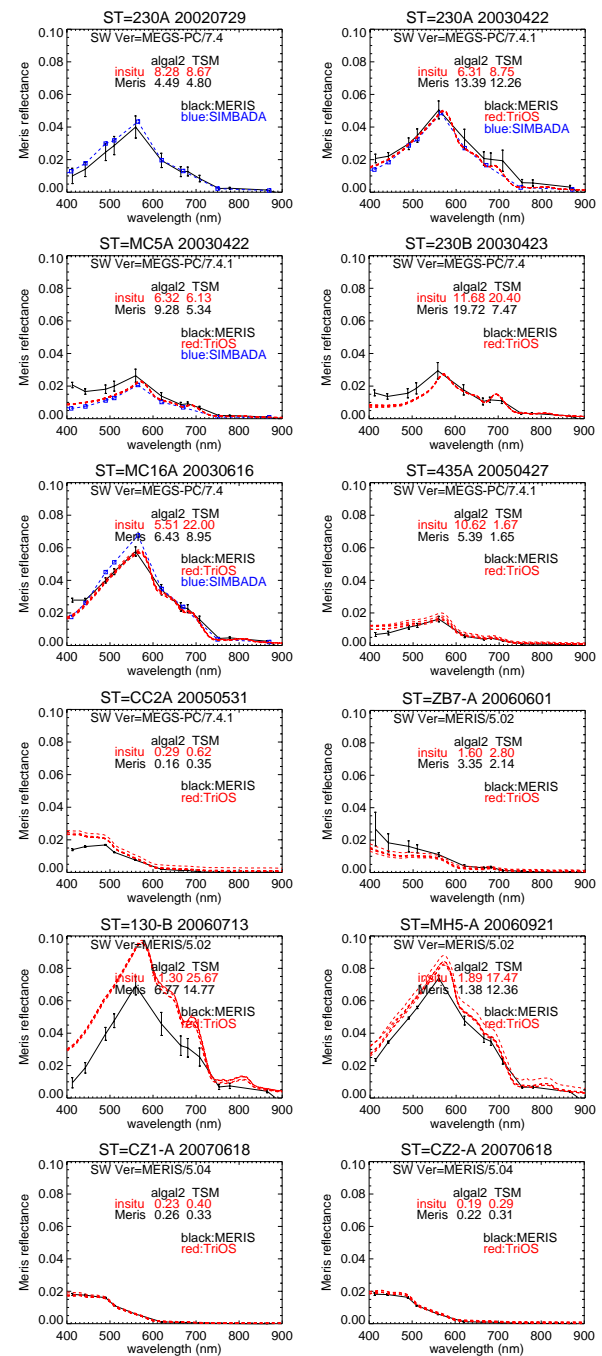


Figure 2. MERIS and seaborne measurements comparison for the 12 best match-ups. For the MERIS spectra, mean (solid lines) and standard deviation for the surrounding 3x3 box are indicated. For the TriOS spectra (dotted red lines), the five replicate measurements are shown.

4.3. Water-leaving reflectance scatter plots

Statistics such as coefficient of determination (R^2), error and regression slope and offset are presented in this section for quantitative comparison. As error indicator, the root-mean-square error (RMSE) is used for water-leaving reflectance and relative error for Chl and TSM.

For the 12 best match-ups, scatter plots of MERIS versus seaborne reflectance are shown in Figure 3 as blue squares for six bands (15 points are shown because for 3 of these matchups data was available from both TriOS and SIMBADA systems). The 560, 620 and 665 bands show good agreement while blue (especially 412nm) and NIR (753nm) bands show lower correlation. The statistics for each band are listed in Table 4 and are similar to previous results [3] except that the current analysis includes some more turbid stations than were previously considered. The green to red bands (488-680nm) show R^2 values of about 0.9 or higher and slopes close to 1, indicating good agreement between MERIS and seaborne measurements. On the other hand, low correlation is seen at both edges of the wavelength range, blue and NIR. At the NIR bands (753, 778 and 865nm) the absolute error, RMSE is small, indicating that the low correlation at NIR bands could be due to a relatively weak signal. On the contrary, low correlation at blue bands (412, 443 nm), where RMSE is large are thought to be caused by an inaccurate extrapolation of the aerosol reflectance in the atmospheric correction. Therefore, the improvement of aerosol spectral properties (e.g. Angstrom exponent) in the atmospheric correction should be prioritized for upgrades of the data processor.

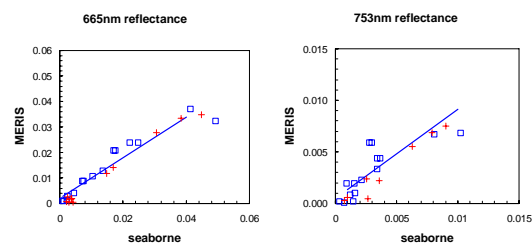
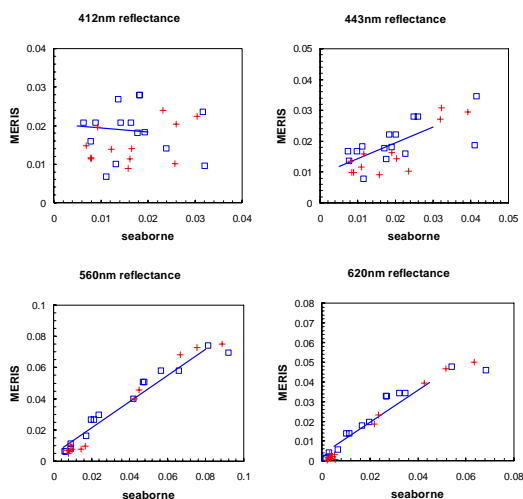


Figure 3. MERIS versus seaborne water-leaving reflectance for selected six bands. High-glint pixels are indicated as red. Regression (blue solid lines) was done for best match-ups only.

High-glint match-ups are shown as red crosses in Figure 3, although they are not included for statistical analysis. Interestingly, many of them are within the variability of the best match-ups. Glint reflectance is relatively weak in Belgian waters or higher latitudes. This implies that some of high-glint pixels could be used if, for example, a high-glint threshold is applied depending on the reflectance of the pixel.

Table 4 Statistics of water leaving reflectance comparison, MERIS vs in-situ. R^2 and RMSE represent correlation coefficient and root-mean-square error. Slope and offset are derived from the reduced major axis fitting.

λ (nm)	R^2	RMSE	slope	offset
413	0.00	0.0101	-0.10	0.0204
443	0.44	0.0077	0.51	0.0093
488	0.87	0.0072	0.68	0.0072
510	0.91	0.0069	0.75	0.0060
560	0.95	0.0072	0.84	0.0048
620	0.90	0.0066	0.81	0.0032
665	0.91	0.0048	0.80	0.0020
680	0.89	0.0046	0.81	0.0024
709	0.77	0.0049	0.82	0.0022
753	0.66	0.0016	0.87	0.0004
778	0.69	0.0015	0.91	0.0005
865	0.68	0.0008	1.00	0.0000

4.4. CHL comparison

A comparison of CHL products was shown previously in [3] and was found to be inconclusive because of the low number of data points.

4.5. TSM comparison

A comparison of TSM products was shown previously in [3] and was found to be encouraging but inconclusive because of the low number of data points.

4.6 Specific Inherent Optical Properties – chlorophyll specific phytoplankton absorption

The MERIS algorithm for chlorophyll *a* retrieval performs a neural network inversion of the water-leaving reflectance spectrum [20] to give the phytoplankton absorption coefficient at 443nm, $a_{\phi}(443nm)$. This is then converted into chlorophyll *a* concentration, C , (officially termed “algal_2” in the MERIS product suite) using the simple empirical relationship:

$$C = 21.0 * a_{\phi}(443nm)^{1.04} \quad (4)$$

Figure 6 shows the *in situ* measurements of C and $a_{\phi}(443nm)$ (all stations, not just matchup stations) compared against this assumed relationship. The correlation coefficient between $a_{\phi}(443nm)$ and C is $R^2=0.71$. The intercept of the regression line (black line in Figure 6) is 1.5 times higher than that used for the MERIS processor [20] (pink line in Figure 6), indicating a lower chlorophyll-specific phytoplankton absorption *in situ* than is assumed by the MERIS processor. Thus, if a regional correction is applied on the basis of the IOP data the regional C product would be higher than the standard MERIS product. The slope of the log-relation between C and $a_{\phi}(443nm)$ is close to 1 for both the present IOP data and the MERIS processor, indicating little evidence for a packaging effect [21] here.

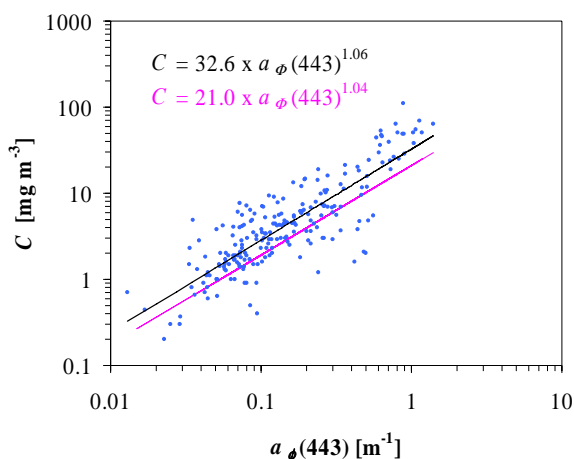


Figure 6. *In situ* measurements of chlorophyll *a* concentration and phytoplankton absorption coefficient at 443nm for the Southern North Sea in blue, compared to the empirical relationships used in the MERIS processor in pink [20].

4.7 Specific Inherent Optical Properties –TSM-specific particulate scattering

The MERIS algorithm for TSM retrieval performs a neural network inversion of the water-leaving reflectance spectrum to give the particulate scattering at 443nm [20], $b_p(443nm)$. This is then converted into TSM concentration, S , using the simple empirical relationship:

$$S = 1.73 * b_p(443nm)^{1.04} \quad (5)$$

Figure 7 shows the *in situ* measurements of S and $b_p(443nm)$ (all stations, not just matchup stations) compared to the MERIS relationship. The correlation coefficient for *in situ* IOP data is $R^2=0.78$. In log space the relationship suggested by the IOP data has a quite different intercept and slope from that used in the MERIS processor [20]. It is possible that this difference is strongly influenced in the regression relationship by the low S and low $b_p(440)$ data, where the highest differences are found.

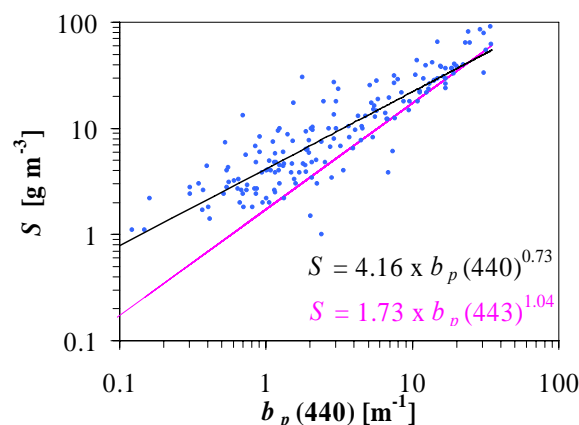


Figure 7. *In situ* measurements of TSM concentration and particulate scattering coefficient at 443nm, compared to the empirical relationships used in the MERIS processor [20].

4.8 Turbidity

Linear regression analysis between turbidity and TSM for 144 samples obtained during seaborne campaigns in 2007 and 2008 is shown in Figure 8. Variability of particle size, refractive index and/or density can give variation of the TSM-specific turbidity. These data were acquired over oceanographic conditions from clear to very turbid water and from mineral-dominated particulate matter to high biomass algal blooms. Despite this wide variety of particulates a very strong correlation is found between TSM and turbidity.

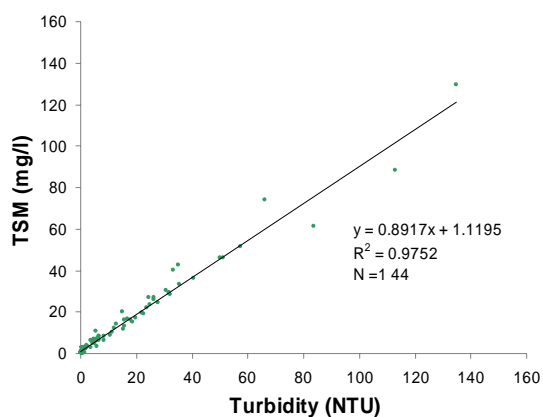


Figure 8. Linear regression between turbidity and TSM for 144 samples obtained during seaborne campaigns in 2007 and 2008.

Comparison of turbidity data before and after filtration (all stations in 2007-8, not just matchups) is shown in Figure 9.

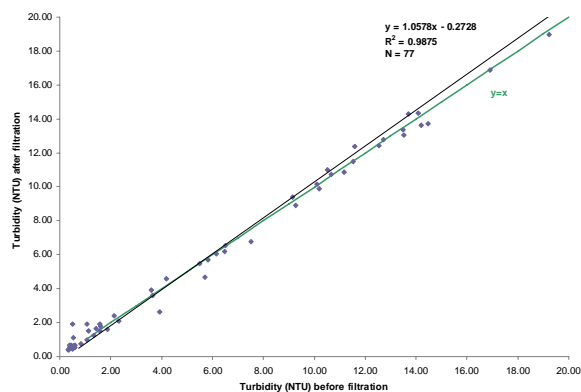


Figure 9. Comparison of turbidity before and after filtration.

As expected the correlation is very high. A few outliers, especially for very low turbidity, can be identified. It is suspected in these cases that the mixing of the sample was imperfect. Following this quality control exercise, the procedure for sample mixing during filtrations was improved giving generally much lower difference between turbidity measurements before and after filtrations.

5. OTHER REMARKS

Occasional anomalies are seen in the MERIS chlorophyll images as noisy data for low concentrations as reported previously for the 22.8.2005 image [3] and additionally for the 27.3.2007 image in Figure 10. These have been reported to ESA and to the case 2 water algorithm developers.

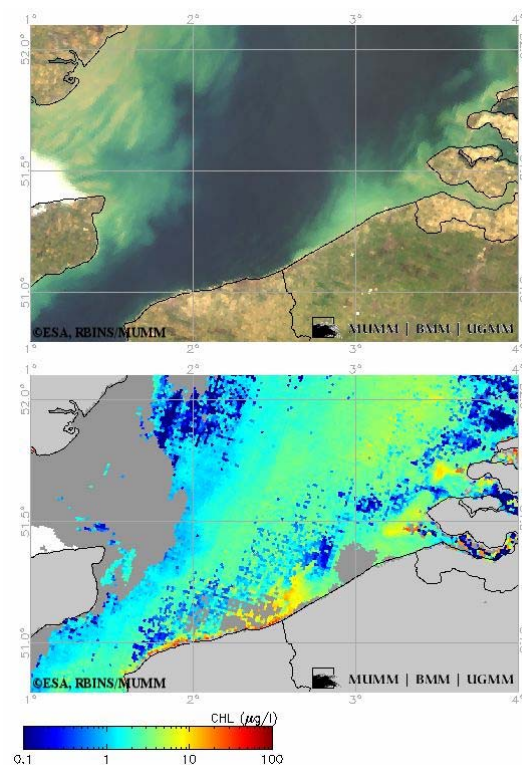


Figure 10. Example of MERIS imagery with suspect noisy low chlorophyll (27th March 2007). (top) RGB composite (bottom) algal2 product.

6. SUMMARY AND RECOMMENDATION

After filtering the original set of 39 match-ups with sea-state condition, sky/cloud condition, less than 1 hour time difference, and PCD flags, the 12 best match-ups were obtained, and have been used to estimate the MERIS product errors.

The water-leaving reflectance comparison shows acceptable agreement in the green to red spectral region while blue and NIR bands are less accurate in turbid waters. This could indicate that the aerosol spectral properties are not retrieved accurately enough. It is recommended to investigate the spectral properties of the selected aerosol models, especially in turbid waters. Spatial irregularity in Chl images was reported previously for the 22.8.2005 image [3] and are illustrated again here for the 27.3.2007 image. Such artifacts are of concern to users and should be investigated and removed.

Many of the high-glint flagged pixels seem usable in Belgian waters or higher latitudes. It is recommended to investigate a new high-glint threshold depending on the water-reflectance in order to increase data usability. Significant differences are found between measured specific inherent optical properties and corresponding relationships used for the standard MERIS processor. The standard products could be regionally calibrated to account for these differences.

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