Abstract Details

Title: **Validation of S3 OLCI observations using one year of semi-continuous WISPstation measurements in the high dynamic area of the Eems Estuary**

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Abstract

The Eems Estuary is a very dynamic area featuring highly variable turbidity and Chlorophyll-a values. There is an interest to decrease the turbidity and monitoring is being put into place to observe the current status and changes. Remote sensing using Sentinel 3 OLCI observations is a candidate monitoring technique but should provide robust and validated results.

Obtaining high quality turbidity estimates starts with validated Bottom of Atmosphere reflectances.

To validate BOA reflectances a WISPstation (Peters et al., 2019) was placed on a fixed structure in open water at 53.4743N and 6.8216W from 13-11-2018 until 05-11-2019. The WISPstation contains 2 sets of sensors (Lup: 40 degrees, Lsky: 40 degrees and Ed): measurements were taken in two directions, N and NE. Some shadowing of the Ed sensors occurred and needed to be filtered out.

The hyperspectral measurements (350-1100 nm; 0.44 nm/pixel or 4.65 nm FWHM) were convoluted to OLCI spectral bands using appropriate spectral response functions. Rrs was calculated using a rho retrieved from the Mobley (1999) table in combination with the similarity spectrum approach (Ruddick et al, 2006). Because the WISPstation is measuring all channels with one spectrometer, it is very unsensitive to any uncertainties in the radiometric calibration.

In total 61 cloud free S3 OLCI matchup measurements could be taken (S3A+B) , some of which were later flagged out. The S3 FR matchup data were collected in 3x3 pixel windows and filtered according to the criteria mentioned in the EUMETSAT validation recommendations document (EUM/SEN3/DOC/19/1092968, v5B).

Since the WISPstation takes a measurement every 15 minutes we were able to take validation measurements close in time to the overpass, although one of the conclusions remains that -for this area- validation at exact overpass times would be better.

We tested the C2RCC-alt v1 and C2X neural networks processors (SNAP v6) together with Polymer v4.10. We will show a detailed analysis of the results of these atmospheric correction processors, in terms of statistical comparison (as e.g. in Warren et al., 2019) and by looking at averaged spectral shape of the OLCI Rrs spectra.

For "all datapoints" scatterplots we find R2 values of 0.6 to 0.8 with slopes from 0.5 to 0.76, Indicating that the atmospheric corrections all underestimate the in-situ measured values with some spread.

For "band averaged" scatterplots we find high R2 values for all three processors (above 0.95) but -again- with slopes significantly deviating from unity: all processors underestimate the reflectance, with Polymer giving the biggest underestimation. The underestimations range from 15% (C2X) to 30% (Polymer). For the neural networks the biggest underestimations are found from 490 to 681 nm.

Plots of mean spectra reveal that especially the neural networks C2RCC-alt and C2X underestimate for wavelengths smaller than about 700 nm. Above that range the performance is much better.

Based on the time averaged WISPstation data series we propose tentative correction spectra to improve the accuracy of BOA reflectances for the studied versions of the atmospheric correction methods. We conclude that the presented method based on stationary in-situ measurements is suitable to validate the performance of current and future updated atmospheric correction methods.

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Introduction

The Ems-Dollard estuary and adjoining Wadden Sea area are highly dynamic in time and space because of tidal influences. The areas have both an international protection status (Natura 2000, World Heritage) and an economic function (shipping, fishing). Because of climate change there is a need to know primary production changes in the estuary and Wadden Sea. There is also an interest to decrease the turbidity and monitoring is being put into place to observe the current status and changes.

Because of tidal dynamics and the extend of the area it is impossible to monitor it efficiently with conventional monitoring methods in a sufficiently high resolution and frequency. Earth observation can provide a valuable addition to an integrated monitoring system (Hommersom, 2009 and 2010).

Remote sensing using Sentinel 3 OLCI observations is a candidate monitoring technique but should provide robust and validated results. Obtaining high quality turbidity estimates starts with validated and -if necessary- calibrated Bottom Of Atmosphere (BOA) reflectances.

Recent studies over inland and coastal waters (e.g. Warren et al., 2019) indicate that specific situations call for specific atmospheric correction methods. Clear water studies may benefit from the use of e.g. Polymer while optical complex waters studies may benefit from the use of e.g. C2RCC or its alternative version, iCOR, Acolite or the standard NASA AC). Very turbid waters studies may benefit from e.g. iCOR or C2RCC-alt (see e.g. Mograne et al., 2019 or Renosh et al., 2020) and the upcoming ACIX-II results). It seems that for any area a substantial amount of validation measurements is necessary to determine the most suitable approach to atmospheric correction.

Introducing the WISPstation instrument for OLCI validation

One recent development to help validating OLCI BOA reflectance is the WISPstation (Peters et al., 2019). The WISP station is an above water optical measuring system. The advantage of an above-water system is that there is no biofouling of the sensors. As a result, invalid measurements are relatively sparse and only very low frequency maintenance is required. This makes it possible to greatly increase the measurement density without recurrent costs for field visits.

The WISPstation instrument is designed both for satellite BOA reflectance validation and for on-line semi-continuous monitoring of some essential ecological water quality parameters. In view of these applications a fixed position design was chosen without any moving parts. Basis for the design is the publication of Mobely (1999), namely that the azimuth angle is optimal around 138° (plus or minus 40°) from the sun, the Lup angle around 42° from the nadir and the Lsky angle around 42° from the zenith. By having an instrument that measures Rrs simultaneously looking in NNW and NNE directions, a valid measurement (according to these criteria) can be obtained during most of the day.

Big advantages of a non-moving sensor are that the time to position the instrument accurately is nihil, the set-up is less prone to malfunctions and the maintenance can be extremely low. In fact the WISPstation only requires some cleaning of the top Ed sensors.

To correct all measurements to the optimal 138° azimuth angle, the table provided by Mobley (1998)) with coefficients for different wind speeds and sun positions is used. In total the WISPstation features 8 channels (Figure 1):

- 2 Radiance channels collecting Lup and Lsky in the NNW direction
- 2 Radiance channels collecting Lup and Lsky in the NNE direction
- 2 Irradiance channels
- 1 unexposed dark radiance channel for evaluation of radiance channel degradation
- 1 unexposed dark irradiance channel for evaluation of the degradation of irradiance channels

All channels are connected to one central spectrometer by means of optical fibres and an optical multiplexer. One of the advantages of this design is that any variability or degradation in the sensitivity of the spectrometer is compensated in the calculation of the reflection. A normal measurement cycle in which each channel is measured 10 times at an optimal integration time usually takes less than 1 minute, depending on ambient light conditions. The system is calibrated with respect to a reference instrument which is calibrated in a certified laboratory using a lamp and integrating sphere with NIST traceable calibrations.

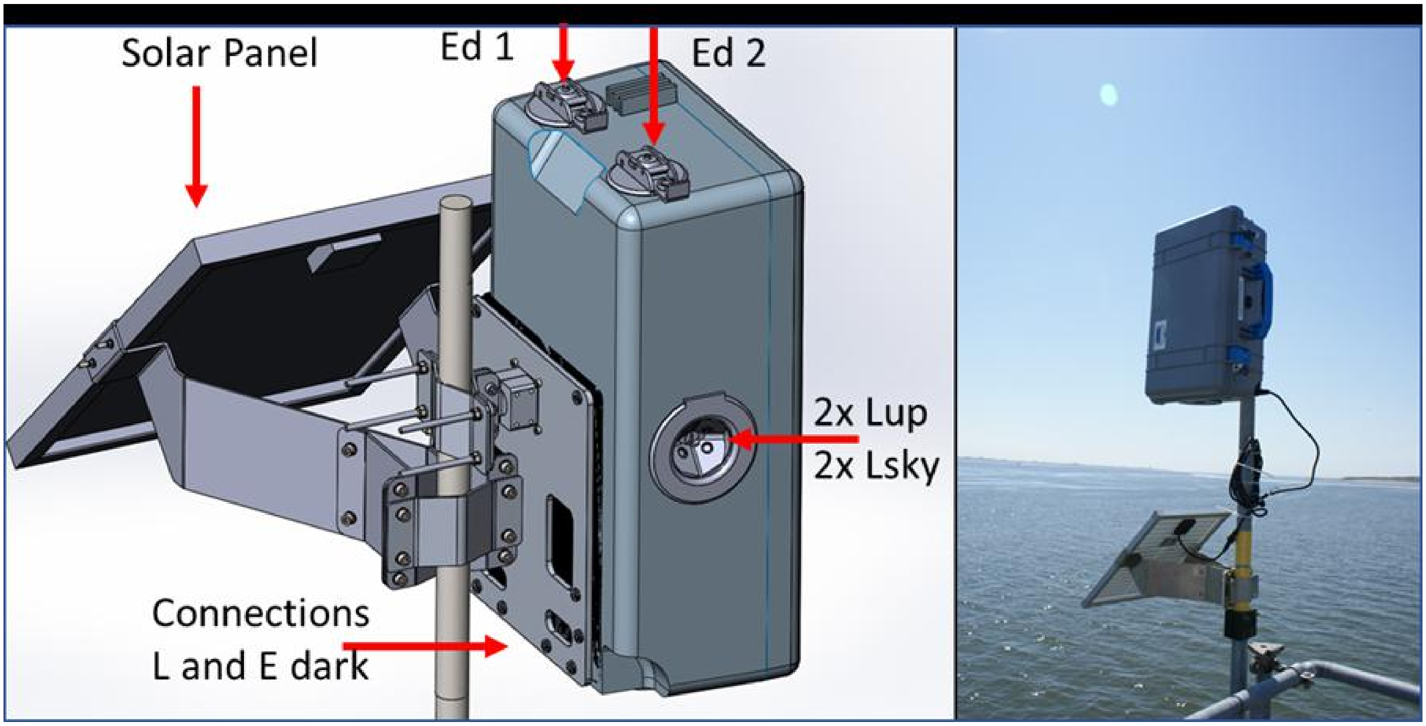

Figure 1: Configuration of the optical sensors on the WISP station (left) and WISP station as mounted (right)

The WISPstation is built around the Avantes Mini mk-1 spectrometer with a maximum wavelength range between 220 and 1100 nm. The "grating" has 300 lines per mm with a "blaze" of 300 nm. Together with a "slit" of 100 um, this leads to a spectral resolution (FWHM) of 4.65 nm. A scalable PostgreSQL database (WISPcloud) is available to receive and store all measurements autonomously, to perform quality control and to apply water quality algorithms. Via an advanced API, users can retrieve data directly. In the H2020 project MONOCLE interfaces are being developed to connect an instrument to a network of sensors via a SOS backbone server (https://monocle-h2020.eu/Home).

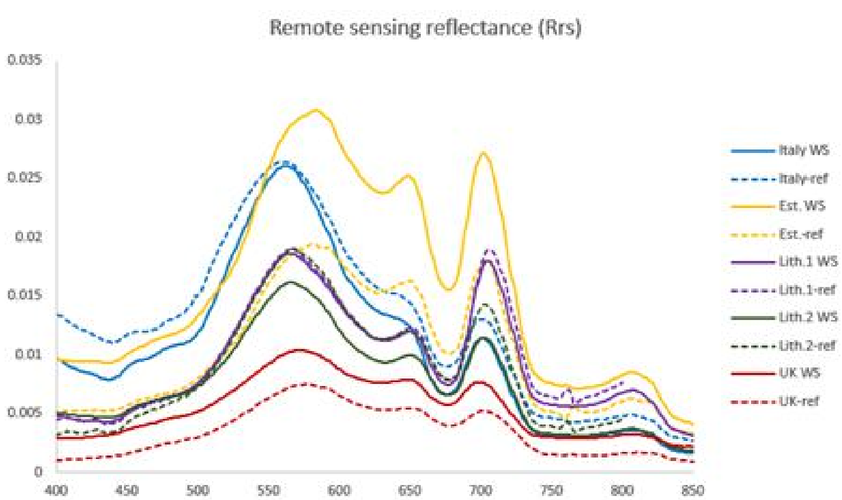

Figure 2 - Examples of matching Rrs spectra from the different regions. WS stands for WISPstation, -ref for the reference instrument (which is different per region). Est. = Estonia, Lith. = Lithuania. In Lithuania there are two WISPstation installed.

In the H2020 EU project EOMORES, spectra and derived concentrations from WISPstations have been extensively validated (Examples of reflectance comparisons can be found in Figure 2). (Riddick et., 2019)

Set up at the measurement location

To validate BOA reflectances a WISPstation was placed on a fixed structure in open water at 53.4743N and 6.8216W from 13-11-2018 until 05-11-2019 (Figure 3).

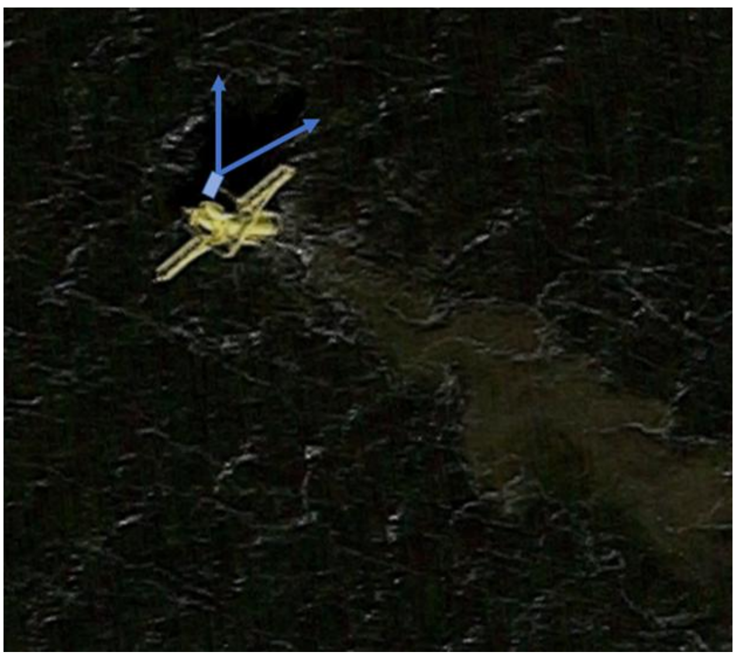

Figure 3: Location in the Dutch Wadden Sea

Figure 4: orientation of measurement pole and WISPstation azimuth angles

As the station could not be attached to one of the arms of the pole, it was attached to the platform on the north side with an NNO orientation. This means that the instrument looks at the N and at the NO (see Figure 4). The upward and downward looking sensors had an unobstructed view. A small part of the construction of the pole is above the instrument and thus in sight of the irradiance sensors. This probably has a negligible influence on the measurement but if the sun is directly to the south, the shadow of the pole will fall over the irradiance sensors. If this happens, the reflection measurements are unreliable. There is also a chance that one of the downward facing sensors will look into the shadow of the pole. In that case, the sensor in the alternative viewing direction is used. The WISPstation was configured to take a measurement every 15 minutes. The measurement was selected that was closest in time with the S3 match-ups.

Data (pre-)processing

The hyperspectral measurements (350-1100 nm; 0.44 nm/pixel or 4.65 nm FWHM) were convoluted to OLCI A/B spectral bands using appropriate spectral response functions. Rrs was calculated using a rho retrieved from the Mobley (1999) table (windspeed fixed at 5 m/s) in combination with the similarity spectrum approach (Ruddick et al, 2006).

Satellite data

The OLCI data were downloaded from the Copernicus Open Access HUB (https://scihub.copernicus.eu) provided by ESA. In total 61 cloud free S3 OLCI matchup measurements were selected (S3A+B). The S3 FR matchup data were collected in 3x3 pixel windows and filtered according to the criteria mentioned in the EUMETSAT validation recommendations document (EUM/SEN3/DOC/19/1092968, v5B).

Satellite data pre-processing

For this study three atmospheric correction processors were compared, C2RCC-v1 (alternative version) (Brockmann and Doerffer, 2016), C2X v1.0 (Brockmann and Doerffer, 2016) and Polymer v4.10 (Steinmetz et al., 2011). C2RCC and C2Xare based on neural networks which was build on the Case2Regional (C2R) and CoastColour (CC) atmospheric correction algorithms. C2X was specifically trained for very turbid waters. Polymer is a spectral optimization algorithm designed for high sun-glint conditions. It combines a bio-optical model with series of polynomials describing sun-glint and atmospheric transmission.

Flags used for selection of valid pixels were:

C2RCC/C2X: NOT invalid, NOT land, NOT fresh_inland_water, NOT cloud/cloudbuffer (Idepix), NOT OOS.

Polymer: standard flagging was applied which includes: negative back-scattering coefficient, out of bounds exception, thick aerosol, high air mass and inconsistency flags.

Pixel extraction

Pixel extraction was done using SNAP at the location of the pole. On the location a window of 3x3 pixels was extracted. If one of the pixels is flagged as land, the whole window is discarded. The mean value of the 9 pixels was used as match-up value and compared to WISPstation measurements.

Statistics

For evaluation of the match-ups the statistical parameters were used proposed by Warren et al., 2019. We have calculated the statistics per OLCI sensor (A or B) to get an impression of the differences between the two.

N = Number of samples (number of images * number of spectral bands)

R^2 = square of the Pearson correlation coefficient (1 is perfect fit)

Slope = the slope of the regression line (1 is perfect 1:1 line)

Intercept = the intercept of the regression line (0 is perfect intercept)

Furthermore we calculated the

BIAS = a measure of consistent over- or underestimation (smaller is better)

MAPD = "Mean Absolute Percentage Difference" is the average error as percentage of the in-situ measurements (smaller is better)

RMSD = "Root Mean Square Deviation" (same as RMSE) provides an impression of the variation between the two datasets (smaller is better)

$$MAPD = \frac{100}{N}\sum\left|\frac{x_i - y_i}{y_i}\right|$$

$$RMSD = \sqrt{\frac{1}{N}\sum(x_i - y_i)^2}$$

$$BIAS = \frac{1}{N}\sum\frac{(x_i - y_i)}{y_i}$$

Selected S3 images

29-3-2019 10:13	19-7-2019 10:10	9-4-2019 09:49
30-3-2019 09:47	23-7-2019 10:06	10-4-2019 09:23
31-3-2019 09:21	24-7-2019 09:40	15-4-2019 10:34
1-4-2019 10:36	26-7-2019 10:28	16-4-2019 10:08
2-4-2019 10:10	8-8-2019 09:51	17-4-2019 09:41
7-4-2019 09:40	11-8-2019 10:13	19-4-2019 10:30
9-4-2019 10:28	22-8-2019 10:28	20-4-2019 10:04
10-4-2019 10:02	23-8-2019 10:02	21-4-2019 09:38
11-4-2019 09:36	24-8-2019 09:36	23-4-2019 10:26
14-4-2019 09:58	26-8-2019 10:24	13-7-2019 10:26
15-4-2019 09:32	27-8-2019 09:58	19-7-2019 09:30
17-4-2019 10:21	28-8-2019 09:32	21-7-2019 10:19
18-4-2019 09:55	30-8-2019 10:21	23-7-2019 09:26
19-4-2019 09:28	31-8-2019 09:55	26-7-2019 09:49
21-4-2019 10:17	24-3-2019 10:04	14-8-2019 09:56
22-4-2019 09:51	29-3-2019 09:34	22-8-2019 09:49
23-4-2019 09:25	31-3-2019 10:22	24-8-2019 10:37
3-5-2019 10:06	1-4-2019 09:56	25-8-2019 10:11
6-5-2019 10:28	2-4-2019 09:30	26-8-2019 09:45
10-5-2019 10:25	8-4-2019 10:15	28-8-2019 10:34
30-8-2019 09:41		

Table 1: Data with cloudfree Match-up pixels from S3 images.

Statistical results of the validation

	S3A					
	C2R CC	C2X	Polymer	C2R CC	C2X	Polymer
	all data			band means		
N	705	420	520	15	15	13
R2	0.67	0.80	0.59	0.97	0.97	0.98
Slope	0.69	0.76	0.507	0.76	0.97	0.64
Intercept	0.0010	0.0010	0.0010	0.0005	0.0003	-0.0001
BIAS	0.127	-0.021	0.253	0.096	0.014	0.348
MAPD	46.07	39.11	42.82	19.71	23.35	34.77
RMSD	0.0036	0.0029	0.0050	0.0023	0.0015	0.0037

	S3B					
	C2R CC	C2X	Polymer	C2R CC	C2X	Polymer
	all data			band means		
N	600	330	429	15	15	13
R2	0.75	0.75	0.59	0.98	0.95	0.95
Slope	0.73	0.73	0.58	0.77	0.84	0.70
Intercept	0.0006	0.0010	0.0010	0.0003	0.0001	0.0001
BIAS	0.208	0.215	0.144	0.104	0.042	0.247
MAPD	47.61	53.93	45.29	20.35	26.4	28.12
RMSD	0.0031	0.0033	0.0041	0.0019	0.0018	0.0028

Table 2: Statistical results of the comparison between WISPstation Rrs and S3A/B Rrs

In the “all data” columns every data-pair S3A/B-band value vs WISPstation-band value is used (see also Figs 5 and 7). Per sensor also the band-mean values were calculated and compared (see also Figs 6 and 8).

All data results

The number of valid pixels differs substantially between the 3 processors, where C2RCC provides the highest number of valid pixels and C2X the lowest number. All atmospheric correction processors have a slope that is significantly below 1. Rrs is underestimated to almost 50% using Polymer for the S3A images.

The uncertainty related indices vary slightly per sensor. R2 is between 0.8 (S3A-C2X) and 0.59 (Polymer). The variability is also expressed in e.g. the MAPD.

Band averaged results

Overall the averaged spectral integrity of the processors is very high expressed by R2 values above 0.95. Also for band-averaged values the slopes are lower than 1 with polymer giving the largest underestimations. Uncertainties in the band averaged comparison follow a slightly different pattern as the “all data” comparison where C2RCC-alt shows the lowest MAPD’s.

Consequences for operational processing of S3 images for water quality mapping

Based on these statistical results a choice was made for further operational processing of S3 images in the area. Polymer was not selected because of the combination: largest underestimation and lowest R2 in the "all data comparison". Operational processing also requires the highest number of valid pixels which is an argument for using C2RCC-alt over C2X. This choice is also supported by the observation that C2X produces significantly more noise in the atmospheric corrected reflectance bands. Therefore C2RCC was chosen for operational processing for Sentinel-3 in this area.

Operational processing is mostly concerned with estimating SPM and Chlorophyl-a as proxy for eutrophication and as model component for primary production estimation. Our algorithms use a band around 705 nm for SPM concentrations (Nechad, 2010) and a ratio of 665/705 bands for Chlorophyll-a estimation (Gons, 1999). To assess the effect of uncertainties in atmospheric correction on the outcome of concentration estimations one can study the mean reflectance of S3A/B compared to the mean reflectance of the WISPstation convoluted to the S3 bands (Figs 6 and 8). It is clear that the C2RCC-alt 705 nm band is very close to the mean in-situ observed value but the C2RCC-alt 665 nm band is underestimated by 20-30%. Therefore the conclusion is that – for this version of C2RCC-alt- the reflectances have to be corrected before they can be entered into a concentration calculation.

We have established preliminary correction factors based on the matchup data (table 4). This illustrates that there are significant differences per band. Probably the accurateness of the correction factors would increase for longer time series.

It is expected that atmospheric correction algorithms will improve over time, becoming more accurate also for the more complex waters like the Ems estuary. This would mean that over time the compensation factors could be decreased. By regular updates of the compensation factors for atmospheric correction based on in situ reflectance matchups, the time series of concentrations could be kept continuous for users. Also for new areas the proposed method to compensate for systematic errors in the atmospheric correction is recommended.

S3 Band	S3A	S3B	All AB
Oa01	1.29927	1.44855	1.37529
Oa02	1.24442	1.3574	1.30241
Oa03	1.29715	1.32448	1.31149
Oa04	1.31201	1.27057	1.28968
Oa05	1.25595	1.20766	1.22977
Oa06	1.18443	1.16675	1.17486
Oa07	1.15316	1.12303	1.13765
Oa08	1.33737	1.25897	1.29741
Oa09	1.40097	1.31085	1.35493
Oa10	1.38116	1.30201	1.34085
Oa11	1.13661	1.0737	1.10587
Oa12	1.27655	1.1587	1.21875
Oa16	1.17008	1.06337	1.11768
Oa17	1.67423	1.58104	1.62761
Oa18	1.61195	1.54443	1.5781

Table 4: Correction factors for C2RCC-alt S3A/B version SNAP 6.0 based on WISPstation match-ups

Literature

Brockmann, C., Doerffer, R., Peters, M., Kerstin, S., Embacher, S., Ruescas, A (2016) Evolution of the C2RCC Neural Network for Sentinel 2 and 3 for the Retrieval of Ocean Colour Products in Normal and Extreme Optically Complex Waters. Living Planet Symposium, Proceedings of the conference held 9-13 May 2016 in Prague, Czech Republic. Edited by L. Ouwehand. ESA-SP Volume 740, ISBN: 978-92-9221-305-3, p.54

Gons, H. J. (1999) Optical teledetection of chlorophyll a in turbid inland waters. Environmental Science & Technology, 33, 1127−1132.

Hommersom A., Peters S., Wernand M., de Boer J., (2009) et al., 2009 Spatial and temporal variability in bio-optical properties of the Wadden Sea, Estuarine, Coastal and Shelf Science 83 (2009) 360-370, Elsevier

Hommersom, A., Wernand, M.R., Peters, S., de Boer, J. (2010). A review on substances and processes relevant for optical remote sensing of extremely turbid marine areas, with a focus on the Wadden Sea. Helgoland Marine Research 64(2): 75-92. DOI: 10.1007/s10152-010-0191-6

Mobley, "Estimation of the remote-sensing reflectance from above-surface measurements," Appl. Opt. 38(36), 7442–7455 (1999), http://dx.doi.org/10.1364/AO.38.007442.APOPAI0003-6935

Mobley, C.D., 2015. Polarized reflectance and transmittance properties of wind-blown sea surfaces. Appl. Optics 54(15), 4828-4849.

Mograne, M.A.; Jamet, C.; Loisel, H.; Vantrepotte, V.; Mériaux, X.; Cauvin, A. Evaluation of Five Atmospheric Correction Algorithms over French Optically-Complex Waters for the Sentinel-3A OLCI Ocean Color Sensor. *Remote Sens.* **2019**, *11*, 668.

Nechad, K.G. Ruddick, Y. Park, (2010): Calibration and validation of a generic multisensor algorithm for mapping of total suspended matter in turbid waters, Remote Sensing of the Environment, 114 (2010), pp. 854-866

Renosh, P.R.; Doxaran, D.; Keukelaere, L.D.; Gossn, J.I. (2020). Evaluation of Atmospheric Correction Algorithms for Sentinel-2-MSI and Sentinel-3-OLCI in Highly Turbid Estuarine Waters. Remote Sens. **2020**, 12, 1285. https://www.mdpi.com/2072-4292/12/8/1285

Riddick, C., Tyler, A., Hommersom, A., Alikas, K., Kangro, K., Ligi, M., Bresciani, M., Antilla, S., Vaiciute D., Bucas, M., Tiskus, E., Dionisio Pires, M., Warren, M., Simis, S. (2019). D5.3: Final Validation Report, EOMORES Project Deliverable. https://zenodo.org/record/4057057#.X3L-fO1S-XI

K. Ruddick, V. De Cauwer, Y. J. Park, and G. Moore, "Seaborne measurements of near infrared waterleaving reflectance: The similarity spectrum for turbid waters," Limnol. Oceanogr. 51(2), 1167–1179 (2006).

Peters S., Laanen M., Groetsch P., Ghezehegn S., Poser K., Hommersom A., De Reus E., Spaias L. (2018) WISPSTATION: A NEW AUTONOMOUS ABOVE WATER RADIOMETER SYSTEM, Proceedings of the Ocean Optics XXIV conference, Dubrovnik, Croatia

Steinmetz, F., Deschamps, P.-Y., and Ramon, D. (2011): Atmospheric correction in presence of sun glint: application to MERIS, Opt. Express 19, 9783-9800.

Warren MA, Simis SGH, Martinez-Vicente V, Poser K, Bresciani M, Alikas K, Spyrakos E, Giardino C & Ansper A (2019) Assessment of atmospheric correction algorithms for the Sentinel-2A MultiSpectral Imager over coastal and inland waters. Remote Sensing of Environment, 225, pp. 267-289.

Additional Figures

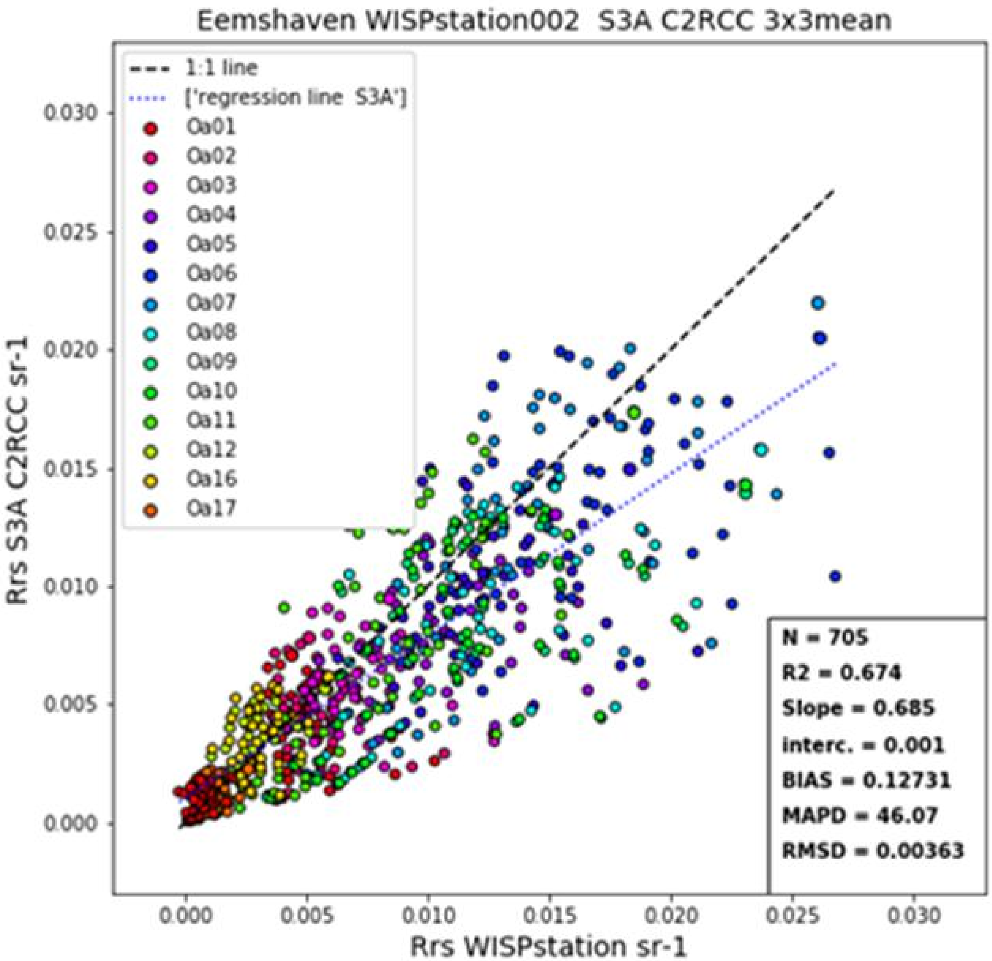

Fig 5: Scatterplot of Rrs Wispstation vs Rrs S3A

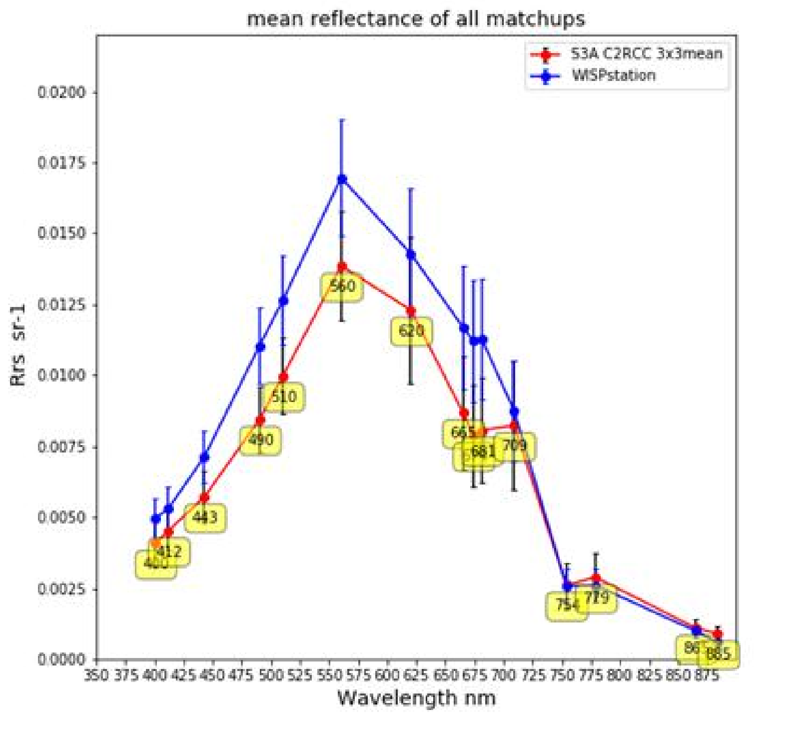

Fig 6: Mean Rrs spectrum WISPstation and S3A C2RCC-alt

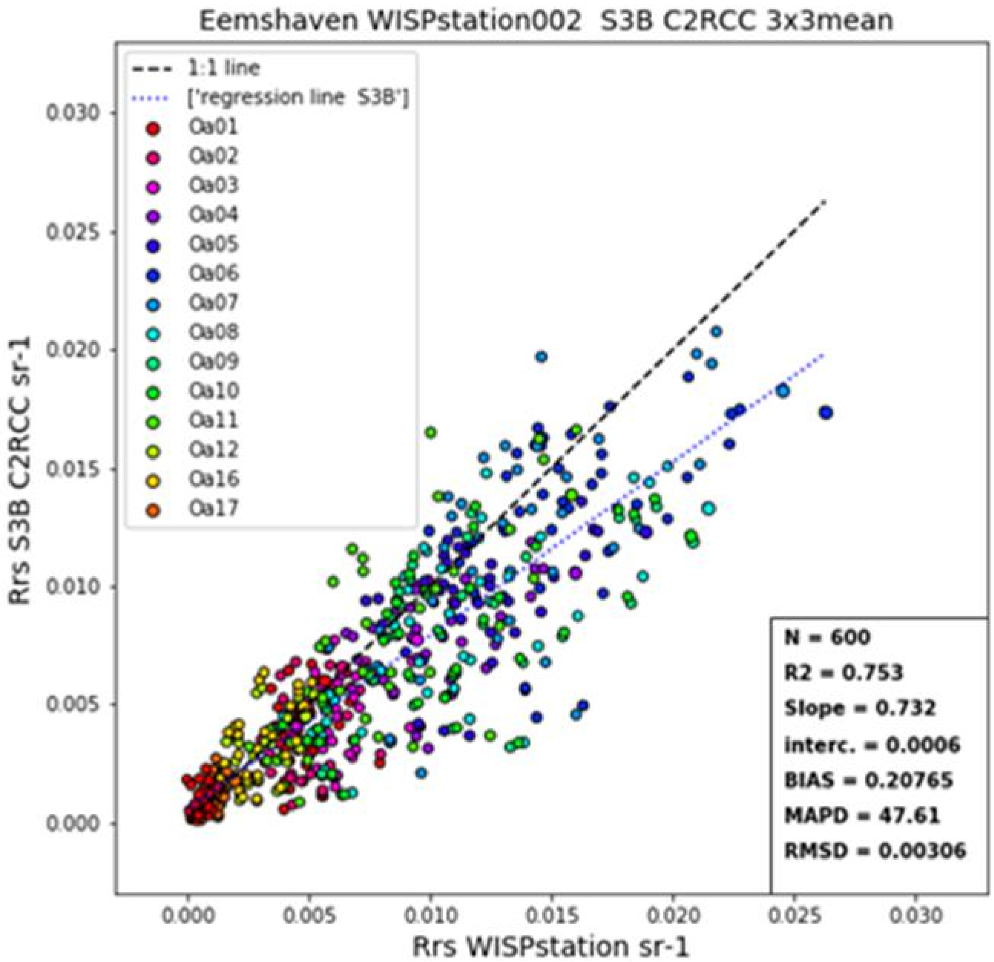

Fig 7: Scatterplot of Rrs WISPstation vs S3B C2RCC-alt

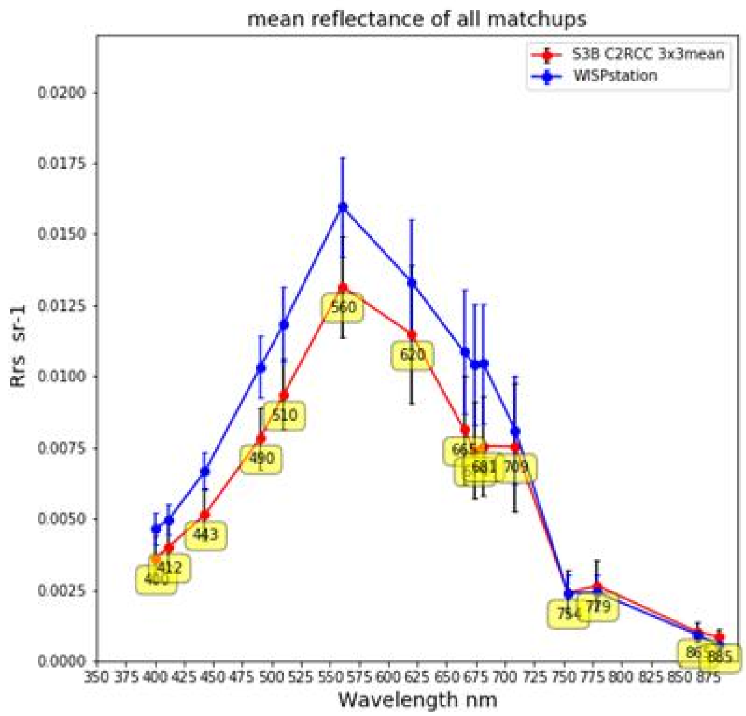

Fig 8: Mean Rrs spectrum WISPstation and S3B