

SEAmBOTH Seamless Bothnian Bay

Remote Sensing – Satellite based water quality assessment in the Gulf of Bothnia









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Contents

| 1. | Int | roduction | 4 |
|-----|--|--|----|
| 2. | На | rmonization of bio-optical protocols | 5 |
| 3. | Ear | th observation data and in situ measurements | 6 |
| 3 | .1. | EO data | 6 |
| 3 | .2. | SEAmBOTH validation campaign data | 6 |
| 3 | .3. | National and regional monitoring data | 10 |
| 4. | Bas | sics of EO processing | 11 |
| 5. | Re | sults and validation | 13 |
| 5 | .1 V | alidation of Sentinel-2 data | 13 |
| 5 | .2 V | alidation of Sentinel-3 data | 14 |
| 5 | .3 lı | norganic suspended matter product from S3 data | 23 |
| 5 | .4 E | O products to support habitat modelling | 24 |
| 6. | EO | publications & outreach | 27 |
| 7. | Dis | cussion and conclusions | 27 |
| Ref | References | | |
| Арр | Appendix I – Optical measurement protocols v. 4, November 2019 | | |
| Арр | Appendix II – Filtration for CDOM measurements | | |
| Арр | Appendix III – Filters for CDOM measurements | | |
| Арр | Appendix IV – Hydrolight reflectance simulations | | |

Glossary

| AC9 | 9-channel absorption (a) and beam attenuation (c) meter (WetLabs, USA) |
|--------------------------|--|
| a _{CDOM} | CDOM absorption at 440 nm, also termed g ₄₄₀ |
| BG | Brockmann Geomatic Sweden, AB |
| CDOM | Coloured Dissolved Organic Matter, also termed Gelbstoff |
| C.V. | Coefficient of variance (=standard deviation/mean) |
| Chl-a | Chlorophyll-a, used as a proxy for phytoplankton biomass |
| EO | Earth Observation |
| Elga® | PURELAB [®] Water Purification System |
| ESA | European Space Agency |
| FNU | Formazin Nephelometric Unit measured at 90 degrees from the incident light beam with an |
| | infrared light source (ISO 7027 method) |
| G440 | CDOM absorption at 440 nm, also termed aCDOM |
| Gelbstoff | Yellow substance, also termed CDOM |
| GF/F filters | Glass fibre filters with a nominal pore size of 0.7 μ m |
| HELCOM | Baltic Marine Environment Protection Commission |
| HPLC | High Performance Liquid Chromatography |
| IOCCG | International Ocean Colour Coordination Group |
| λ | lambda, wavelength (nm) |
| Macropixel | 3x3 pixel box around a specific sampling station or location |
| MAE | Mean Average Error |
| Microtops | Solar Light's Model 540 Microtops II [®] Sunphotometer 5 channel instrument for measuring |
| | aerosol optical thickness, direct solar irradiance, and water vapour column |
| Milli-Q® | Water purification system to make ultrapure water (UPW) |
| MSFD | Marine Strategy Framework Directive |
| MSI | 13 channel Multi-Spectral Instrument launched on S2 |
| Ν | number of samples |
| NASA | National Aeronautics and Space Administration |
| NIVA | Norwegian Institute for Water Research, Norway |
| OLCI | Ocean Land Colour Instrument (launched on Sentinel-3) |
| Pixel | Abbreviation for picture element; smallest part of a digitized or digital image. |
| Rhow | Water-leaving reflectance, dimensionless (rhow= $\operatorname{Rrs}^*\pi$) |
| Rrs | Remote-sensing reflectance, unit: sr-1 |
| S2 | Sentinel-2 satellite, part of ESA's Copernicus programme |
| S3 | Sentinel-3 satellite, part of ESA's Copernicus programme |
| SD | Secchi depth (unit: m) |
| SPM | Suspended Particulate Matter, also termed TSM |
| SQRT | Square Root, |
| SE | Standard error of the mean $=\frac{St.Dev.}{\sqrt{N}}$ |
| Sonicator | Device to applying sound energy in order to disrupt cells in a sample |
| St.Dev. | Standard deviation of a population |
| SU | Stockholm University, Sweden |
| SYKE | Finnish Environment Institute (Suomen ympäristökeskus), Helsinki |
| TACCS | Tethered Attenuation Coefficient Chain Sensor (Satlantic Inc., Canada) |
| TSM | Total Suspended Matter |
| UMF | Umeå Marine Sciences Centre (Umeå marina forskningscentrum) |
| UPW | Ultrapure water |
| WFD | Water Framework Directive (EU Directive from 2002) |
| WISP | Water Insight Spectrometer, Water Insight, The Netherlands |

1. Introduction

SEAmBOTH project uses satellite observations to detect spatial and temporal changes in the water quality (WQ) in the area of the Bothnian Bay. The estimation of water quality using satellite observations, often referred to as Earth Observation (EO), is based on the measurement of Sun light reflected from water. The instruments in satellites observe the reflected light in various channels (or bands), typically covering the optical and infrared wavelength regions. The water quality parameters are derived from the signal observed by the satellite instruments using various mathematical models (algorithms). The most common WQ parameters are:

- Concentration of Chlorophyll-a (a proxy for phytoplankton biomass)
- Turbidity (a measure of scattering in water, which is related to the concentration and type of particles suspended in water)
- Absorption by Coloured Dissolved Organic Matter (CDOM, a measure of the amount of decomposed vegetation matter in water)
- Water transparency (a measure of the overall clarity of water)
- Surface temperature

For more information about these please see e.g. www.syke.fi/EOstorymap.

The main advantages of using EO for aquatic monitoring are the superior spatial and temporal coverage of satellite instruments. A satellite image actually provides a continuous grid of measurements from a target area in cloud-free conditions. Thus, the amount of observations is manifold in comparison to point-wise observations provided by station sampling and transects measured on-board ships.

The Baltic Sea is observed every cloud-free day by instruments such as OLCI onboard the two Sentinel-3 (S3) satellites. These observations are made with 300 m resolution, which allows for frequent observations in open sea and outer archipelago/coastal areas. The inner parts of the coastal waters require higher resolution instruments, and these are provided by the Sentinel-2 (S2) series. These instruments have less frequent overpasses, but still the series provides observations 2-3 times per week in the northern latitudes. S2 provides observations with 10 or 20 m accuracy for most wavelength bands. Even though the products are often provided in 60 m pixels (in order to reduce noise), this allows estimation of water quality much closer to the shore compared to the medium resolution OLCI (onboard S3 series). Satellite observations cannot be utilised for water quality detection in shallow areas (where the bottom is visible and effects on the observations).

Sentinel satellite series (S2 and S3 satellites) are part of the highly ambitious Copernicus programme of the European Union. The programme provides satellite observations to scientists and environmental monitoring experts with unprecedented coverage and data quality. The EU is committed to keeping the satellite constellation operational long term (2030 and beyond), which allows improved environmental monitoring and climate change assessments tools and services to be built.

The Baltic Sea and especially the Bay of Bothnia are challenging areas for the utilization of EO for water quality estimation. In comparison to other sea areas in the world, these areas are dark waters, and therefore the EO products are sensitive to errors. This is due to the high absorption by CDOM combined with relatively low particle concentration. Thus, it is necessary to formulate the algorithms applicable especially for this optically challenging region before they can be utilized for water quality determination with high accuracy. This highlights the importance of accurate in situ measurements in the development of EO methods.

There are certain factors that limit the use of EO in the Bay of Bothnia. One is the lack of light during winter. The instruments stop making observations when the solar elevation angle is too low and in the Bay of Bothnia this leads to a gap in the availability of data from early November until early February. Another problem is ice cover which can prevent measurement of water quality in the coastal areas of the Bay of Bothnia until late April or early May. Nevertheless, during the summer period satellites are able to make frequent observations throughout the season. Regular station sampling (not intensive stations), on the other hand, tends to take place only during certain time periods. Thus, EO covers the seasonal ecological cycle much better.

In the following sections we describe the EO related work performed and results obtained during the SEAmBOTH project.

2. Harmonization of bio-optical protocols

One of SU's contributions to SEAmBOTH was to harmonize the determination methods for chlorophyll-a, coloured dissolved organic matter (CDOM), turbidity, suspended particulate matter (SPM) and Secchi depth measurements and to write and distribute optical protocols. This work task was requested by the County Board Administration Norrbotten as to secure good data quality for the validation of satellite data. Also, an overview of the errors involved in the measurements was required so that the contracts with the subcontractors could be specified and good data quality of the deliverables could be ensured.

In early 2018, Susanne Kratzer (SK) wrote the optical protocols and distributed them to the Swedish monitoring groups (v.3). During 14-15 November 2019, SK organized a bio-optical training workshop for the key Swedish monitoring groups (SU, UMF, Kristineberg, SMHI) funded by HaV. For this workshop, the protocols were revised (v.4; attached to this report as appendix I). If funded, there is a plan to organize more bio-optical training workshops and to also involve Finnish and Norwegian monitoring groups in this effort if requested by the water authorities.

In addition, optical methods used in Sweden and Finland were compared. The main differences were that in Finland the subcontractors do not measure the full spectrum for CDOM. They only use a restricted number of wavelengths which do not allow to reliably derive the CDOM slope. Another key issue is the way the monitoring groups both in Sweden and Finland measure chlorophyll-a (Chl-*a*). According to international standards (JGOFS, NASA protocols) one should flush-freeze the samples in liquid nitrogen and also extract them using a sonicator (under ice-cooling). This is especially important in the presence of cyanobacteria as these have very strong cell walls. None of the monitoring groups use this method which implies a systematic underestimation of Chl-*a* as indicated by comparisons performed at Stockholm University.

3. Earth observation data and in situ measurements

3.1. EO data

Observations made with both high and medium resolution (S2 and S3, respectively) satellite instruments were utilized in this study. For S2, both S2A (June 2015-to date) and S2B (March 2017-to date) data were used. For S3, both S3A (April 2016-to date) and S3B (July 2018-to date) observations were used, which means that from summer 2018 onward the S3 data availability effectively has been doubled. No significant differences between the S3A and S3B datasets were observed so the two data sources were combined for analysis and are displayed as one, combined, EO dataset in Ch. 5.2.

Satellite observations corresponding to the in situ sampling stations were extracted from the image data and compared to the in situ data described in Ch. 3.2 and 3.3. Match-up plots and time series have been produced to explore the performance of the different algorithms. Match-up analyses use only remotely sensed products that coincide with the time and location of *in situ* measurements. For product evaluation, the allowed time difference between satellite and *in situ* measurements can be more or less strict. In this pilot study, all measurements within the same day of the satellite overpass were allowed for the analysis. Time series consider all remotely sensed products available from a sampling station, i.e. even when no simultaneous in-situ measurement was performed. Match-ups can either be evaluated with statistical metrics (r², MAE, bias) for comparisons, but they are by nature based on much fewer data points than time series comparisons. The satellite method provides time series with very high sampling frequency (see figure 8 and figures 10-36) on which the values measured *in situ* can be superimposed (shown as red dots in these figures). This type of comparison thus allows for a direct visual comparison of both datasets, including the variability of each set, and evaluating if a plausible seasonal variability is retrieved.

From the EO data, we extract either only data represented by a single pixel values (i.e. 'satellite location') corresponding to the sampling location, or all data available within a 3x3 pixel box around the sampling location, a so-called 'macropixel'. Macropixels enable much more options for filtering valid pixels and deriving statistics such as the coefficient of variance (C.V.) which is an indication of the heterogeneity of the sampled water body. However, when only relying on the mean or median values, this approach blurs the spatial sampling in particular for horizontally patchy water bodies, and thus spatially variable water constituents. For the S3 data 3x3 macro pixels were extracted and used in the analysis.

Together with remotely sensed parameters, we also extracted a number of data quality flags for each pixel, which indicate whether the pixel is valid or not, e.g. due to cloud coverage. These flags have been used to remove invalid data, but the result is not perfect, as it can add noise/outliers to the data set.

3.2. SEAmBOTH validation campaign data

The sea-truthing protocols established by the marine remote sensing group at SU were followed to measure optical properties as well as physical-chemical data during SEAmBOTH dedicated optical campaigns. In 2018, SU joined the weekly monitoring cruises from UMF's monitoring group during week 20, 24 and 28 (Figure 1). In June and July SYKE participated in the cruises and the field work.



Figure 1. Sampling stations visited during SEAmBOTH cruises weeks 20,24 and 28 during 2018.

A whole range of optical properties were measured: in situ reflectance (TACCS), absorption and scatter (AC9), aerosols (Microtops), turbidity as well as CDOM. UMF measured chlorophyll-a, SPM and turbidity. An inter-comparison of Secchi depth measurements was done using a 30 cm diameter Secchi disk (SU) and a 20 cm disk (UMF). There was no significant difference between the methods.

The standard filtration method for CDOM using a glass filter apparatus was compared to the method using a plastic syringe for filtration. The results showed that the derived CDOM values were reliable when using plastic ware, but the slope value for CDOM had a very high relative error which means that there is a difference in the nature of the CDOM (see appendix II). So, the recommendation is to filter with glassware rather than plastic syringes when taking CDOM samples.

Additionally, the turbidity bench methods by UMF and SU were compared. It was found that the UMF bench turbidity meter was faulty (more than 50% error). Thus, during summer 2018 UMF bought the same bench turbidity meter and introduced the same method as established by the marine optical group at SU in 2010, and also adopted by SU's marine monitoring group.

Previous research indicates the following error metrics:

- Chlorophyll-a (spectrophotometer) in-water measurements: 7-10% standard error of the mean (Kratzer, 2000; Kratzer and Tett, 2009)
- SPM (gravimetric method) (Kratzer, 2000; Kratzer and Tett, 2009): 10-13%
- Turbidity ~ 10-12% error (Kari et al., 2017)
- CDOM: ~6% error (Harvey et al. 2015).

This information was then provided to the County Board Administration Norrbotten so that they could define the required data quality in the contracts with the subcontractors measuring the optical properties for the SEAmBOTH project.

Figure 2 and Figure 3 shows satellite and sky state data from the 11th July 2018 when there was both a S3 and a S2 overpass during the cruise. The water samples from the cruises with UMF were measured by SU and UU during spring and summer 2018, and the data from the radiometer, sun

photometer and the AC9 were processed in autumn 2018 and early 2019. The TACCS was recalibrated by Tartu Observatory in January 2019.

Different methods of measuring reflectance using the TACCS in-water radiometer (SU) and the WISP on loan to SYKE that measures reflectance above the sea surface were applied and compared. The TACCS had problems measuring reflectance at very high CDOM values, e.g. in the Öre Estuary (station B7) and in the inner Råneå estuary. A special adaptation had to be made for the measurements (i.e. the Kd-chain had to be shortened) to derive Kd490 (Figure 4).





11/7-2018, OLCI Sentinel-3 (300 m)11/7- 2018, MSI Sentinel-2 (60 m)Figure 2. Example of OLCI Sentinel-3 and MSI Sentinel-2 overpasses on 11 July 2018.



Figure 3. Sea and sky state 11 July 2018 – Station RA2; 16:36.





Figure 4. Adaptation of TACCS radiometer (i.e. shortening of Ed chain) to measure reflectance in the Bothnian Sea.

The TACCS is a multispectral instrument and measures only at 7 wavelengths, but the spectra could then be used to decide which of the WISP spectra (hyperspectral data) were valid water reflectance spectra. The TACCS data was evaluate which of the WISP spectra were valid (by comparing the spectral slopes in the blue). The TACCS has been calibrated and intercompared in several international intercalibration exercises funded by ESA. So, although it is only a multi-channel instrument it still provides reliable reflectance. The processor that calculates the reflectance uses spectral K_d derived separately from the AC9 data, which allows to regress the upwelling radiance at 50 cm to the surface, and to derive reflectance from a ratio of the downwelling irradiance and the upwelling radiance. Aerosol optical properties measured with the Microtops are used in the TACCS processor to correct for the effects of locally measured aerosols. The WISP gave an overestimation of remote sensing reflectance in the range of a factor of around 2. So, more work has to be done to correctly calibrate the WISP, although a clear advantage is that it gives the full spectral signature. Figure 5 shows an example of both WISP and TACCS measurements as well as spectra derived for 10 July 2018.



WISP hyperspectral reflectance spectra (SYKE)

Figure 5. Comparison of TACCS and WISP reflectance measurements (example from 10 July 2018). Note that the TACCS spectra shows the average of 120 measurements.

The results from the water sample analysis were included in the Swedish monitoring data base sustained by SMHI, and the more specialized optical data was made available directly to SYKE and Brockmann Geomatics Sweden AB to be used in the validation of EO products.

3.3. National and regional monitoring data

Some of the in-situ data used for validation of EO products was specifically collected for SEAmBOTH project purposes as described above, but the main bulk of optical data for validation was retrieved from national databases and collected within the Swedish and Finnish national and regional monitoring programs. The national and regional authorities are responsible for the monitoring programs, but the actual data collection is often out-sourced to consultants who collect and analyse the samples. In all cases the sampling personnel used in monitoring are certified. The laboratory analyses are based on international standards and the laboratories have accredited their methods.

Most sampling stations are fixed and a part of the networks since many years/decades. The sampling frequency varies according to the existing monitoring programme and ranges from one per year to weekly samples. Chl-a, Turbidity, SPM/TSM, water absorption and transparency (Secchi Disk Depth) data was extracted from the data bases and used in the validation of EO products. All Finnish and Swedish stations used in the analysis, including the additional SEAmBOTH stations, are plotted in Figure 6.



Figure 6. Location of routine monitoring sampling stations in Sweden and Finland.

4. Basics of EO processing

The estimation of water quality from satellite images is usually done with a two-step approach:

- 1. **Atmospheric correction**: This step removes the effects of the atmosphere (scattering by particles and absorption by gases) from the signal received by the satellite. The result of this step is the so-called remote sensing reflectance (Rrs) which represents the shape and magnitude of the spectra at the surface of water.
- 2. **In-water inversion**: This step converts Rrs into water quality parameters using simple methods such as band ratios or more complex ones such as neural network algorithms.

A number of processors using this approach has been developed and are publicly available such as the C2RCC-processor (Doerffer et al., 2012 and Brockmann et al. 2016). These processors have not, however, been developed for the water type of the Bay of Bothnia and thus require additional testing and in many cases also calibration before the results are reliable.

In the two-step approach, the algorithm must estimate the reflectance accurately before the optical components (indicating the actual water quality) can be estimated. If the atmospheric correction is not able to provide accurate reflectances the in-water part of the model is also likely to fail. Thus, it is important to also validate the Rrs values as this test may indicated if there is a problem with the atmospheric correction model.

The number of actual reflectance measurements from the Bay of Bothnia is still small. Fortunately, it is possible to utilize reflectances simulated with radiative transfer modelling in this kind of analysis. Radiative transfer models describe the way light is absorbed and scattered in water or air. The models are an intrinsic part of the processors that are used to process ocean colour data. Usually,

there is one model part that solves the radiative transfer in air and corrects for atmospheric effects in the data and another part that describes the spectral scattering and absorption properties (i.e. the inherent optical properties) in the water. The model also describes the relationship between remote sensing reflectance and the inherent optical properties. The latter are used to derive the concentrations of the main three optical components in the water: chlorophyll-a, suspended matter and dissolved organic matter.

SYKE has been using the collected data for radiative transfer modelling with the radiative transfer software Hydrolight (Mobley & Sundman 2016a and 2016b) which allows to simulate remote sensing reflectance based on optical properties (see example in Figure 7). The inherent optical properties (IOPs) measured by SU were used by SYKE to further develop a regional in-water model using Hydrolight (version 5.3.1). The software allows to derive reflectance via forward modelling if the main optical properties – chlorophyll-a and SPM concentration as well as CDOM absorption as well as the SPM-specific scatter (b*) and other specific IOPs are known (see tables 1 and 2). SYKE used both the data measured by SU during 2018 as well as data from the literature (Fournier and Forand 1994, Kallio 2005, Simis et al. 2017, Kratzer and Moore 2018) to simulate the reflectance (Table 1). The reflectance showed to be strongly dependent on the SPM-specific scattering coefficient (b*) as exemplified in Figure 7. More details about the simulations are available in Appendix IV.

| SIOP | Symbol | Value | Reference |
|---------------------------------|--------------------------|--------------------------|-----------------------------|
| Specific scattering coefficient | b* _{part} (440) | Measured at each station | |
| at 440 nm | | | |
| Scattering exponent | nb | 0.55 | Kratzer&Moore (2018) |
| Backscattering ratio | b _b /b | 0.015 (wavelength | Simis et al. (2017), summer |
| | | independent) | |
| Scattering phase function | | | Fournier and Forand (1994) |
| Specific absorption coefficient | a* _{ph} (λ) | | Simis et al. (2017), |
| of phytoplankton | | | summer, package effect |
| Slope factor of CDOM | S _{CDOM} | Measured at each station | |
| absorption | | | |
| Specific absorption coefficient | a* _{nap} (λ) | | Simis et al. (2017), summer |
| of non-algal particles | | | |

Table 1. The best SIOPs for the SEAmBOTH TACCS stations in 2018.

Table 2. bpart* at 443 nm and bb/b measured in the Baltic Sea and Finnish lakes.

| Data | Area/season | b* _{part} at 400, 442 or 443 nm m2/g | bb/b |
|----------------------|--------------------------------------|--|-------------------------------|
| SEAmBOTH | Swedish coast of GOB | 1.06 ± 0.35 (min 0.49, max 1.49) | - |
| Kratzer&Moore 2018 | NW Baltic Proper Summer | 1.016 ± 0.326 | 0.017 ± 0.0103 (443 nm) |
| Simis et al. 2017 | Open Baltic sea Spring | 0.200 ± 0.093 | 0.0197 (mean of all bands) |
| Simis et al. 2017 | Open Baltic sea Summer | 0.468 ± 0.382 | 0.0151 (mean of all bands) |
| Kallio (2005) | Finnish lakes (Spring and summer) | 0.95 | - |
| C2RCC, default value | | 0.58 (blue) | - |
| | | 0.32 (white) | - |



Figure 7. Example of reflectance simulations using Hydrolight and different specific inherent optical property (SIOP) parameterisations.

5. Results and validation

5.1 Validation of Sentinel-2 data

SYKE has utilized S2 data to provide water turbidity products that can be used as input data in models. An example of this is shown in Figure 8, which displays a time series of turbidity measured with monitoring samples measured in the laboratory (MS in red) and S2 images. The two datasets correspond very well. The station in question is a so-called intensive measurement station of routine monitoring, which means it is sampled by boat about 10 times per year. EO data can provide many more estimates during the same time period. Furthermore, one can observe elevated values in the EO data during August 2018. These data points are from a time period affected by resuspension, presumable due to wind-wave stirring. This leads to the stirring-up of bottom sediments which subsequently become resuspended in the water column. This effect is strongest in shallow waters. In situ samples were not taken during this resuspension event. So, the traditional sampling method by boat completely missed the increased values in suspended particulate matter. A turbidity map of the same event is shown in Figure 9, left panel. For comparison, also the normal situation (without resuspension) is shown (right panel).



Figure 8. Turbidity time series at Hailuoto intensive station measured from in situ samples and with S2 data using the SYKE algorithm (C2RCC processor and calibration based on in situ data). The location of the station is shown in Figure 9.



Figure 9. Turbidity map in the Bay of Bothnia estimated from S2 data taken on Aug 19, 2018 and July 10, 2018. The Hailuoto station (Figure 8) is indicated with a triangle and a number 30372. The left panel shows the turbidity in the event of strong wind, the right panel shows the normal situation, indicating the run-off from land.

5.2 Validation of Sentinel-3 data

Data from the full S3 archive was processed using a number of different algorithms to derive different water quality parameters. For OLCI, the relevant products for validation within the SEAmBOTH project were:

- Inherent optical properties derived with C2RCC processing, e.g. absorption from detritus and Gelbstoff (CDOM) (Doerffer et al., 2012 and Brockmann et al. 2016)
- Water constituent concentrations derived with C2RCC processing, e.g. chl-a and suspended matter (Doerffer et al., 2012 and Brockmann et al. 2016)
- Attenuation coefficient derived with C2RCC processing (Doerffer et al., 2012 and Brockmann et al. 2016)
- Suspended matter concentration and turbidity derived from a semi-empirical algorithm (Nechad et al. 2010) based on C2RCC atmospheric correction (Doerffer et al., 2012 and Brockmann et al. 2016)
- Empirical Secchi disk depth algorithms developed for the Baltic Sea and/or humic lakes (Alikas and Kratzer, 2017 and Florén et al., 2012)
- Chl-a concentration derived from MPH algorithm (Matthews et al., 2015, Pitarch et al., 2017)

Chlorophyll-a

None of the investigated chl-a algorithms performed well for all water types, i.e. for all stations, in the investigated region. However, for most stations good alternatives could be identified, and a number of examples, both in Sweden and Finland, have been included below. In all figures the situ data (IS) is plotted with red dots and the satellite based estimations (EO) in blue. However, the best performing chl-a algorithm(s) (MPH) was not developed for low chlorophyll/high a_{CDOM}

(brown/humic) waters and the good results might be more of a coincidence rather than appropriate processing routine for the respective water type. Dedicated development of a high a_{CDOM} algorithm to estimate Chl-a is a task for future EO research and development projects.



Figure 10. Chl-a time series between 2016-2019 for station Råneå 1R plotted with in situ data from station 1R and Råneå-6 (same position). The in situ data corresponds to surface samples.



Figure 11. Chl-a time series between 2016-2019 for station Råneå 2R plotted with in situ data from station 2R and Råneå-7 (same position). The in situ data corresponds to surface samples.



Figure 12. Chl-a time series between 2016-2019 for station Råneå 3R plotted with in situ data from station 3R and Råneå-8 (same position). The in situ data corresponds to surface samples.



Figure 13. Chl-a time series between 2016-2019 for station Råneå-1. The in situ data corresponds to integrated samples between 0-5 m.



Figure 14. Chl-a time series between 2016-2019 for station Råneå-2. The in situ data corresponds to integrated samples between 0-10 m.



Figure 15. Chl-a time series between 2016-2019 for station Slumpfjärden. The in situ data corresponds to surface samples.



Figure 16. Chl-a time series between 2016-2019 for station KA12 / LÅNGÖREN. The in situ data corresponds to surface samples.



Figure 17. Chl-a time series between 2016-2019 for station Vav-6 I-5A. The in situ data corresponds to integrated samples between 0-10 m.



Figure 18. Chl-a time series between 2016-2019 for station Monäsviken. The in situ data corresponds to integrated samples between 0-3/5 m.



Figure 19. Chl-a time series between 2016-2019 for station Välimatala Ö59. The in situ data corresponds to integrated samples between 0-appr. 3 m.

Transparency

Secchi Disk Depth is a measure of water transparency. Some of the empirical Secchi disk depth algorithms developed for the Baltic Sea and/or humic lakes seem to work well in the investigated waters. A number of examples, both in Sweden and Finland, have been included below. In all figures the situ data (IS) is plotted with red dots and the satellite based estimations (EO) in blue.



Figure 20. Secchi Depth time series between 2016-2019 for station Råneå-1.



Figure 21. Secchi Depth time series between 2016-2019 for station Råneå-1R (and Råenå-6).



Figure 22. Secchi Depth time series between 2016-2019 for station Vav-6 I-5A.



Figure 23. Secchi Depth time series between 2016-2019 for station Haukiputaan edusta KIE12.

Turbidity

The turbidity products derived based on the semi-empirical Nechad algorithm seem to work well in the investigated waters. A number of examples, both in Sweden and Finland, have been included below. In all figures the situ data (IS) is plotted with red dots and the satellite based estimations (EO) in blue.



Figure 24. Turbidity time series between 2016-2019 for station P70 YTTRE FJÄRDEN. The in situ data corresponds to different discrete depths between 0.5-10.5 m.



Figure 25. Turbidity time series between 2016-2019 for station P300 BAGGEN. The in situ data corresponds to different discrete depths between 0.5-3 m. See also Figure 26.

Figure 26. Turbidity time series between 2016-2019 for station P300 BAGGEN. The in situ data corresponds to different discrete depths between 0.5-3 m. Different scale used compared to Figure 25 for improved readability.

Figure 27. Turbidity time series between 2016-2019 for station Råneå-1. The in situ data corresponds to different discrete depths between 0.5-7 m.

Figure 28. Turbidity time series between 2016-2019 for station Tottesund. The in situ data corresponds 1 m depth.

Figure 29. Turbidity time series between 2016-2019 for station Haukiputaan edusta KIE12. The in situ data corresponds discrete depths between 1-15 m.

Figure 30. Turbidity time series between 2016-2019 for station Öljysatama 11. The in situ data corresponds discrete depths between 1-10 m

Absorption

Absorption from detritus and Gelbstoff can be estimated based on the C2RCC algorithm. A number of examples, both in Sweden and Finland, have been included below. In all figures the situ data (IS) is plotted with red dots and the satellite based estimations (EO) in blue. The performance is very good at some stations, but not convincing at others and further analysis is needed in order to better conclude on its applicability.

Figure 32. Absorption (443 nm) time series between 2016-2019 for station Råneå-2.

Figure 33. Absorption (443 nm) time series between 2016-2019 for stations Haraholmsfjärden.

Figure 35. Absorption (443 nm) time series between 2016-2019 for stations PERäMERI LAV4.

5.3 Inorganic suspended matter product from S3 data

The SEAmBOTH measurements together with optical data from the NW Baltic proper allowed for the development of a novel regional algorithm to derive inorganic suspended matter (ISPM) from satellite data using the specific scatter of ISPM (Kratzer et al., 2020). Figure 36 shows an example of an OLCI Sentinel-3 composite image during April 2018. During this time, parts of the Bothnian Bay were still covered in ice and are therefore not displayed in the image. Other algorithms that were further developed and tested were various turbidity algorithms (Kari et al. 2017) as well as Secchi depth, SPM, Chl-a and CDOM algorithms (Kyryliuk, 2019; Kyrykliuk and Kratzer, 2019).

Figure 36. Example of regional SPM and ISPM algorithms applied to a composite satellite image (OLCI Sentinel-3) of the Baltic Sea during April 2018. Note that the Bothnian Bay was still covered in ice during this time period.

5.4 EO products to support habitat modelling

As satellite observations are often prevented by cloud cover, it is advantageous to merge all observations collected over a certain time period, such as a month. This can be done by averaging the non-cloudy image areas or with other binning methods that provide a temporal composite of the images. Also, oceanographic models often require input data that covers the target area as well as possible. An example of such a temporal composite image is shown in Figure 37. Those locations at which elevated values of turbidity are consistently found are visible as yellow to red areas. These areas with relatively high turbidity include e.g. river estuaries and areas where dredging is taking place, leading to a strong resuspension of sediments.

SYKE publishes its EO results through the TARKKA service (<u>www.syke.fi/tarkka/en</u>). TARKKA includes true color images, maps of water quality parameters, and time series plots over reference stations with water sampling. TARKKA service enables the users to conveniently browse various water quality maps to zoom in and out and to pan into an area of interest. The service also provides various GIS datasets, like shoreline, drainage basin division and WFD water bodies to overlay them on top of the satellite data. Figure 8, Figure 9 and Figure 37 have all been extracted from TARKKA.

Figure 37. Turbidity composite of summer 2017 (1.7-7.9). Note the increased values of turbidity (measured in FNU) in river estuaries (indicating run-off from rivers) and dredging areas (indicating resuspended sediments).

In addition to turbidity, SYKE also provides CDOM and water transparency (Secchi depth) maps produced from single day observations through TARKKA. An example of a CDOM map and a time series of estimated values at a monitoring stations are shown in Figure 38.

TARKKA also includes daily sea surface temperature products. These are made with an instrument that has lower spatial resolution (1000 m) and thus cannot cover the areas closest to the shore. However, the thematic accuracy of the product is excellent; the satellite observations correspond with field measured surface temperature (~1m depth) with r² more than 0.96.

Figure 38. (a) Values of absorption by CDOM a_{CDOM}(400 nm) estimated with S2 satellite on 14.5.2019. The elevated values along the coast are caused by humic substances brought into the area by melting snow water. (b) a_{CDOM}(400 nm) values at the Hailuoto intensive monitoring station (number 30372) measured with EO and in situ (MS, based on Pt water colour measurements).

6. EO publications & outreach

The S2 products generated by SYKE are available to the public via TARKKA. BG and its partners are presently developing a service where daily S3 products will become available. The service is called CyanoAlert and will be launched before summer 2020, but is not available as yet.

Some of the data measured in SEAmBOTH has contributed to a PhD thesis (Kyryliuk, 2019) to a scientific manuscript published in Remote Sensing Environment (Kratzer et al. 2020), the top journal in remote sensing and to a popular science article in Havsutsikt (Kratzer, 2019). The paper was also presented at the Baltic Sea Science Congress in Stockholm on 22 August 2019 and at the Nordic Remote Sensing Conference 2019 (NoRSC'19) at the Aarhus Institute of Advanced Studies (AIAS), Aarhus University, from 17-19 September 2019.

Petra Philipson participated in the bio-optical training workshop arranged by SU and presented the Copernicus programme, including S2 and S3 data, for the key Swedish monitoring groups. Susanne Kratzer participated in the Final SEAmBOTH seminar in Oulu on 20 February 2020 and presented our joint results. Finally, some of the data from SEAmBOTH have been used in a paper (Kari et al. 2020).

7. Discussion and conclusions

As shown in the results above, water quality parameters such as turbidity and CDOM can be estimated well in the Bothnian Bay using Sentinel-2 observations. The water quality estimates provided by high resolution instruments are especially valuable in coastal regions, whereas moderate resolution instruments can cover open sea areas with more frequent coverage. With Sentinel-3 OLCI data, examples of Chl-a time series with good correspondence with station sampling were shown at many of the investigated stations. However, the best performing Chl-a algorithm (MPH) was not developed for areas with low Chl-a concentration and extreme a_{CDOM} (brown/humic) waters and over stations with this combination of water type the performance was not convincing. Dedicated development of an algorithm to estimate Chl-a in high a_{CDOM} waters is a task for future research and development projects.

The SEAmBOTH validation efforts provided insights on the performance of some publicly available algorithms in Gulf of Bothnia waters. As one example, the Neural Net algorithm (C2RCC) that also is available and downloadable as a standard Sentinel-3 product from EUMETSAT, was tested with unsatisfactory results for e.g. chlorophyll a. Promising results could be identified for some stations, but the same algorithm did not perform well everywhere. Hence, no fixed processing chains, or "on-the-shelf" product, for generation of water quality products with Sentinel-3 data in the Gulf of Bothnia could be defined through this study.

The in-situ dataset collected during SEAmBOTH has been a valuable resource for the algorithm testing and development. However, development of water quality algorithms over dark water types requires long time series before a sufficient level of confidence in the results can be reached. We recommend that water quality sampling is kept at high level in this region, and that the sampling follows the optical protocols utilized here. In addition to determining the in-situ concentrations of Chl-a, CDOM and turbidity, it is also important to collect more data on the inherent optical properties (see Table 1). Getting improved information about the water depth in coastal areas is also important.

The algorithms analysed here are being continuously updated. Thus, it will be valuable to repeat these analyses with additional data and new versions at a later date. Usually, at least 25-30 match-

ups between satellite and in situ data are required, to derive the uncertainties statistically. Hopefully, this can be accomplished in a follow-up project on the Bothnian Bay.

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Appendix I – Optical measurement protocols v. 4, November 2019

by Susanne Kratzer, Stockholm University (SU), Sweden and Therese Harvey, Norwegian Institute for Water Research, Norway

The following methods are based on Kirk (2011), the SeaWiFS protocols (Mueller and Austin, 1995), the MERIS protocols (Doerffer, 2002), Susanne Kratzer's PhD thesis (Kratzer, 2000) and the IOCCG protocol series (2018).

General procedures

In the field: Note that for all water samples, the respective sampling bottle is rinsed twice with sea water before the sample is taken. All samples are stored cool and dark. Filtration: All sample bottles are turned gently in order to mix them before filtration. Measuring cylinders are rinsed twice before filtration with the sample water. To effectively resuspend sinking particles/phytoplankton and for evenly distribution, the water bottle should be swirled 3 times clockwise, then 3 three times counter-clockwise, followed by 3 times clockwise, again. Sample bottles should never be shaken vigorously. Analysis: Analysing cuvettes are rinsed 2 x with sample water before measurements. All tissues used for wiping and drying of cuvettes should be done with e.g. Kimwipes[®] or other tissues that that do not shed any particles. We would also like to strongly recommend each lab starting to work with bio-optical measurements to buy a copy of Kirk (2011) which explains the basics of bio-optics, the publications from IOCCG (International Ocean Colour Coordinating Group) are also very useful https://ioccg.org/what-we-do/ioccg-publications/.

Chlorophyll analysis (Chl-a)

For the estimation of chlorophyll a (Chl-a) 1-2 l of sea water samples are filtered through 47 mm GF/F filters (triplicates) using a mild vacuum (~40Kpa, 1/2 atmospheric pressure or 5.8psi). In order to avoid overloading and clogging of the filters, filter only as much water of the sample as required. Make sure to gently swirl the sample before filtration. The filters with samples are stored in liquid nitrogen for a maximum of 2 months. For analysis, the filters are extracted in 10 ml 90% acetone, sonicated under ice cooling for 30 seconds, centrifuged for 10 min at 3000 RPM. After 30 min extraction the sample is decanted into a 1 cm quartz cuvettes and scanned against 90% acetone in a Shimadzu UVPC 2401 dual beam spectrophotometer. The Chl a concentration is then calculated according to the trichromatic method (Parsons et al., 1084; Jeffrey and Welschmeyer, 1997). The method has been calibrated against HPLC measurements from NIVA (Oslo), for n=32 sampling stations and showed no significant difference for the Chl *a* concentration. The standard error of the method is 7-10 % dependent on the range of Chl a (Kratzer, 2000). The measurement error was shown to be within 10% in an international intercalibration performed by the ESA MERIS Validation Team (Sørensen et al., 2008). The intercalibration exercised showed that the main causes of errors lie in the storing and extraction method. The best procedure to minimise errors are to filter, extract and measure directly after sampling using a sonicator. If this is not possible the samples should be flush frozen in liquid nitrogen (for storing); after that they can be kept at -80 °C (for up to 3 months). For extraction, the samples should be sonicated under ice cooling in order to avoid pigment degradation (Jeffrey and Welschmeyer, 1997).

CDOM measurement protocol

For determining CDOM absorption the water is sampled in 250 ml amber glass bottles (rinse bottle 2 x with sea water) and filtered through 0.22 µm membrane filters using a Whatman glass filtration unit (with a metal mesh). GF/F filters can contaminate the samples and should be avoided (IOCCG, 2018). Note that each sample must be well mixed before filtration and usually one rinses the filtering apparatus and the bottle to collect the filtrate 2 x each with filtered water. The filtered samples can be kept in the fridge in 100 ml amber glass bottles for up to 3 months. The samples are then removed from the fridge and should reach room temperature before being scanned in a 10 cm optical cuvette against ultrapure water as a blank using (for example) a Shimadzu UVPC 2401 dual beam spectrophotometer (300-850 nm). The blank should be treated in the same time as the samples and be stored in the same fridge and placed in room temperature at the same time as the samples. This is to avoid any temperature effects on the absorption measurements (IOCCG, 2018). The scanning spectrophotometer should have a 1 nm resolution. The spectral absorbance (abs) is then corrected for the absorbance at 700 nm (Bricaud et al., 1995) in order to account for measuring errors, and the spectral absorption for CDOM, is then derived according to Kirk (2011) as:

 $a_{CDOM}(\lambda) = ln(10) OD(\lambda) L^{-1},$ [m⁻¹]

where: $OD(\lambda)$ is the optical density; L is the path length of the cuvette in meters (in this case 0.1 m).

One usually uses the CDOM absorption at 440 nm, a_{CDOM} (440) (also termed g440), for comparison to ocean colour data. MERIS and Sentinel-3 use the absorption at 443 nm.

CDOM absorption decreases exponentially according to the following equation Kirk (2011):

$$a_{CDOM}(\lambda) = a_{CDOM}(\lambda_0)e^{-S_{CDOM}(\lambda-\lambda_0)}$$

where: S_{CDOM} is the slope factor, and λ is the reference wavelength, nominally 440 nm.

The slope factor of a_{CDOM} , S_{CDOM} , is derived through non-linear curve fitting between 350 and 500 nm. It can indicate different types of water masses. An alternative method is to In-transform the CDOM absorption spectrum and to fit a linear trendline, with the slope of the line corresponding to the CDOM slope factor, S_{CDOM} . However, there is a slight off-set between the non-linear and the linear fitting method (IOCCG, 2018). The standard error for deriving g440 is 3-6%, dependent on the measurement range. For the slope the error is around 3% (Harvey et al., 2015).

An intercomparison of methods by SU and UU showed that if the samples are filtered with a plastic syringe there is no significant difference for the CDOM absorption at 440 nm (t-test: P=0.96) when using the linear fitting method. However, for the slope value there was a significant difference (t-test: P=0.048); so this method should be avoided if possible.

SPM measurement protocol

The concentration of organic and inorganic suspended matter (SPM) is measured by gravimetric analysis (Strickland and Parson, 1972). **Preparation of filters:** GF/F filters are rinsed with a similar volume as the expected samples of ultrapure water to remove any lose filter bits, and then

combusted at 480 °C in order to burn off any possible organic contamination (Doerffer, 2002). These clean filters are then weighed (tare filter weight) using a microbalance ($\pm 1 \mu g$) and stored in folded square aluminium foils (0.020 x 100 x 100 mm) with scored numbers until filtration. **Sampling and analysing**: 1-2 l of water samples are filtered in triplicates through the pre-weighed and pre-combusted filters. The funnel and the filters are then rinsed with 50 ml ultrapure water to remove any remaining salt. To avoid overloading and clogging of the filters, filter only as much sample water as necessary.

The filters are dried overnight at 60 °C and kept in a desiccator until weighing using the same microbalance. Total suspended matter is then derived from the difference between the tare and the dry weight. Then the samples are combusted at 480 °C in a furnace, followed by another weighing step. The weight of inorganic suspended matter equals the weight of the combusted filters (corrected for the tare weight). The organic fraction is derived from the difference of the total and the inorganic suspended matter. In order to correct for handling errors 10 blank filters are processed in the same way, and the results from these are used to correct the sample filters. For SPM sampling it is especially important to swirl the sample bottle before filtration.

Quality control: The triplicate results for each station are quality checked as it is easy to lose a part of the filter in the handling process. If a replicate deviates more than 10% from the other samples it is not used for deriving the average value for the respective station. The standard error of the method is 10% (Kratzer 2000).

Turbidity measurement protocol

Turbidity is measured according to ISO 7027 with a portable turbidity meter (Hach Lange 2100Qis, Düsseldorf, Germany). The instrument has a light-emitting diode in the near-infrared range (at 860 nm), and the detector measures the side-facing scatter (90° angle). The light source in the nearinfrared is important for waters with high CDOM absorption (such as all Baltic Sea waters), since the effect of CDOM absorption decreases to zero at about 700 nm and is negligible in the near-infrared. Before each sampling campaign the turbidity meter is calibrated at 20, 100, 800 and 10 FNU steps against a dedicated calibration kit from the supplier. The water sample is measured in a sampling vial that is carefully cleaned before each measurement. Double check if the vial is fully dried and does not contain visual artefacts (e.g. fingerprints or similar) and that the sampling water is bubble free by holding the sample against a low light source. Take care to mix each sample before each measurement by carefully turning the sample 3 times up-side down. Make sure you do not shake the sample vigorously as this may create air bubbles that scatter light. Do not use a squeezy bottle for filling the sampling vial as this may also create air bubbles. The sampling vial should always be place in the same orientation inside the turbidity meter. One can make sure the vial is always in the same position by placing the arrow in the vial directly against the arrow in the instrument. The measurement accuracy of the Hach Lange turbidity meter is $\pm 2\%$. In the 'normal mode' the instrument takes three measurements and calculates the average value as output, with high measurement quality up to 20 FNU. Triplicate samples are registered for each water sample. A sample of ultrapure water (UPW; e.g. MilliQ or Elga water) is measured at each sampling occasion as a blank, and all measurements must be corrected for the turbidity of ultrapure water. Make sure you use the same bottle for the blank measurements as for the samples. The UPW should be well settled as it may contain air bubbles if it comes directly from the MilliQ system. The standard error of the bench turbidity method is 12 % (Kari et al, 2016).

Turbidity is strongly correlated to SPM concentration. Once one has done a calibration of SPM concentration vs. the turbidity method and derived a local algorithm (Kari et al, 2016) the turbidity measurements may replace the SPM measurements. For this, a statistically valid number of samples (30+) should be compared for the respective area spanning over a representative range of SPM

concentrations. For turbidity measurement it is especially important to swirl the sample bottle before pouring the sample into the vial.

Turbidity meter (used by SU and UU):

https://se.hach.com/2100q-portabel-turbidimeter-epa/product?id=24930148270&callback=qs Calibration kit:

https://se.hach.com/stablcal-100-ml-calibration-kit-2100q/product?id=26427850940&callback=qs

Appendix II – Filtration for CDOM measurements

Comparison of syringe CDOM filtration to standard method (using glass ware)

The optical protocols by NASA and IOCCG suggest the use of glassware for CDOM filtration as plastic can leak into the CDOM sample. During 2018, Stockholm University made a comparison of the syringe method vs. the glass filtration method for measuring CDOM. 12 CDOM samples were measured in the Gulf of Bothnia with both methods and 8 samples in Bråviken bay (with a strong CDOM influence). A t-test showed that for the CDOM absorption the difference was not significant (t-test: P=0.96) when using the linear fitting method. However, for the slope value there was a significant difference (t-test: P=0.048).

Figure 1 Comparison of CDOM measurements after filtration with a plastic syringe vs. a Whatmann glass filter apparatus.

Appendix III – Filters for CDOM measurements

Using GF/F filter for CDOM measurements (not recommended)

The revised NASA protocols (NASA, 2008) suggested to use GF/F filters for coastal waters, but not the latest optical protocol by the International Ocean Colour Coordination Group (IOCCG, 2018). However, GF/F filters allow for smaller particles and viruses to pass through which creates errors. This method is thus not to be recommended. S.Kratzer (SK) has done a comparison of the methods during her PhD (University of Wales, Bangor). She participated in the Cirolana cruise (DEFRA, UK) in the Irish Sea/North Sea where she sampled 10 duplicates of CDOM samples and filtered one sample each through Whatman GF/F and one sample each through 0.22 µm Millipore membrane filters. These samples provided a rather low range of CDOM (0.03-0.19 m⁻¹). Then SK also sampled during the Argos cruises (SMHI, SE) in June and August 1998. The g440 in these samples ranged from (0.05-0.47 m⁻¹), n=24. The GF/F method had a relative error (RMS) of 30 % and a systematic off-set (MNB) of 15 % (overestimation) when compared to the standard method using 0.22 µm Millipore membrane filters. The comparison of the two methods is shown in Figure 1. If one wants to derive the correct 0.2 µm filtered CDOM, one can apply the following algorithm:

 $G_{440} = 0.87 * G_{440(GF/F)} + 0.05$ $R^2 = 0.90; n=34$

However, this algorithm is only valid for the specified range of CDOM ($0.03-0.47 \text{ m}^{-1}$). If one wants to use GF/F filters a full comparison of using 0.2 µm membrane filter vs. GF/F filters must be performed for the high CDOM absorption as found in the Gulf of Bothnia and the Bothnian Sea. SYKE have done a comparison in Finnish lakes and found that using GF/F leads to an overestimation of about 15%. This is in accordance to the RMS error found in the comparison in figure 1 below. If one uses GF/F filters one should make such a calibration line and also rinse the GF/F filters with ultrapure water prior CDOM filtration in order to remove lose filter bits (Doerffer, 2002; IOCCG, 2018) that can cause scatter.

Figure 2 Comparison of CDOM measurements after filtration with both 0.22 μ m Millipore membrane filters and Whatman GF/F. The GF/F method overestimates by about 15%; the relative error (RMSE) is 30%. Note that for higher CDOM values, the GF/F filtered data can lie below the 1:1 line.

Appendix IV – Hydrolight reflectance simulations

Reflectance simulations of the Swedish SEAmBOTH stations by Hydrolight and comparisons with the TACCS measurements of 2018

Kari Kallio, Finnish Environment Institute (simulations)

Susanne Kratzer, Stockholm university (optical data, concentrations)

SEAmBOTH Work package 2.1 (Remote sensing)

March 12th, 2020

1. Introduction

The main objectives this sub-task of the SEAmBOTH satellite remote sensing work package (2.1) were 1) to simulate water reflectance with the Hydrolight model using concentrations and specific inherent optical properties (SIOPs) measured at the Swedish SEAmBOTH stations and 2) to compare them with the reflectances measured with the TACCS instrument. The SIOPs measured at the stations were CDOM absorption spectra (a_{CDOM}), and total absorption (a_{tot}) and total scattering (b_{tot}) at nine wavelengths.

Most of the SIOPs needed for the simulations were taken from published optical studies from the Baltic Sea. This report also includes comparison of some published SIOPs in the Baltic sea region.

The results are used to find out how accurately reflectance can be simulated in the studied coastal region. Reflectance spectra can also be simulated for routine monitoring stations were the concentrations of the key optical water constituents are measured and where SIOPs are known with a reasonable accuracy (based on measurements and/or literature). The simulated reflectance specta can be additionally utilized e.g. in the validation of atmospheric correction of the satellite image processors that are used for the interpretation water quality.

2. Material

For the simulations we selected 15 SEAmBOTH stations, where sufficient optical and water constituent concentration measurements were available. The stations were located in the Swedish coast of the Gulf of Bothnia. All data is from 2018.

At station 16a scattering measurement was not available and therefore it was not included in the reflectance simulations based on the specific scattering coefficient of particles at 440 nm (b_{part} * (440)) measured at each station. Time was not recorded for station 14e, but it (UTC 1452) was interpolated from the times of previous and next station.

Total suspended matter (TSM) concentration was estimated from turbidity according to Kari(2018). The water constituent concentrations (TSM, Chl-a, $a_{CDOM}(443)$), $b_{part}*(440)$, date and time of each station are presented the reflectance figures (Figs. 3-4).

3. Input for Hydrolight simulations

Three simulations were made using different SIOPs:

 Best SIOPs, with station specific slope factor of CDOM absorption (s_{CDOM}) and b*part(440) (Table 1). In addition, sun altitude of each measurement was input to Hydrolight.

- As 1) but b*_{part}(443) was the same for all stations (mean of the 14 stations: b*part(440) = 1.06 m2/g).
- 3) Average SIOPs reported by Simis et al. (2017) for summer condition in the open Baltic sea.

| SIOP | Symbol | Value | Reference |
|------------------------------------|--------------------------|--------------------------|------------------------------|
| Specific scattering coefficient of | b* _{part} (440) | Measured at each station | |
| particles at 440 nm | | | |
| Scattering exponent | nb | 0.55 | Kratzer&Moore (2018) |
| Backscattering ratio | b₀/b | 0.015 (wavelength | Simis et al. (2017), summer |
| | | independent) | |
| Scattering phase function | | | Fournier and Forand (1994) |
| Specific absorption coefficient | a* _{ph} (λ) | | Simis et al. (2017), summer, |
| of phytoplankton | | | package effect |
| Slope factor of CDOM | S _{CDOM} | Measured at each station | |
| absorption | | | |
| Specific absorption coefficient | a* _{nap} (λ) | | Simis et al. (2017), summer |
| of non-algal particles | | | |

Table 1. The best SIOPs (Option 1) for the SEAmBOTH TACCS stations in 2018.

Sun altitude was calculated from coordinates, date and time. The Hydrolight simulations represent the nadir view reflectance. Reflectance at different viewing angles can also be calculated by Hydrolight.

TACCS reflectance is Rho_w . Hydrolight simulates R_{rs} and it was converted to Rho_w by: $Rho_w = 3.14*R_{rs}$. The Hydrolight simulation were made with version 5.3.1, that was published in 2016.

4. SIOP comparisons

Comparisons were made for scattering (b^*_{part} and b_b/b) and phytoplankton absorption.

4.1 Scattering

Table 2. b_{part}^* at 443 nm and b_b/b measured in the Baltic Sea and Finnish lakes.

| Data | Area/season | b* _{part} at 400, 442 or 443 nm m2/g | b _b /b |
|-----------------------------------|--------------------------------------|---|-------------------------------|
| SeamBoth | Swedish coast of GOB | 1.06 ± 0.35 (min 0.49, max 1.49) | - |
| Kratzer&Moore 2018 | NW Baltic Proper Summer | 1.016 ± 0.326 | 0.017 ± 0.0103 (443 nm) |
| Simis et al. 2017 | Open Baltic sea Spring | 0.200 ± 0.093 | 0.0197 (mean of all bands) |
| Simis et al. 2017 | Open Baltic sea Summer | 0.468 ± 0.382 | 0.0151 (mean of all bands) |
| Kallio (2005) | Finnish lakes (Spring and summer) | 0.95 | - |
| C2RCC processor, default value | | 0.58 (blue scattering) | - |
| | | 0.32 (white scattering) | - |

Figure 1. Average $b_{part}^*(\lambda)$ measured in the Baltic Sea and Finnish lakes, and the default $b_{part}^*(\lambda)$ for blue and white scattering in the C2RCC processor. The mean of the $b_{part}^*(440)$ measured at the SEAmBoth stations (N=14) is indicated by '*'. K&M is Kratzer & Moore (2018), SS is Simis et al. (2017) and Finnish lakes is Kallio et al. (2016). The vertical line is: $\lambda = 443$ nm.

4.2 Phytoplankton absorption

Figure 2. Chl-a specific absorption of phytoplankton in the Baltic Sea and Finnish lakes. Horizontal line is a*ph= 0.03 m2/mg. a*ph(443) of K&M2018 (Kratzer & Moore 2018) is Chl-a independent. Other data takes into account package effect (a*ph(443) is Chl-a dependent). S2017 is Simis et al. 2017 and FIN lakes is Ylöstalo et al. (2014).

5. Results

Reflectances are presented in figures 3 and 4. Simulated reflectances include results of three SIOP options (see Section 3). In addition, normalized reflectances are presented in figure 4. Simulations were made for 380-800 nm and TACCS measures reflectance at seven wavelengths.

Figure 3. Simulated (HL) and measured (TACCS) Rho_w of stations 9b - 14e. bstar is $b*_{part}(440)$.

Figure 4. Simulated and measured Rho_w of stations 14f - 18c. bstar is $b^*_{part}(440)$.

Figure 5. Normalized reflectance spectra of all stations. Rhow at 560 nm = 1.

6. Discussion

- Simulations with Simis et al. (2017) summer SIOPs (Option 3) under-estimated Rho_w at most stations.
- In some cases, average b*_{part}(440) yielded better results than station specific b*_{part}440 (see also comment on b_b/b later).
- The magnitude of Rho_w spectrum also depends on b_b/b (and scattering phase function), which was not measured in the field. Its variation can be high e.g. Kratzer&Moore(2018) reported 0.017 ± 0.0103 for bb/b in NW Baltic Proper. This adds uncertainty in the simulated spectra.
- TACCS Rho are unrealistically low at station 10e particularly in the short wavelengths. The same is probably the case at station 10b (see also normalized spectra). These are stations with the highest CDOM concentrations of the dataset. TACCS was mainly developed for ocean conditions, and therefore it probably is not able to measure reliably low radiance/irradiance in the short wavelengths.
- The TACCS Rho_w(671) was in many cases higher than simulated values (e.g. stations 14a-16a), when looking the normalized spectra.
- Additional options for SIOPs to be used in Hydrolight simulations
 - b_b/b (0.0151) was from Simis et al. (2017) summer SIOPs. Another option is to use
 0.017, published by Kratzer & Moore (2018).
 - The scattering exponent is fixed (from Kratzer&Moore (2018)). It could be calculated from ac-9 data for each SEAmBOTH station.
 - \circ a^{*}_{nap}(λ) comparison based on published values in the Baltic sea could be made.

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