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Contents

Abstract

This document describes the analysis and comparisons of model, EO and in situ data generated in WP4 and quantifies the impact and benefits of model and EO developments performed in WP3.

Glossary

AC	Atmospheric Correction
aCDOM	Absorption coefficient of Coloured Dissolved Organic Matter
ATBD	Algorithms Theoretical Basis Document
C2RCC	Case 2 Regional Coast Color
CDOM	Coloured Dissolved Organic Matter
Chl a	Chlorophyll a
CMEMS	Copernicus Marine Environment Monitoring Service
COD	Chemical oxygen demand
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
EO	Earth Observation
ERGOM	Ecological Regional Ocean Model
IOP	Inherent Optical Properties
N	Number of data points
NN	Neural Network
OLCI	Ocean and Land Color Imager
P	Phosphorous
PAR	Photosynthetically active radiation
PLC	Pollution Load Compilation
TN	Total Nitrogen
R^2	Coefficient of determination
RMSE	Root Mean Square Error
S2	Sentinel-2
S3	Sentinel-3
TOA	Top of Atmosphere
TOC	Total Organic Carbon
TP	Total Phosphorous
TSM	Total Suspended Matter

List of Symbols

Symbol	Definition	Dimension/Unit
aCDOM(400)	Absorption coefficient of CDOM at 400 nm	m^{-1}
ay440	Absorption coefficient of yellow substances (CDOM) at 440 nm	m^{-1}

1 Introduction

The overall goal of the WP4 of the Baltic+ SeaLaBio project was to generate EO and model datasets using the methods developed in WP3 and then assess the impact that these new and/or improved products have on the understanding of biogeochemical processes and carbon cycle. One specific goal formulated during the project was to assess if the accuracy of the ERGOM model can be improved by using EO based data as input values. This document describes the comparisons of EO, in situ and model data performed during WP4 and the impacts of the results for the monitoring of the state of the Baltic Sea. The generated datasets and the methods to access them are described in Dataset User Manual.

2 Summary of modifications

This chapter describes the main modifications done to ERGOM and EO processors during the SeaLaBio project. For more details please see the ATBD V2.

2.1 ERGOM

The main modifications made to ERGOM during the SeaLaBio project were:

1. Improvement of spatial resolution from 3 n.m. to 1 n.m.
2. Introducing an explicit CDOM state variable
3. Allow CDOM values of river water to be used as input data in addition to river runoff.
4. Introduction of the photo bleaching of CDOM

The 1st modification is essentially a technical one. The processes of the model did not change, only the cell size of the horizontal grid where the values are computed. This improvement allows finer features to be seen in the data. This modification increases the processing time by a factor of about 30 causing a significant strain on the computing resources.

The 2nd modification is an upgrading of the model and primarily a technical issue. After validation of the CDOM variable, CDOM is used for estimations of the under-water PAR. It replaces the former CDOM parametrization with salinity.

The 3rd modification is more significant as it leads to a more realistic light climate which has an impact on the biological processes in water.

The 4th modification was added after the first tests with the EO based CDOM values as input data led to unrealistically high concentrations in the Central Baltic.

2.2 EO algorithms

2.2.1 Atmospheric correction

The development here aimed to combine the advantages of the C2RCC and Polymer processors, which were identified as the two best algorithms over the Baltic while not performing well in the most challenging optical conditions near the coast and towards the easternmost and northernmost parts of the Baltic Sea. C2RCC is based on artificial Neural Networks (NNs) and its marine model aggregates a large knowledge of natural variability, with realistic covariance in the IOPs (Inherent Optical Properties), thanks to training on relevant dataset. When the NN is trained, it is also very fast to process a whole scene at once. On the other hand, the spectral matching technique of Polymer is known to be robust over many atmospheric conditions and perturbations (such as thin clouds, residual Sun glint, adjacency effects), while its marine model with two components is not optimal over absorbing or very turbid waters. The Baltic+ AC merges both advantages. The marine reflectance model is given as a function of five IOPs by a forward NN, specifically trained over the Baltic. For a given combination of IOPs, the marine reflectance is computed, removed from the total signal, and the best atmospheric path reflectance is searched based on Polymer approach. The discrepancy between the modeled marine reflectance and the one retrieved by removing the atmosphere is minimized with an optimization method (Nelder-Mead simplex). The method can be seen as an overall non-linear least-square minimization on five IOPs. It allows to rigorously compute the uncertainty of the retrieved IOPs, hence subsequently of the atmosphere and final marine reflectance, on a per-pixel basis.

2.2.2 In-water inversion

A Baltic Sea specific bio-optical model was developed to facilitate the development of a new in-water inversion algorithm. The model is based on parameter (CDOM, Chl-a, TSM) ranges determined according to data collected from Finland, and Sweden. The model was used to create a simulated dataset which then was used for training a new neural network for the inversion. Parallel to this, an empirical band ratio was calibrated with in situ data.

3 Dataset comparisons

3.1 ERGOM vs. in situ data

The objective of this comparison was to see how well ERGOM can simulate CDOM values when EO-based CDOM values are used as input data. Figure 1 shows the locations of the measurement stations used in the comparison. The in situ aCDOM dataset (see the Dataset Description) only covers Finland and the northern part of Sweden. However, the range of aCDOM values is large in the area and thus this dataset is suitable for this kind of validation.

The extraction of ERGOM matchups was done directly from THREDDS (from the dataset with 12 h time step, see the Dataset User Manual) based on in situ station locations and dates. Since there are no clouds, the number of data points is high. Both salinity and CDOM values were extracted. Figure 2 shows the comparison of in situ salinity values vs. ERGOM salinity. The correspondence is very good which means that 1) the extraction works as expected and 2) ERGOM can estimate salinity accurately.

Figure 3 shows the comparison of in situ CDOM values vs. ERGOM CDOM when the old version (CDOM from salinity) is used. The correlation is poor. Most ERGOM values are low while some are very large (not all high values are shown).

Figure 4 shows the comparison of in situ CDOM values vs. ERGOM CDOM with the new version of the model. The improvement is clear. Correlation is much better, there are no over-estimated (very large) values and the data follows the 1:1 line much better. The high in situ values (> 6 m^{-1} at 400 nm) are underestimated by the model. Possible reasons for this are:

- Some rivers are not included in ERGOM and their impact is missing.
- The input CDOM values given to the model are too low since - due to dilution - river water typically has higher CDOM values than coastal water and the EO based method is only able to estimate CDOM close to the river mouth.
- It is not known how well the EO CDOM is estimated in Sweden. More in situ data needed to evaluate this.

Adding more rivers to ERGOM is beyond the scope of the present project. The use of higher CDOM input values (P95) was tested and the results are presented in Figure 5. The data points generally move upwards while the correlation stays the same. The low values are now overestimated. The photo bleaching was calibrated with the P75 input data and a recalibration of the coefficients is likely to be needed. This would, however, require extensive model runs which were beyond the scope of the project.

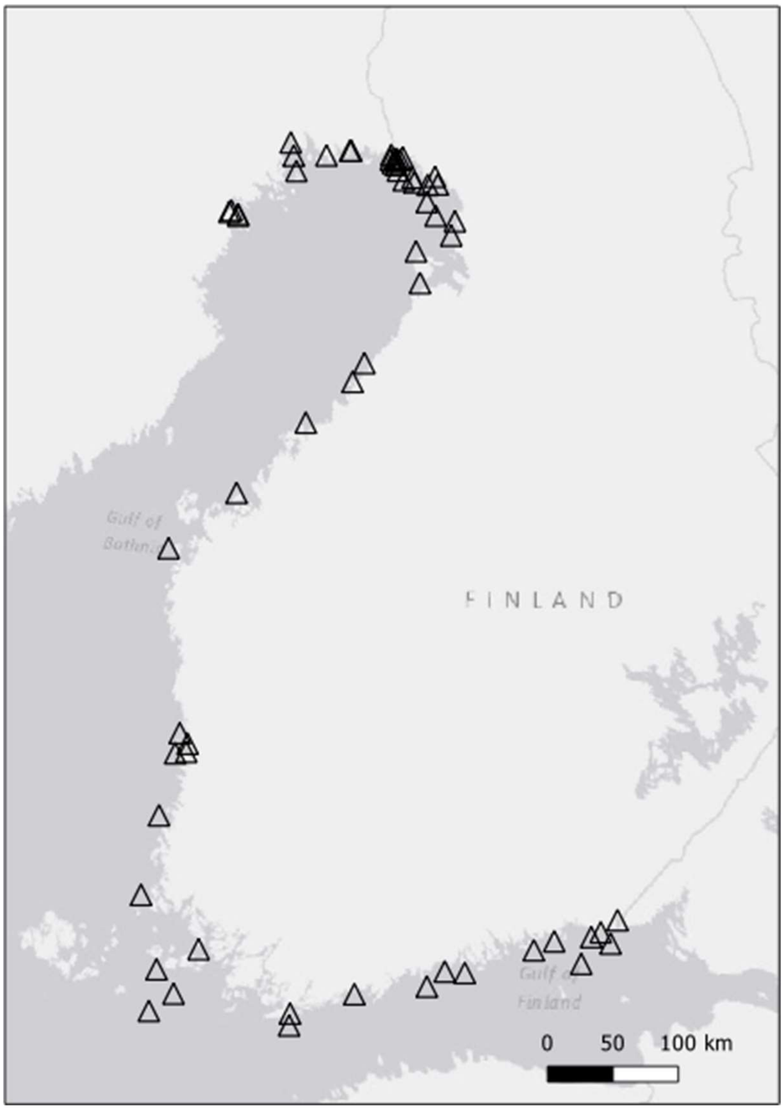


Figure 1. In situ measurement station sites used in the comparison of ERGOM simulations.

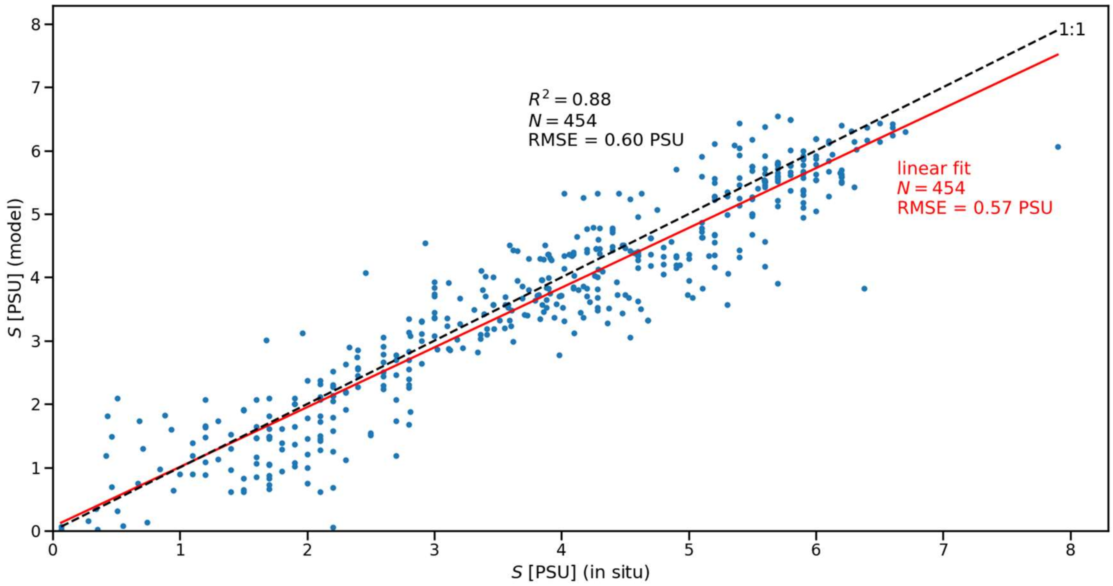


Figure 2. In situ salinity vs. ERGOM salinity at monitoring stations in the Northern Baltic. Salinity was not estimated in all stations, hence there is a different number of data points here and in Figure 3.

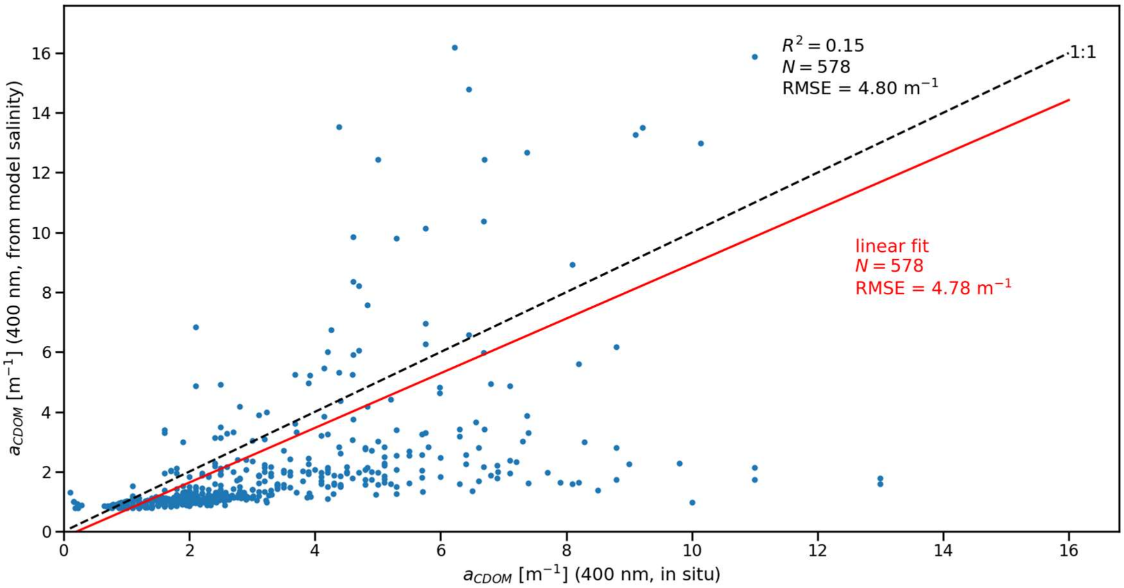


Figure 3. In situ aCDOM vs. ERGOM aCDOM derived from salinity at monitoring stations in the Northern Baltic.

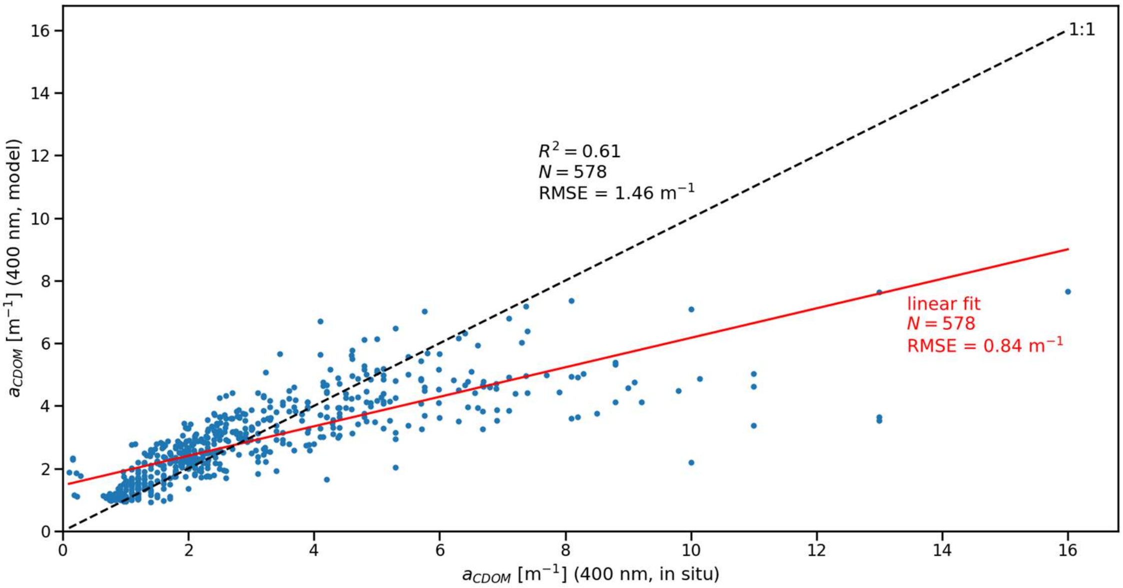


Figure 4. In situ aCDOM vs. ERGOM aCDOM simulated using the 75th percentile EO values as input data at monitoring stations in the Northern Baltic.

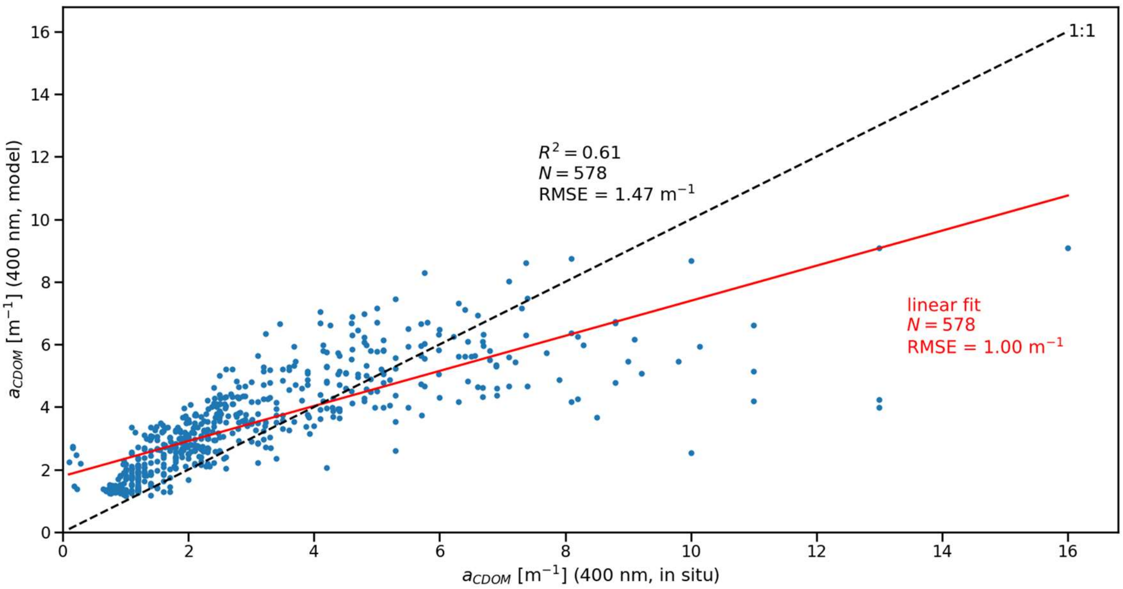


Figure 5. In situ aCDOM vs. ERGOM aCDOM simulated using the 95th percentile EO values as input data at monitoring stations in the Northern Baltic.

In addition to the scatter plots, we show time series from ERGOM results together with *in situ* data and how it compares to the salinity parametrization. All model CDOM concentrations are converted into absorption values for 440nm. Figure 6 shows the location of the stations while the results are shown in Figure 7, Figure 8 and Figure 9.

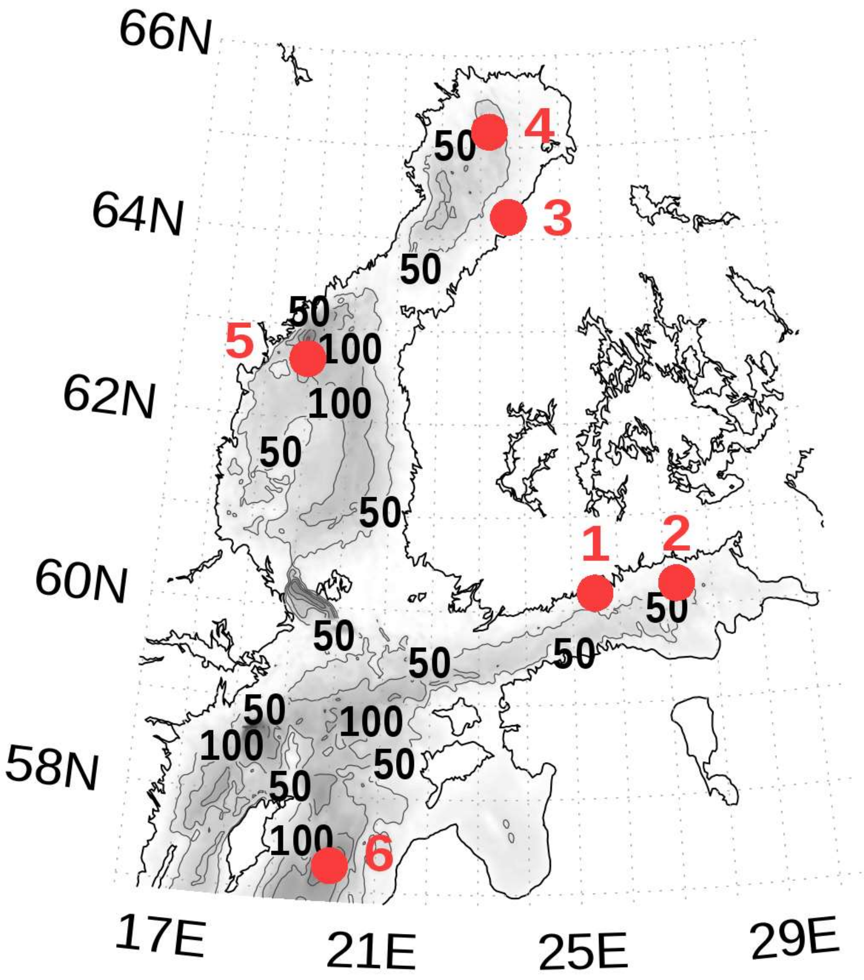


Figure 6. Stations for model and observation comparison.

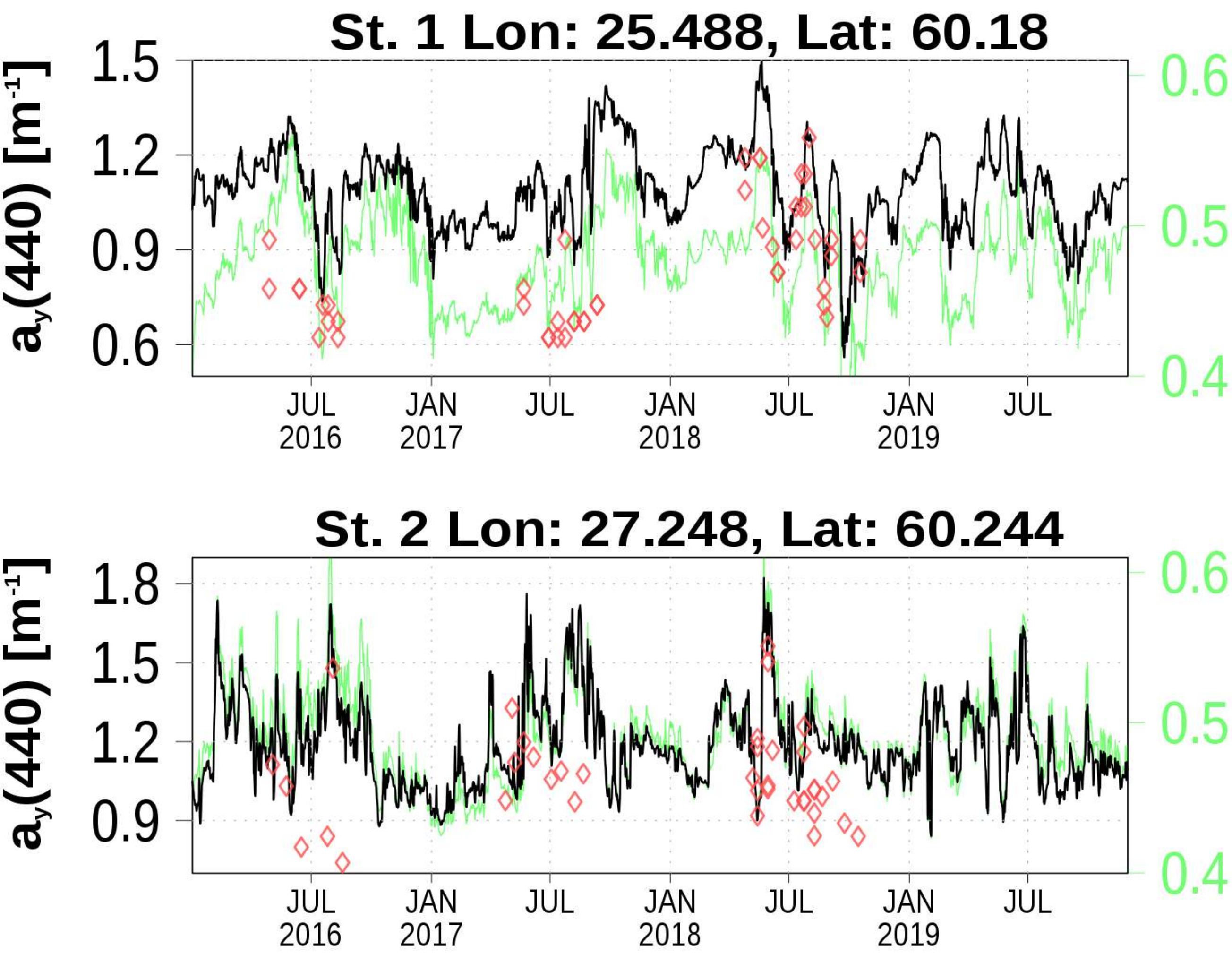


Figure 7. CDOM absorption simulated by ERGOM (black), estimated with a salinity parametrization (green), and observed (red) in the Gulf of Finland. For the location of the stations see Figure 6. Note the different scale for the green curve (right y-axis).

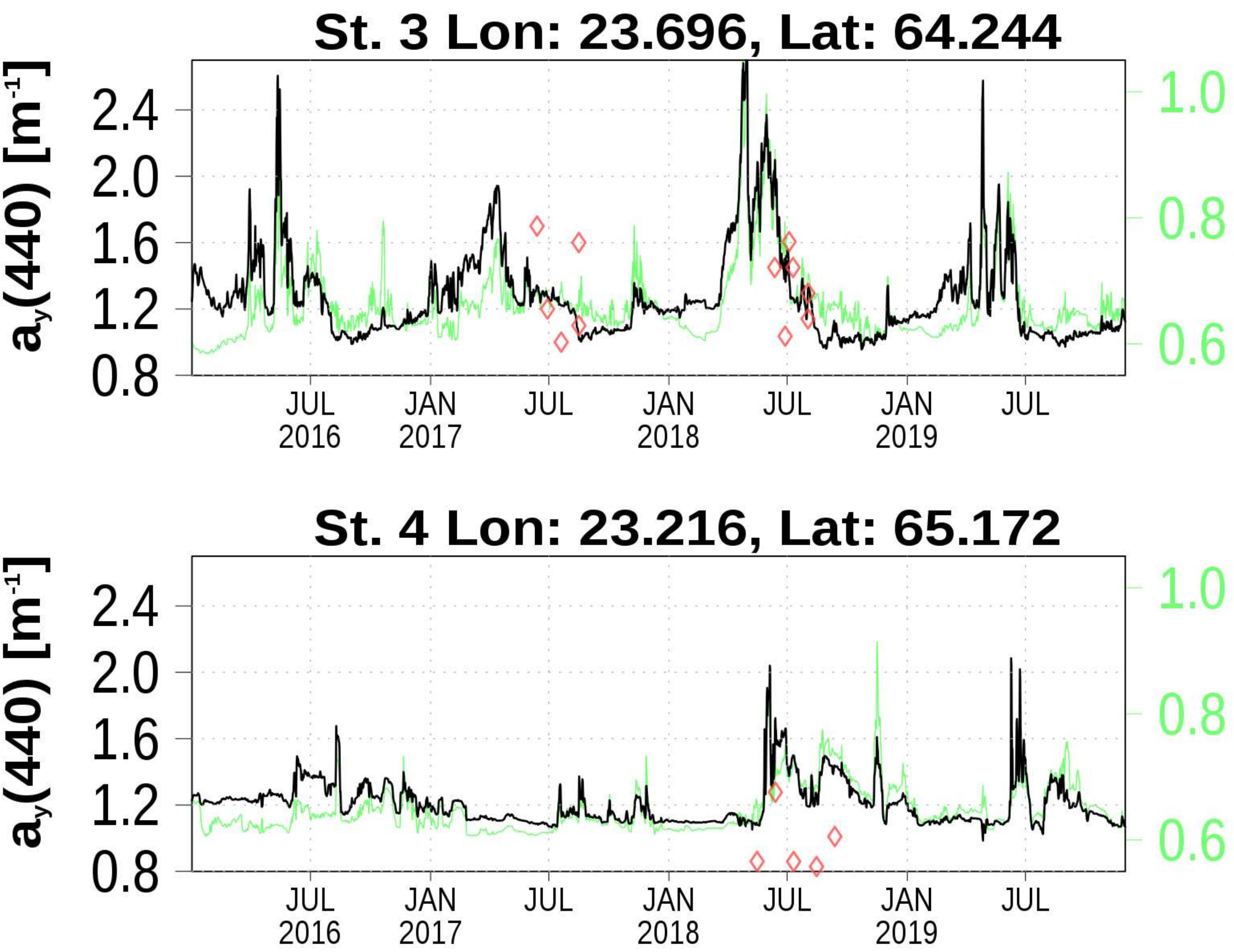


Figure 8. CDOM absorption simulated by ERGOM (black), estimated with a salinity parametrization (green), and observed (red) in the Bay of Bothnia. For the location of the stations see Figure 6. Note the different scale for the green curve (right y-axis).

Especially for the Gulf of Finland and the Gulf of Bothnia, the simulated CDOM data improved considerably compared to the salinity parametrization. At the stations in the Bothnian Sea and Gotland Sea, the difference between simulated data and data from the parametrization is small while the dynamics of the simulated CDOM is stronger. A convincing improvement could be achieved especially in the Gulf of Finland and the Bay of Bothnia.

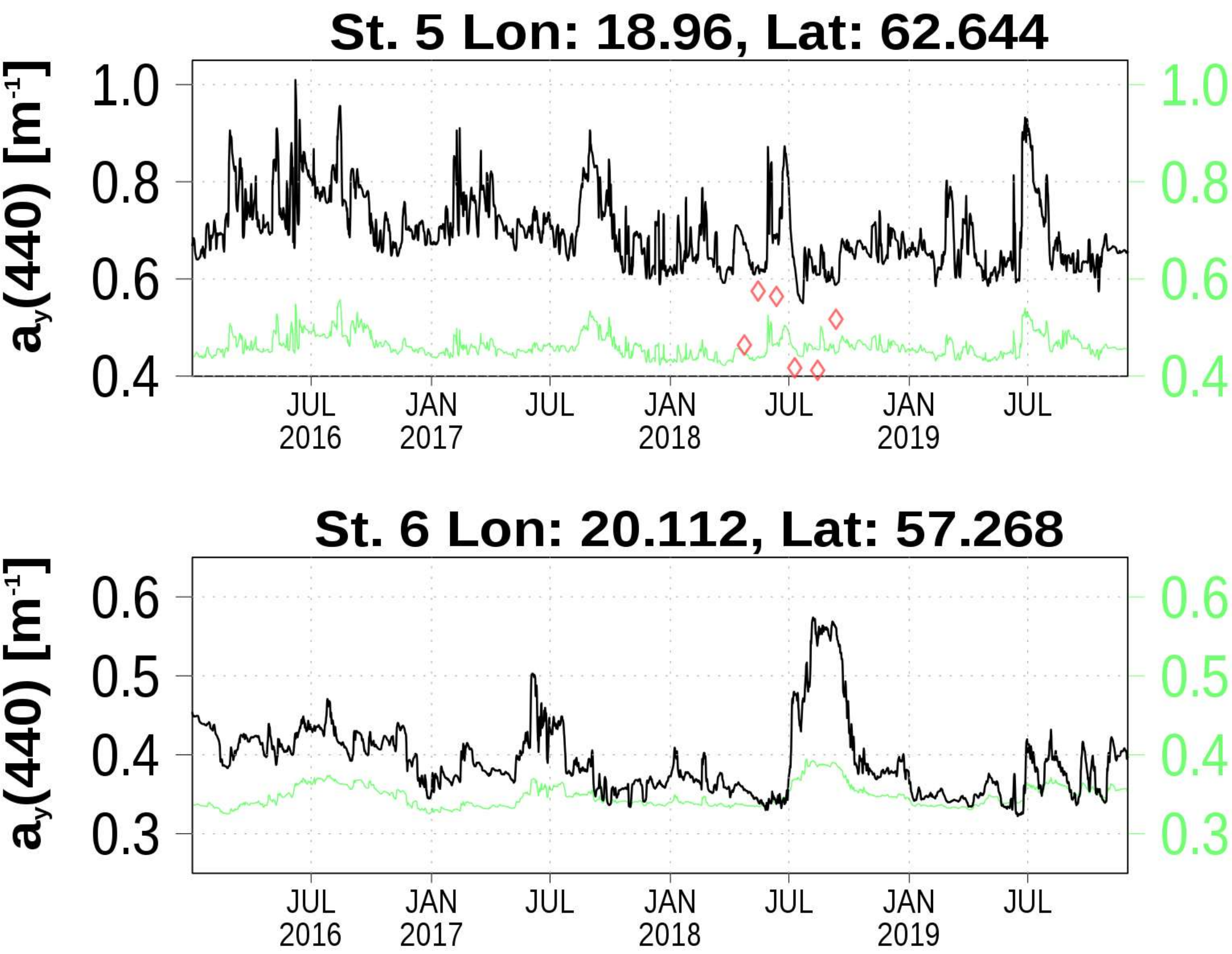


Figure 9. CDOM absorption simulated by ERGOM (black), estimated with a salinity parametrization (green), and observed (red) in the Bothnian Sea and Gotland Sea. For the location of the stations see Figure 6. For the Gotland Sea, no data were available.

3.2 Other EO data

According to the validation report the algorithms developed in SeaLaBio clearly outperform the other available processors (C2RCC, IPF, Polymer) in the estimation of aCDOM. Thus, further comparisons with these processors were not made here. EUMETSAT provides aCDOM values which are based on OLCI and C2RCC and thus fall into the same category.

CMEMS provides EO based Chl-a concentrations but not aCDOM. Since SeaLaBio has concentrated on the estimation of aCDOM, it was not possible to make comparisons with the CMEMS data.

3.3 ERGOM vs. EO data

Figure 10 shows examples of aCDOM maps estimated with OLCI and simulated with ERGOM. In May both data sources show elevated concentrations along the coast caused by high terrestrial influx during the snow melting period. In July the concentrations have decreased along the coast and increased in the open sea areas (less terrestrial influx and transport of CDOM from coast to open sea). The monthly composites generated from OLCI data appear smooth and contain no apparent artefacts.

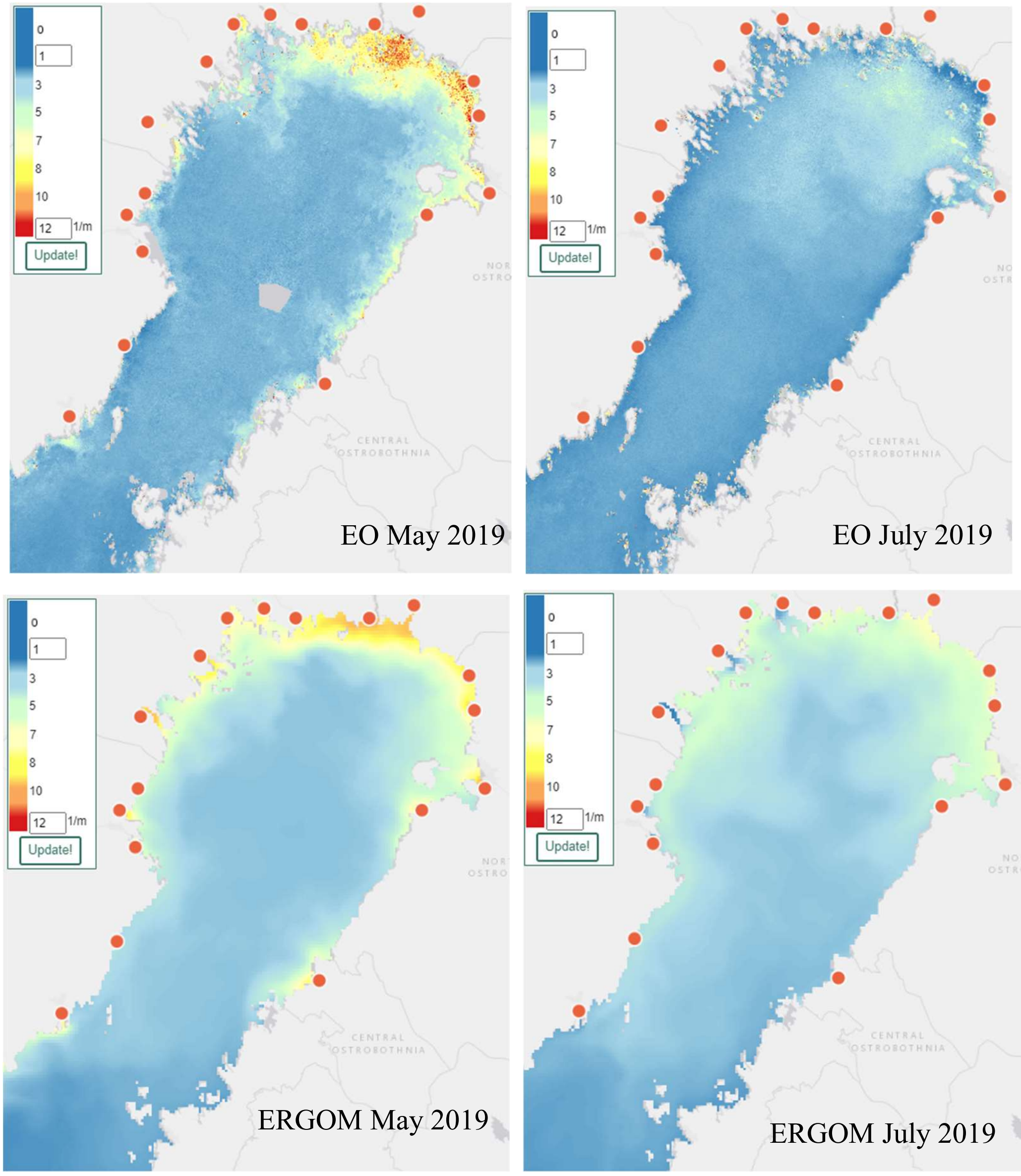


Figure 10. Monthly composite aCDOM maps (top) estimated from Sentinel-3 OLCI images with band ratio rho_wn_8/rho_wn_6 (665 nm/560 nm) after atmospheric correction with the Baltic+ AC processor and (bottom) simulated with ERGOM for May and July 2019 in the Bay of Bothnia (images from the TARKKA map service). Red dots are load points in the ERGOM model.

3.4 S2, S3 and ERGOM synergy

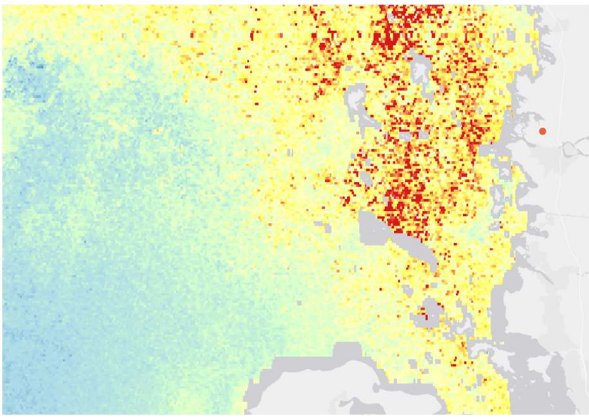
One of the objectives of the study was to explore the potential synergies offered by Sentinel-2 MSI and Sentinel-3 OLCI. HR data, such as Sentinel-2, can provide information closer to the shore than OLCI while OLCI is expected to have better thematic accuracy and temporal resolution. We tested the synergetic use through data fusion.

SYKE has a data fusion tool originally designed to merge raster and in situ data. This was adapted to work with several raster datasets. The data fusion system first resamples all products into the same grid and then runs a Kalman smoother for the harmonized data. This operates both in spatial and temporal dimensions. The number of pixels is limited to about 1 000 000 due to memory demands.

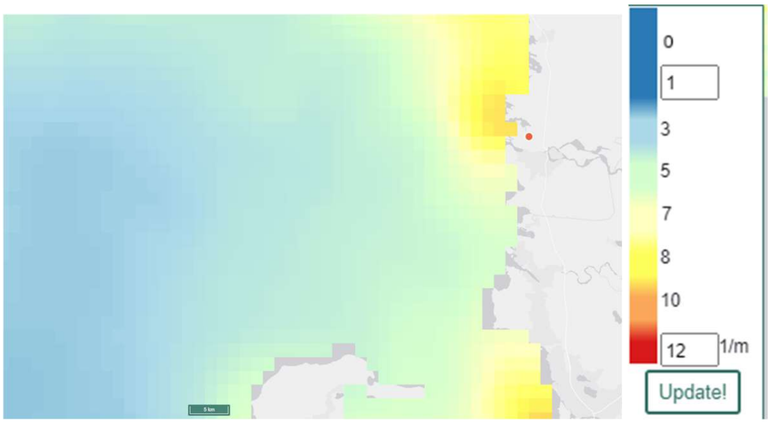
We tested merging with monthly S2 and OLCI CDOM rasters. The OLCI values were obtained with the method described above while the S2 results were based on C2RCC. Figure 11 shows examples of the input data.

Figure 12 shows the results of the data fusion with 300 m resolution. S2 allows estimations near the coast with no apparent artefacts in the results (e.g. border of OLCI results). The fusion method can also fill a shallow water area where the EO values are masked. We also tested merging the two EO datasets with ERGOM results. These results are now shown here but, in general, the lower CDOM values of ERGOM make the fusion results lower near the coast.

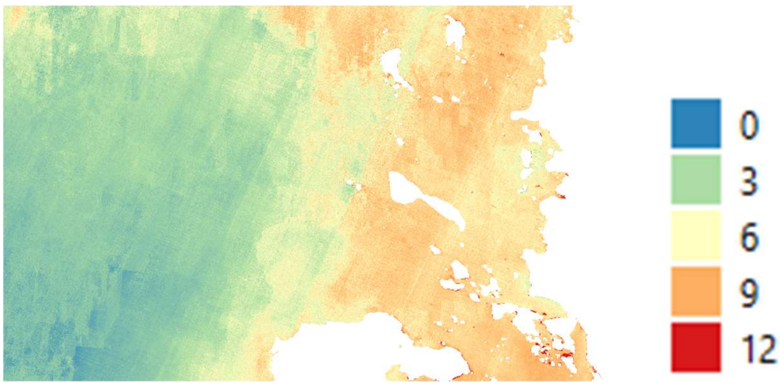
This test shows that the merging of dataset is technically possible. In situ data was not used in this test but it is possible include it. The system has several tunable parameters and it was not possible to test different combinations in this project. Furthermore, the quality of the data fusion result depends on the quality of the input data. Figure 13 shows an example time series with CDOM values estimated with EO, ERGOM and laboratory methods. At this station the ERGOM values have a lower dynamic range than the other methods while the EO results may contain noise. Nevertheless, there is also clear agreement in the values.



(a)



(b)



(c)

Figure 11. The input data used in the data fusion test. The examples show the May 2018 monthly CDOM values with: (a) OLCI with Baltic+ AC & band ratio with 300 m resolution, (b) ERGOM with 1 n.m. resolution and (c) S2 with C2RCC. Note that the color scale in (a) and (b) is the same but different in (c).

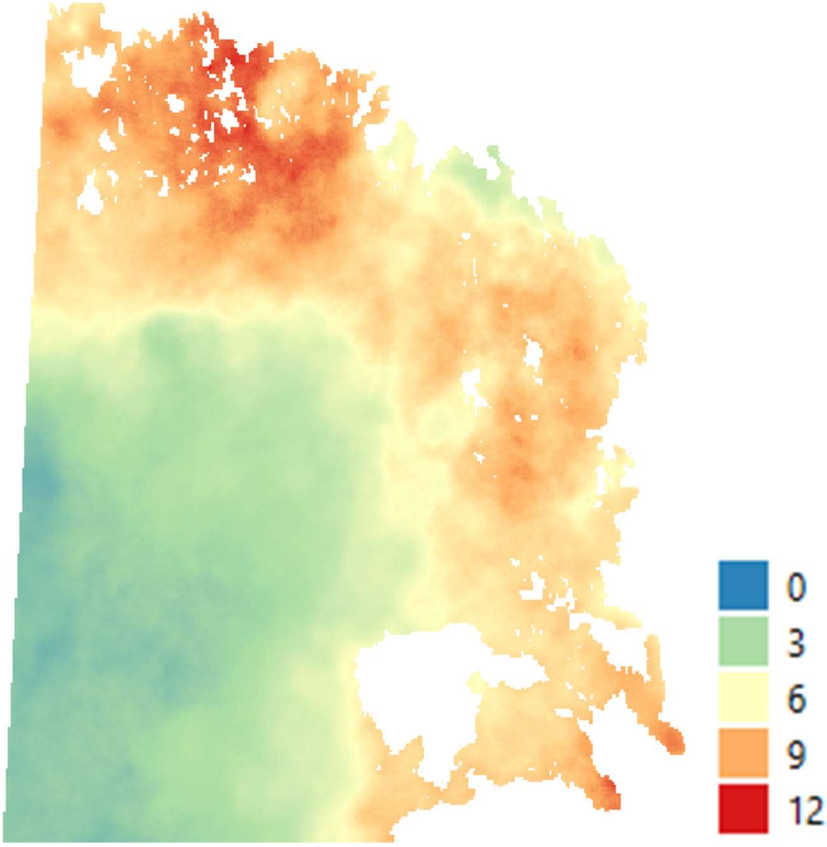


Figure 12. CDOM values after data fusion with S2 and OLCI data.

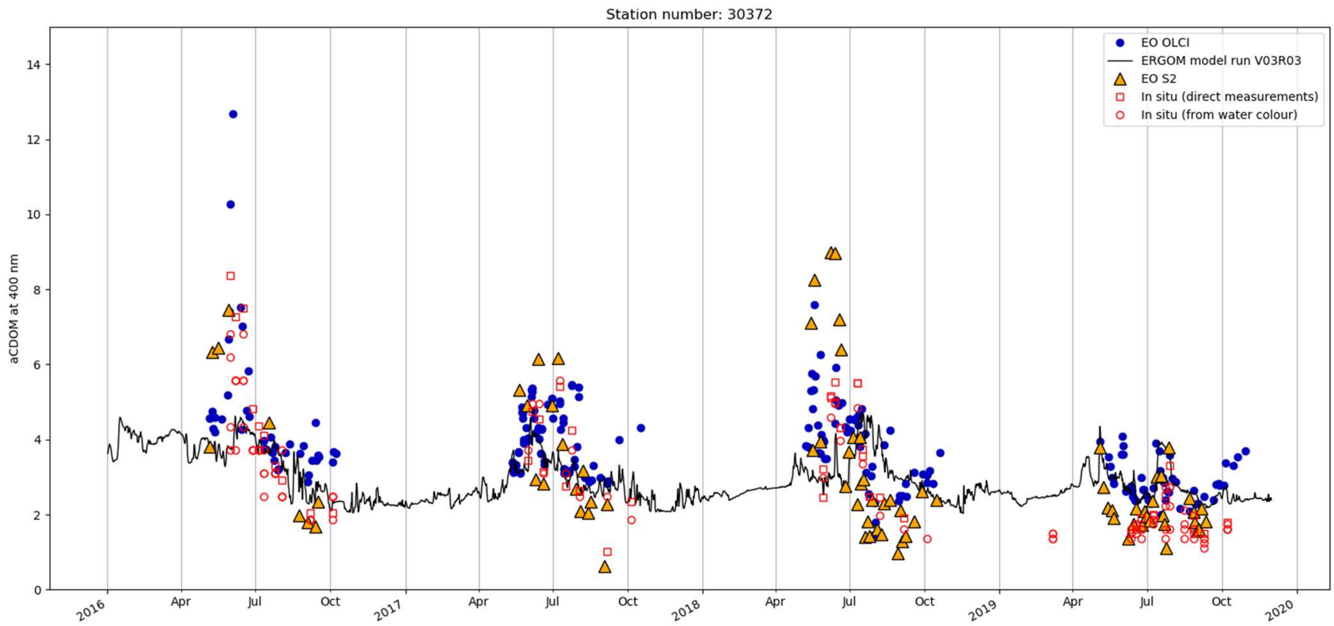


Figure 13. CDOM time series with different methods at the Hailuoto (in Finland) intensive monitoring station.

3.5 DOC/aCDOM and DOC/TOC ratios

Satellite data can be used to estimate aCDOM, but not directly the concentration of Dissolved Organic Carbon (DOC) or Total Organic Carbon (TOC). However, aCDOM can be converted to DOC, if there is clear correlation between them in the study area of interest.

We analyzed the DOC/aCDOM relation in the SeaLaBio in situ dataset (Kallio et al. 2019, Figure 14) and in river Kyrönjoki estuary in Finland (Figure 15). These measurements were all from the Bay of Bothnia, because DOC and aCDOM were not simultaneously measured in other regions that were included in the SeaLaBio dataset.

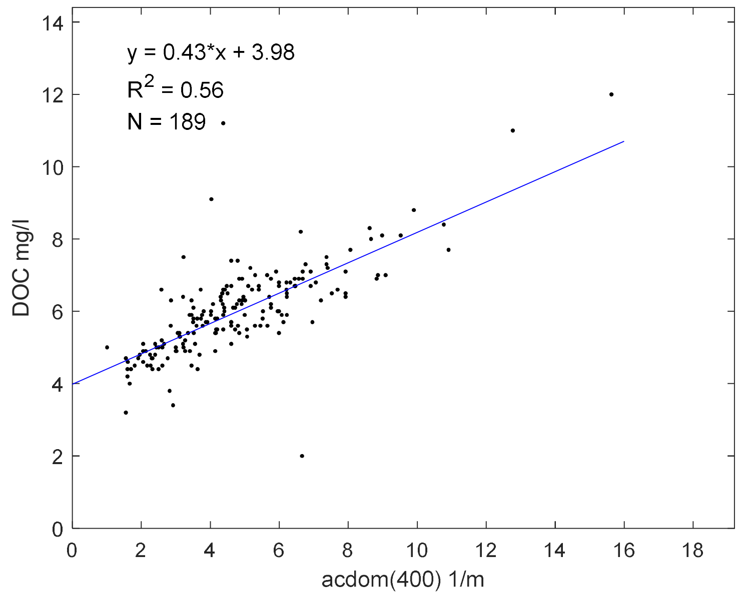


Figure 14. Relation between DOC and aCDOM(400) in the SeaLaBio dataset. Data consists of Finnish and Swedish in situ measurements in the Bay of Bothnia and is described in the SeaLaBio Dataset description-document (Kallio et al. 2019). Sampling depth was < 1.1 m.

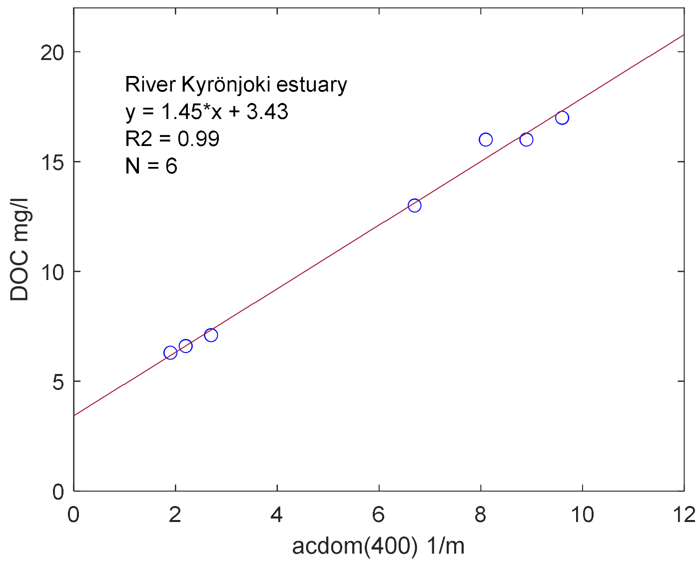


Figure 15. Relation between DOC and aCDOM(400) in the EO validation campaign of SYKE in Kyrönjoki estuary (Bay of Bothnia) in high discharge conditions in May 10th, 2018. Unpublished data.

Table 1. Relation between DOC and aCDOM(400) in the Baltic Sea studies. DOC is in mg/l and aCDOM(400) in 1/m. aCDOM(412) in Simis et al. (2017) was converted to aCDOM(400) assuming an absorption slope of 0.018 1/nm and in Harvey et al. (2015) aCDOM(440) was converted to cdom(440) assuming an absorption slope of 0.016 1/nm.

Area	Equation	Min - Max aCDOM(400)	Reference
Gulf of Bothnia	DOC = 0.43 x aCDOM(400) + 4.0	1.0 - 13	SeaLaBio dataset
	DOC = 0.41 x aCDOM(400) + 3.3	1.5 - 17	Harvey et al. 2015
	DOC = 0.34 x aCDOM(400) + 3.8	0.5 - 2.2	Simis et al. 2017
	DOC = 1.45 x aCDOM(400) + 3.4	1.9 - 9.6	SYKE campaign
Baltic Proper & Nyköping	DOC = 1.5 x aCDOM(400) + 3.3	0.6 - 8	Harvey et al. 2015
Gulf of Finland, Northern Baltic Proper and Gotland basin.	DOC = 1.25 x aCDOM(400) + 3.7	-	Simis et al. 2017

Simultaneous DOC and TOC in situ measurement were only available from the Bay of Bothnia in the SeaLaBio dataset (Kallio et al. 2019). The average DOC/TOC ratio was 0.97 (sampling depth < 1.1 m, N=215). In the northern Baltic sea rivers, the reported average DOC/TOC ratios are ≥ 90%. In 15 rivers in Finland the average ratio was 95% (Mattsson et al. 2005) and in Kiiminkijoki (Finland) 90% (Heikkinen 1989). Ostapenia et al. (2009) reported an average ratio of 93% for Lake Ladoga.

The relation between DOC and aCDOM varies in the Baltic Sea (Table 1 and Ylöstalo et al. manuscript). In the Gulf of Bothnia, the conversion equations were quite similar except in River Kyrönjoki estuary (SYKE campaign). The SYKE campaign was conducted during spring flood and the ratio of river water in the sampling location was high. This indicated that in river estuaries the DOC/aCDOM ratio can differ from the open sea values.

The DOC maps of the Gulf of Bothnia (Figure 16) were calculated from ERGOM average aCDOM(400) maps of May and August in 2019. We used the following conversion equations: DOC = 0.39 x aCDOM(400) + 3.72, where DOC is in mg/l . This equation was obtained by calculating average parameter values of the conversion equations of the following Gulf of Bothnia studies: Harvey et al. (2015), Simis et al. (2017) and SeaLaBio dataset (Table 1).

The concentration levels in Figure 16 were similar to the DOC maps that were based on point and transect in situ measurements (e.g. Ylöstalo et al., manuscript). The DOC in the coastal waters in the SeaLaBio products are more realistic but the DOC maps could be improved by adding own extraction areas to the estuaries of all large and medium sized rivers. In addition, more field studies on the spatial and temporal variation of the DOC/aCDOM ratios are needed.

3.6 Validation of aCDOM in Neva bay

Neva is the largest river (by discharge and basin area) draining to the Baltic sea. However, no recent aCDOM nor TOC&DOC observations were available from the river or the Neva bay. Therefore, we compared SeaLabio aCDOM estimated from the Neva Bay extraction area to the in situ observations published in the literature (Table 2).

The locations of sampling stations use by Ylöstalo et al. (2016) and Aarnos et al. (2012), and the SeaLabio-extraction area are shown in Figure 17.

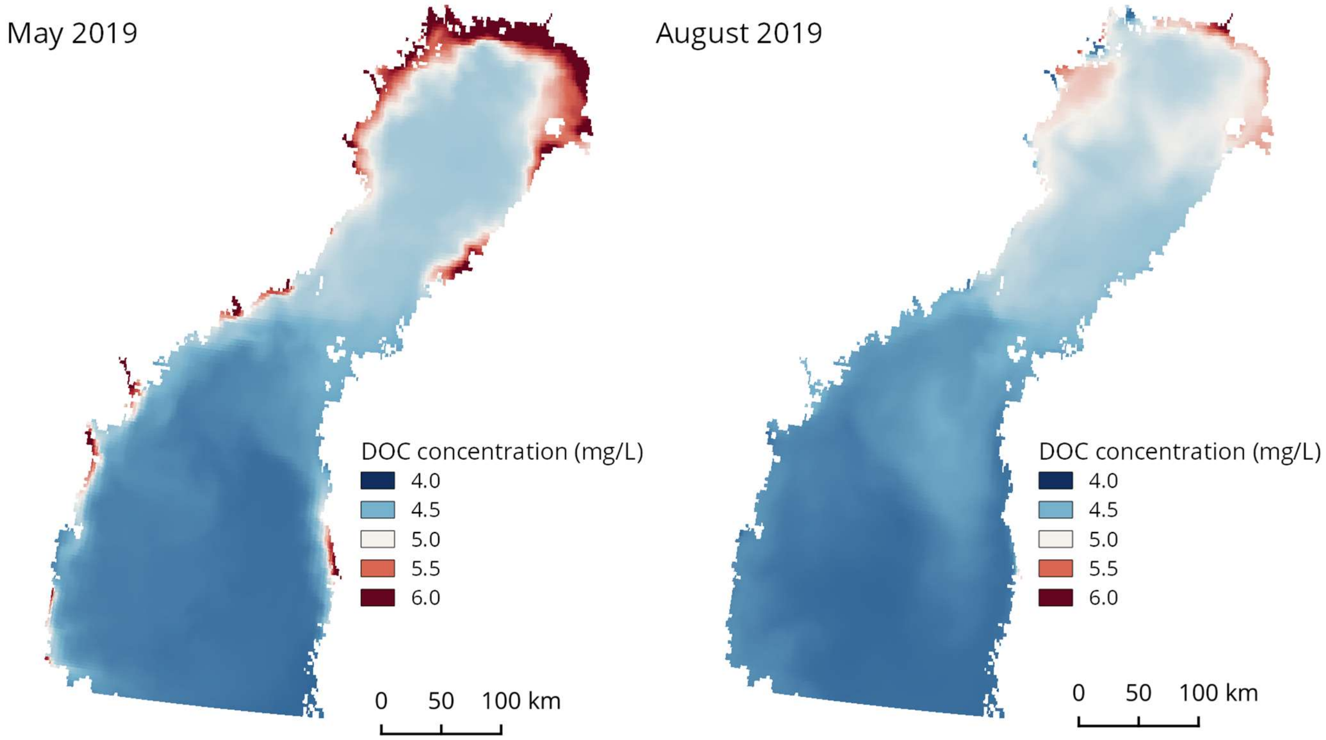


Figure 16. Average DOC distribution in May (left) and August (right) 2019.

Table 2. Average aCDOM of the Neva bay (NB) and Inner Neva estuary (INE) based on in situ measurements and aCDOM estimated by EO in the SeaLaBio extraction area of the Neva Bay. aCDOM(442) was converted to aCDOM(400) by assuming a slope factor of 0.018 1/nm. p95 in 95th percentile.

	Ylöstalo et al. (2016) Mean (min - max)	Aarnos et al. (2012) Mean (min - max)	p95 of extraction area Mean of 2018-2019
aCDOM(442) 1/m	2.28 (1.39 - 3.77)	1.89 (1.38 - 2.29)	-
aCDOM(400) 1/m	4.56 (2.78 - 7.54) Calculated from aCDOM(442)	3.78 (2.76 - 4.58) Calculated from aCDOM(442)	7.27
Sampling location	NB in Figure 17	In the INE area in Figure 17	See Figure 17

Figure 17. The Neva Bay (NB) sampling station location used by Ylöstalo et al. (2016) (left) and the SeaLaBio EO extraction area of Neva Bay (right, red area). Sampling in Aarnos et al. (2012) was conducted in the Inner Neva estuary (INE). The Saint Petersburg Ring Road, which goes through Kotlin Island, is shown in both figures.

The aCDOM estimated by EO was somewhat higher than presented in the literature. This can be due to 1) overestimation of aCDOM by the EO algorithm, 2) aCDOM has increased after the in situ samples were taken and 3) observation areas were different. The estimation accuracy of the EO algorithm could not be validated, because in situ aCDOM data was not available from the SeaLaBio study years.

The in situ observations of Ylöstalo et al. (2016) and Aarnos et al. (2012) were taken 11 - 14 years before the SeaLaBio study and aCDOM level may have changed during this period. The study period in Ylöstalo et al. (2016) was from mid-April 2005 to late-January 2006. In Aarnos et al. (2016) water samples were taken in March, July and September in 2006-2007. The SeaLaBio EO observation were from 2018-2019 and covered the April-October period. The CDOM level in the Inner Neva estuary (INE) was lower than in the Neva bay (NB) probably due to mixing of river water with sea water (Table **2**). The extraction area has pixels closer to river mouth when compared to the location of the NB sampling station of Ylöstalo et al. (2016). In these pixels aCDOM can be higher than at the mentioned NB sampling station.

3.7 River in situ aCDOM vs. estuary EO aCDOM

In order to find out the correspondence between extraction area aCDOM and river aCDOM, a comparison was made in five river estuaries on the Finnish side of the Bay of Bothnia. Good correspondence means that aCDOM load is estimated accurately with the SeaLabio method.

The in situ data was obtained from the water quality (VESLA) and hydrology (HYDRO) databases of the Finnish Environmental Administration and estuary aCDOM (95th percentile) from the extraction areas (Figure 18, Figure 19, Figure 20). The River Kemijoki figure (Figure 18) also includes the monthly average discharge used in the ERGOM model. Only river Tornionjoki is in natural state, the rest of the rivers are regulated for the needs of hydroelectric power plants. The rivers and their extraction areas are shown in Figure 21.

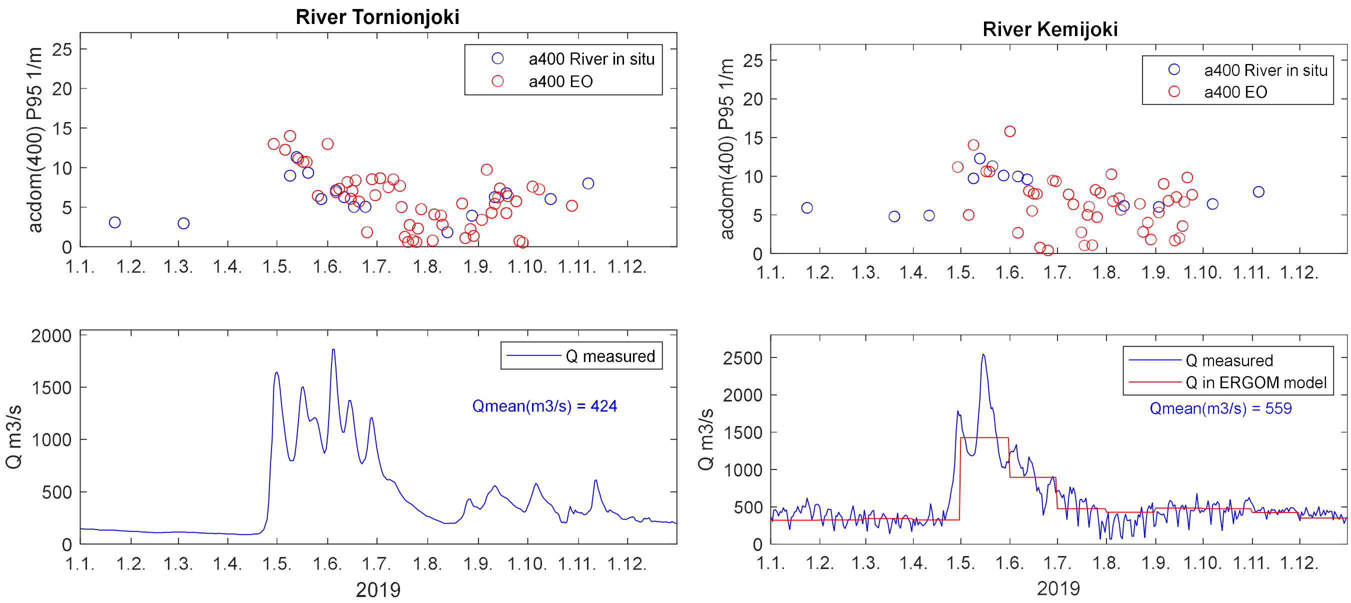


Figure 18. aCDOM measured in situ at the river load monitoring station and in the EO extraction area, and measured discharge (Q) in River Tornionjoki (left) and River Kemijoki (right) in 2019. For River Kemijoki, the discharge (monthly mean) used in the ERGOM model is shown.

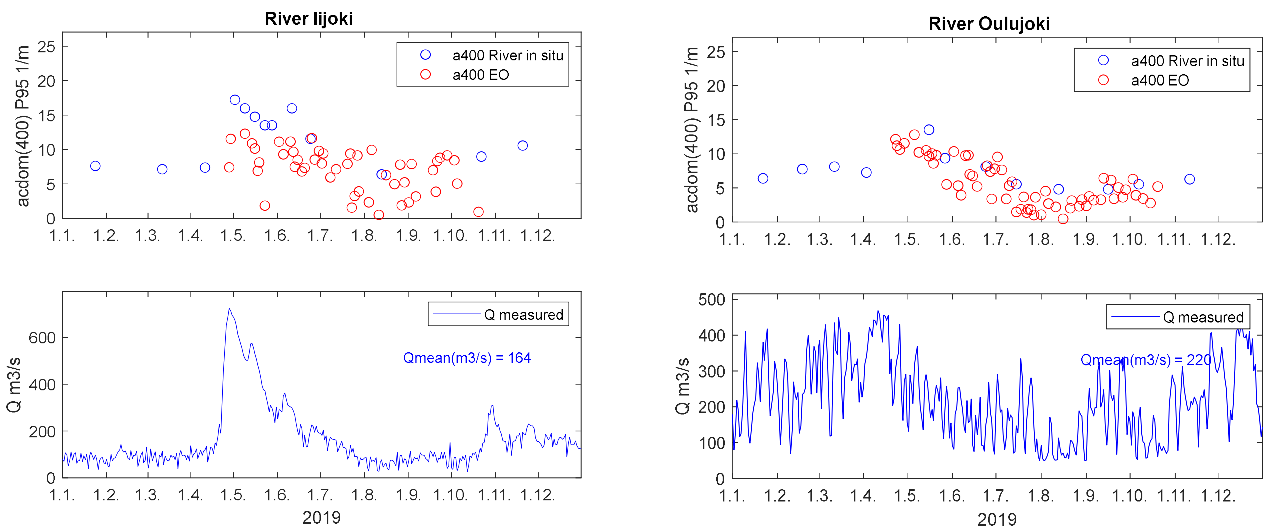


Figure 19. aCDOM measured in situ at the river load monitoring station and in the EO extraction area, and measured river discharge (Q) in River Iijoki (left) and River Oulujoki (right) in 2019.

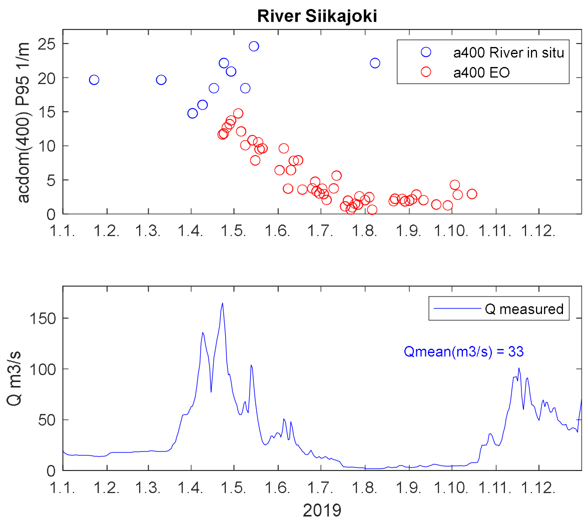


Figure 20. aCDOM measured in situ at the river load monitoring station and in the EO extraction area, and measured river discharge (Q) in 2019.

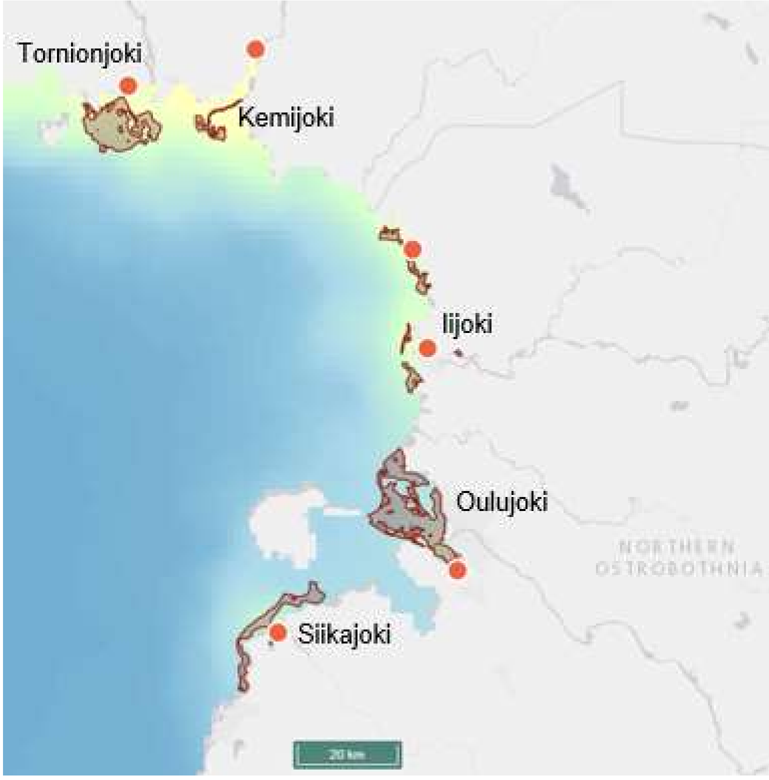


Figure 21. Extraction areas of Tornionjoki, Kemijoki, Iijoki, Oulujoki and Siikajoki rivers on the Finnish coast in the Bay of Bothnia. Red dots are load points in the ERGOM model.

The correspondence in the three largest rivers Tornionjoki, Kemijoki and Oulujoki is good (Figure 18 and Figure 19). There is some clear underestimation by EO, but these can be excluded in the future by constraining the selection of the p95 value. The possible other discrepancies can be due to problems with the EO algorithm and/or that the P95 value of the extraction area does not represent the river water quality. In the large rivers the extraction area extends close to the river mouth, which together with high discharge, ensures that EO aCDOM represents river water. In the smallest river, Siikajoki, the estuary is open towards the pelagic areas and due to the exclusion of shallow areas, the extraction area does not extend close to the river mouth (Figure 21). Therefore, the EO aCDOM is underestimated especially in summer, when discharges are low.

3.8 TOC load of selected rivers using the SeaLaBio method

The SeaLabio method based on the EO estimation of aCDOM in estuaries and monthly river discharges can also be used for the estimation of TOC loads from land. Within HELCOM, the Pollution Load Compilation (PLC) project is missioned to supply the most up-to-date information on land-based input of selected substances to the marine environment, their sources and pathways. These substances are TN (and dissolved N), TP (and dissolved P), hazardous substances and organic matter, which countries report (annual loads) to HELCOM. Organic matter is reported as TOC, in few cases as Chemical oxygen demand (COD). The PLC-recommends that the number of water samples in the rivers should be > 12/year. The reported river loads are stored in the PLC database (http://nest.su.se/helcom_plc/).

In practice only Sweden, Finland and Estonia report organic matter (as TOC) loads to HELCOM regularly. Recently, here has been growing interest of TOC load in the PLC due to climate change. Regular information on organic carbon load would also support modelling of organic carbon dynamics in the Baltic sea. Fransner (2018), for example, had to simulate years 1996-2000 instead of more recent years due to lack of load data. We demonstrated the potential of the SeaLaBio method by calculating the TOC load for eight largest rivers of the Baltic sea (Figure 22). The monthly mean TOC concentration was obtained from the aCDOM of the EO extraction areas and mean river discharge from the ERGOM model. Annual TOC loads were obtained by summing the calculated monthly loads. The aCDOM(400) was converted to TOC (mg/l) by TOC = 0.78 * aCDOM(400). This ratio was based on in situ measurement in Tornionjoki and Kiiminkijoki (Finnish side of the Bay of Bothnia) with corresponding aCDOM(400) levels of 6 and 17 1/m.

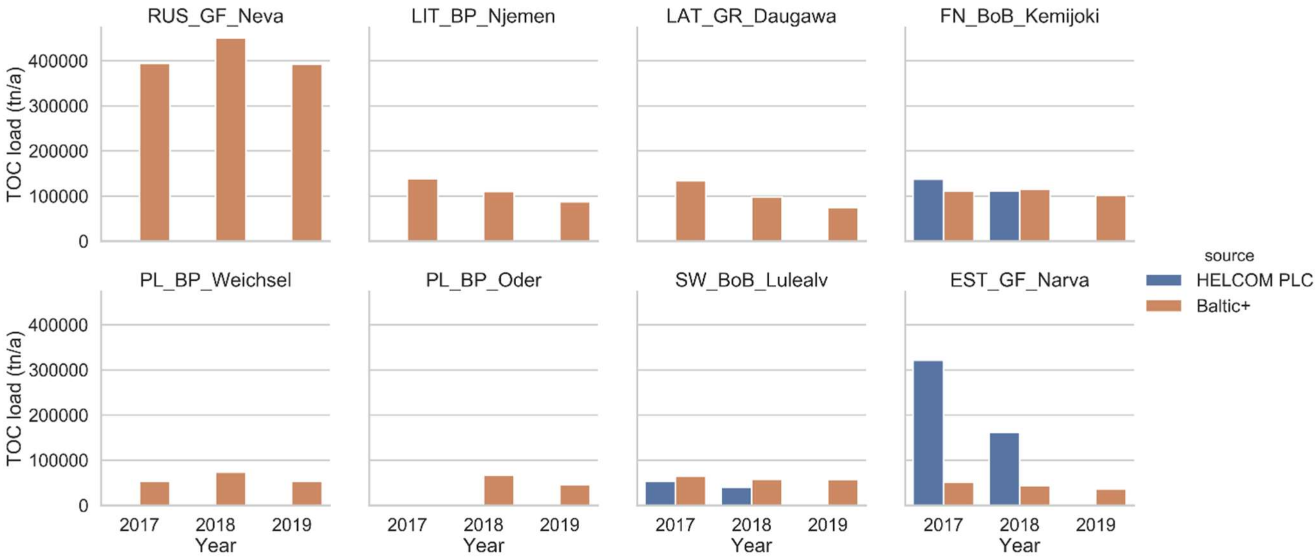


Figure 22. Annual TOC load estimated by the SeaLabio (Baltic+) method and available in the HELCOM PLC database in eight largest rivers of the Baltic sea (ranking by https://www.worldatlas.com/articles/the-major-rivers-draining-into-the-baltic-sea.html) in 2017-2019.

Only three rivers out of eight were reported to HELCOM in 2017-2018 (Figure 22). Deadline for reporting the 2019's loads to HELCOM is December 2020. The correspondence between reported and SeaLaBio estimated TOC loads are good in Rivers Kemijoki and Lule Alv. In river Narva load was clearly underestimated by EO. This can be due to the fact that Narva estuary is open. Therefore, river waters are effectively mixed with sea water and the extraction area, which is located at some distance from the river mouth due to the exclusion of shallow areas, hardly includes any river water.

The advantages of the SeaLaBio TOC load estimation method are:

- Load estimates can be obtained for all rivers with extraction areas.
- Load estimates are available sooner than in the HELCOM PLC database.
- The number of concentration estimates, that the load calculations are based on, can be higher in the EO based estimations than in the water sampling-based load estimations.
- The improved method could be used to fill caps in the estimation of TOC load to the Baltic Sea.

The SeaLaBio TOC load method could be improved by:

- More detailed selection of the extraction areas. In some coastal area several rivers are combined to one load point. In these cases, each river should have their own extraction area. In some estuaries the extraction area could probably situate in the river instead of estuary (e.g. River Narva).
- More aCDOM in situ measurement are needed for EO validation in various parts of the Baltic Sea, especially in the estuaries.
- Simultaneous aCDOM and TOC(DOC) in situ measurements in estuaries/rivers are needed to find out the conversion factors in different river types in various parts of the Baltic sea.

4 Impacts of new developments

4.1 Biogeochemical modelling in the Baltic Sea

Photosynthetically active radiation (PAR) is the driver for all biogeochemical processes in marine ecosystems and especially, in the ERGOM model. PAR controls the primary production and therefore, the energy flow in the system. The PAR climate in marine ecosystems is regulated by absorption properties of pure water and optically active substances in the water. CDOM could have an important impact on absorption mostly in coastal waters where terrestrial CDOM dominates. The Baltic Sea, and especially the northern parts, is a marine ecosystem with high CDOM loads of terrestrial origin. The CDOM effect on light is obvious from Secchi depth data which range from the order of 1m in the North up to 20 m the Kattegat area while in the open ocean the Secchi depth is deeper than 50 m.

Getting the PAR climate right is essential for ecosystem models. Different approaches are used, e.g. water body classes, salinity dependent parametrizations, and fixed absorption for different regions. The most obvious approach, modeling CDOM explicitly, is hampered by the lack of high quality riverine CDOM loads data, especially since the salinity parametrization delivers reasonable results.

However, since high resolution EO satellites are in operation, CDOM loads in a sufficient high quality can be derived from EO products. The new developments in SeaLaBio use such data to force the Baltic Sea model ERGOM. This approach has some advantages over e.g. the salinity parametrization:

- CDOM is independent on salinity, i.e. uncertainties in model salinity will not propagate into the biogeochemistry
- Different CDOM concentrations in different rivers can be considered
- The annual cycle in riverine CDOM concentration can be included

A seemingly drawback is a necessary re-calibration of some model parameters like e.g. phytoplankton growth rates. The reason is that errors in the PAR climate so far have been “delegated” into parameters of the ecosystem model. However, if we now are able to reasonably reproduce the PAR, the model has to be re-calibrated in order to be more realistic.

In the following figures, we show simulated data as annual means from year 2018. The model has been run since 1948 and has adjusted to the new CDOM formulation. In Figure 23, the light absorption difference between the new model with an explicit CDOM state variable and the model with CDOM-salinity parametrization is shown. Pronounced differences are obvious in the Bay of Bothnia and the Gulf of Finland. The higher CDOM concentration in Nordic-Baltic rivers results in higher absorption. In estuaries and river mouths, the low salinity yields unrealistic high CDOM concentrations with the CDOM-salinity parametrization seen as blue color.

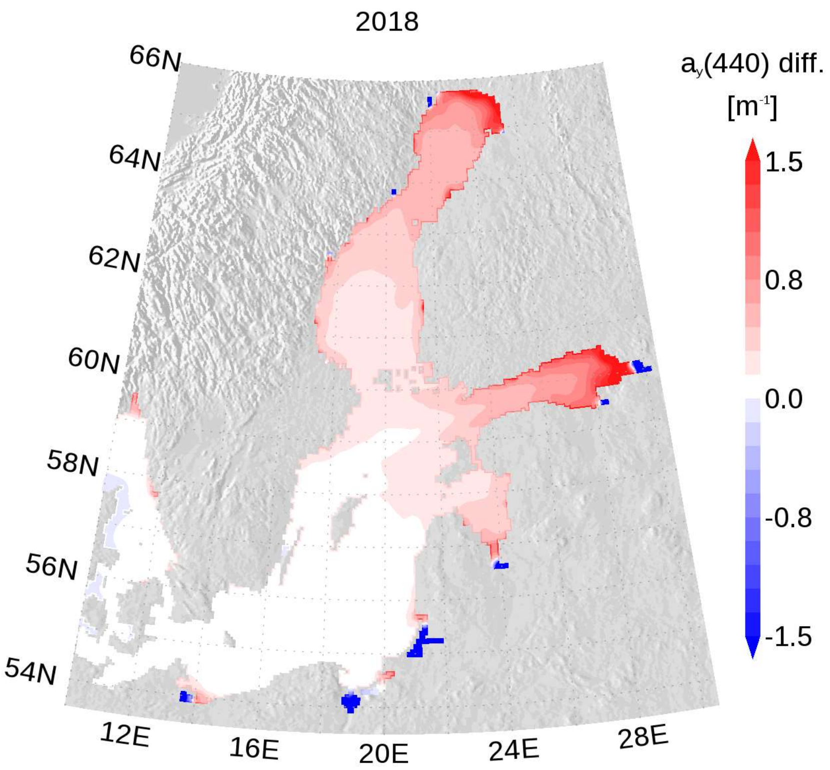


Figure 23. Differences between the CDOM absorption (at 440 nm) values of two versions of ERGOM ("new" – "old"). "new" is the model with an explicit CDOM variable and "old" the model with CDOM-salinity parametrization.

The impact of changed CDOM starts in the available light for primary production as shown in Figure 24. Available PAR is reduced in the modified model. The increased phytoplankton concentration in the surface layer is somewhat unexpected at the first glance. Also primary production is increased in the uppermost 6 m but decreased below that depth. The impact on temperature is as expected but small: Temperature increase in the upper layer and decreases below.

A possible cause-effect chain could be: Less light reduces the primary production and as a consequence more nutrients are left. Nutrient concentrations increase and nutrient limitation of primary production is less strong. Therefore, there is more phytoplankton in the surface layer where sufficient light is available but below a certain depth, less primary production occurs and phytoplankton concentration decreases. Finally, a new dynamic equilibrium establishes as seen in Figure 24.

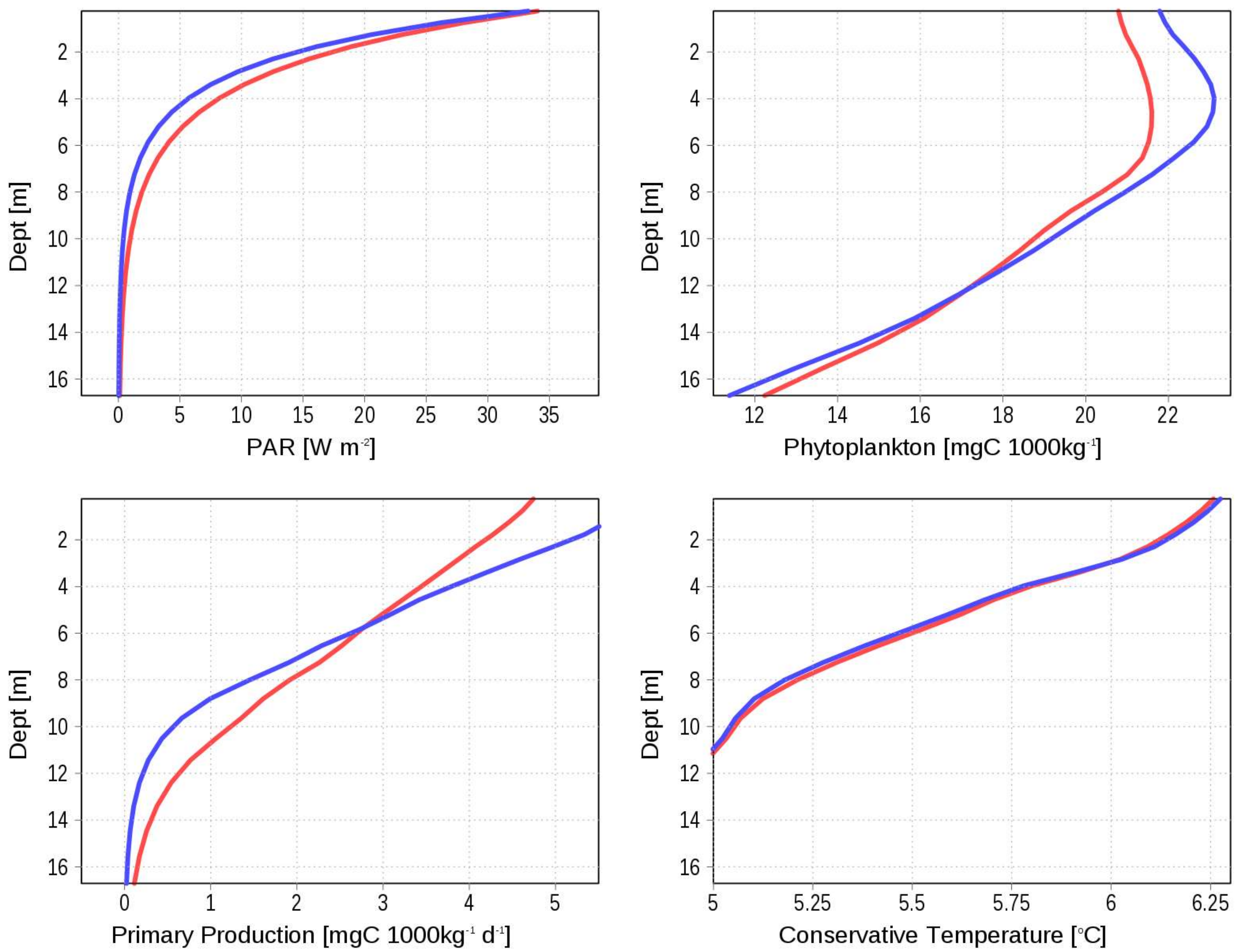


Figure 24. Annual mean profiles at a station in the Botnian Bay (22.4E; 64.6N) simulated with the "new" (blue) and "old" (red) model version.

The net effect of changed primary production can be demonstrated by changes in the bottom water oxygen concentration. Less primary production produces a reduced downward flux of organic particles and in turn less oxygen consumption. In Figure 25, changes in bottom oxygen concentration are shown. Oxygen is increased in regions with increased CDOM concentration – the Gulf of Bothnian and the Gulf of Finland.

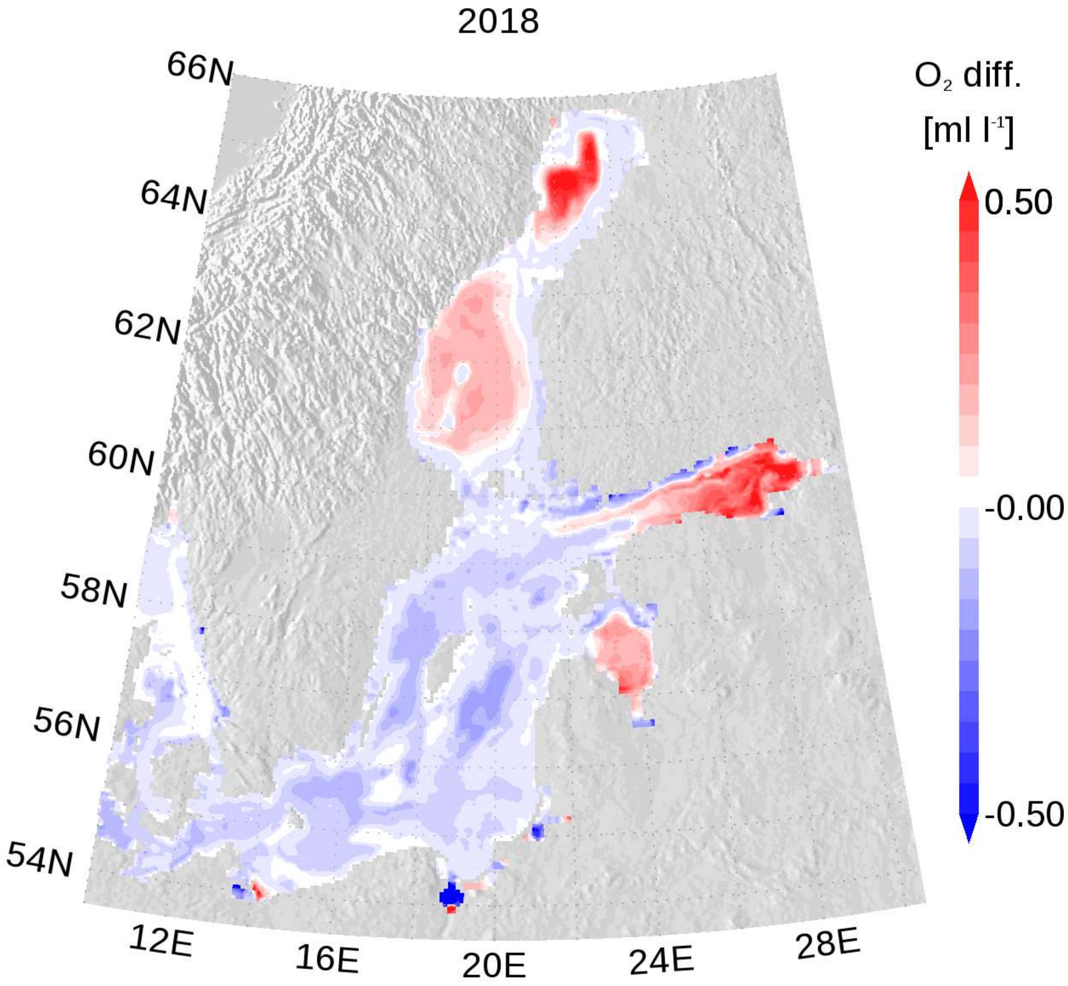


Figure 25. Bottom oxygen difference "new" - "old" model version.

The impact on nitrogen and phosphate surface concentrations is shown Figure 26. The winter concentration is increased for nutrients nitrate and phosphate. Compared with observations, nitrate values have improved but not the phosphate values. Another issue is the delayed spring bloom. The bloom starts about 10 days later in the "new" model version due to reduced PAR. This example demonstrated that the changed and improved PAR climate requires a revision of the parametrization of the impacted biogeochemical processes, starting with primary production.

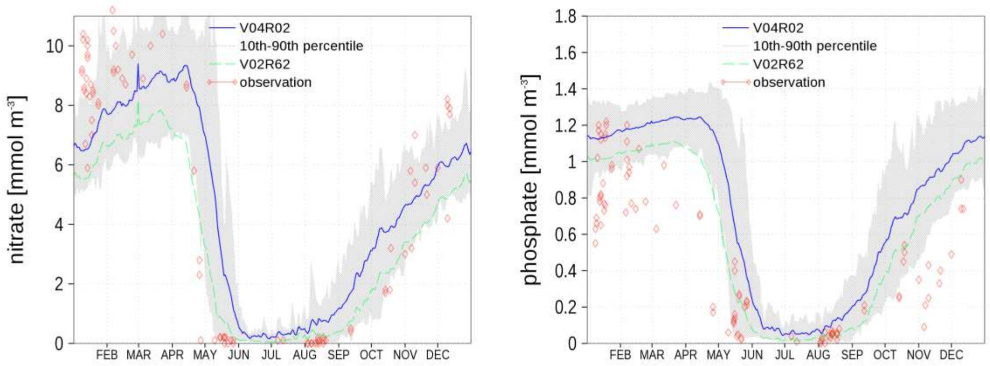


Figure 26. Surface nitrogen (left) and phosphate (right) climatology (1990-2019) at station LL5 (25.6E; 60.0N) in the Gulf of Finland. "new" model: blue, "old" model: green, observations: red.

4.2 Use of EO for the monitoring of the Baltic Sea

The SeaLaBio project has concentrated on the estimation of aCDOM from EO data and the new atmospheric correction and in-water estimation methods have improved aCDOM estimation accuracy significantly. Other water quality parameters have not yet been tested. High concentrations of CDOM have caused problems for the estimation of other parameters such as Chl-a in the past. The developments of SeaLaBio are thus expected to improve the reliability of Chl-a estimations especially in coastal regions with high CDOM. This in turn is expected to lead to more extensive information about processes such as eutrophication along the vulnerable coastline of the Baltic Sea.

As shown in Figure 22 EO can be used to estimate annual TOC loads from rivers to the Baltic Sea. The method still requires refinements (e.g. the extraction areas must be redefined in some cases) and additional in situ data to confirm the conversion factors between aCDOM and TOC in different areas and seasons. Once these are done EO can provide additional information about loading from rivers. This is especially valuable for rivers that are currently not reported according to the HELCOM recommendations.

5 Summary

The developments done in the SeaLaBio project have advanced the state-of-the-art in three important fields:

1. **Biogeochemical modelling:** The ERGOM model can now utilize EO based aCDOM values as input data and, as a result, provide more reliable estimates of light attenuation in water, which potentially provides more realistic simulations of several other state variables. This has consequences especially in the norther parts of the Baltic Sea where CDOM has a large effect on water transparency.
2. **EO data processing:** A new method for atmospheric correction of satellite images – based on combining the advantages of Polymer & C2RCC – can now provide more reliable water leaving reflectance values. This is a major step towards the formulation of an optimal AC for the Baltic Sea. When combined with a band ratio algorithm, the new processor can generate better CDOM estimates than the previous processors.
3. **Use of EO for monitoring carbon fluxes:** EO based data can e.g. provide information about the Total Organic Carbon loads from rivers.

Further improvements in all fields are still possible and even required. For example, ERGOM now requires extensive calibrations in order to further improve its reliability. EO processing algorithms will benefit from further testing and validation while the carbon flux monitoring requires more in situ data. Data fusion can be used for merging data from different sources, but requires further analysis before it can be fully included in a monitoring system. All these are discussed in more detail in the Scientific Roadmap deliverable.

6 References

Aarnos, H., Ylöstalo, P., Vähätalo, A.V., 2012. Seasonal phototransformation of dissolved organic matter to ammonium, dissolved inorganic carbon, and labile substrates supporting bacterial biomass across the Baltic Sea. J. Geophys. Res 117 (G01004). http://dx.doi.org/10.1029/2010JG001633.

Fransner, F. 2018. Organic carbon dynamics in the Baltic Sea – a modelling perspective. PhD thesis. Department of Meteorology, Stockholm University. 54 p. http://su.diva-portal.org/smash/get/diva2:1175372/FULLTEXT01.pdf

Harvey, E.T., Kratzer, S. & Andersson, A. 2015. Relationships between colored dissolved organic matter and dissolved organic carbon in different coastal gradients of the Baltic Sea. Ambio 44(3):392–401. DOI: 10.1007/s13280-015-0658-4

Heikkinen, K., 1989. Organic carbon transport in an undisturbed boreal humic river in northern Finland. Arch. Hydrobiol 117, 1–19.

Kallio, K., Attila, J., Koponen, S., Keto, V., Stelzer, K., Brockmann, C. & Philipson, P. 2019. Dataset Description. SeaLaBio project. 26 p. http://eo.ymparisto.fi/data/water/Baltic_SeaLaBio/SeaLaBio_Dataset_Description_V1.2.pdf

Mattsson, T., Kortelainen, P., Räike, A., 2005. Export of DOM from boreal catchments: impacts of land use cover and climate. Biogeochemistry 76, 373–394. https://link.springer.com/article/10.1007/s10533-005-6897-x

Ostapenia, A.P., Parparov, A., Berman, T., 2009. Lability of organic carbon in lakes of different trophic status. Freshw. Biol 54, 1312–1323.

Simis, S.G.H., Ylöstalo, P., Kallio, K.Y., Spilling, K., Kutser, T. 2017. Contrasting seasonality in optical-biogeochemical properties of the Baltic Sea. PLoS ONE 2017, 12, e0173357.

Ylöstalo, P., Seppälä, J., Kaitala, S., Maunula, P., & Simis, S. (2016). Loadings of dissolved organic matter and nutrients from the Neva River into the Gulf of Finland – biogeochemical composition and spatial distribution within the salinity gradient. Marine Chemistry, 186, 58–71. https://www.sciencedirect.com/science/article/pii/S0304420316301050