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Contents

Abstract

This document summarizes the work done in the Baltic+ SeaLaBio project. Please see the deliverables of each WP for further details.

Glossary

a400	CDOM absorption coefficient at 400 nm
a700	CDOM absorption coefficient at 700 nm
a750	CDOM absorption coefficient at 750 nm
AC	Atmospheric correction
BGC	Bio Geo Chemical
C2RCC	Case 2 Regional Coast Color
CDOM	Coloured Dissolved Organic Matter
Chl a	Chlorophyll a
CMEMS	Copernicus Marine Environment Monitoring Service
DOC	Dissolved Organic Carbon
EO	Earth Observation
ERGOM	Ecological Regional Ocean Model
HELCOM	Helsinki Commission
IOP	Inherent Optical Properties
ISM	Inorganic suspended solids
MERIS	Medium Resolution Imaging Spectrometer
MODIS	Moderate Resolution Imaging Spectroradiometer
MSI	MultiSpectral Instrument
N	Number of samples
NIR	Near infrared
NN	Neural Network
OLCI	Ocean and Land Color Imager
POLYMER	POLYnomial based algorithm applied to MERIS
PtCo	Pt water colour
RMSE	Root Mean Square Error
S2	Sentinel-2
S3	Sentinel-3
SAG	Scientific Advisory Group
Sal	Salinity
SDT	Secchi disk transparency
SSTS	Sea surface temperature, measured using a water sampler
SSTC	Sea surface temperature, measured with CTD
TOA	Top of Atmosphere
TOC	Total Organic Carbon
TSM	Total Suspended Matter

List of Symbols

Symbol	Definition	Dimension/Unit
a_{CDOM}	Absorption coefficient of CDOM	m^{-1}
$\rho_{Rc}(\lambda)$	Rayleigh corrected signal	dimensionless
$\rho_w(\lambda)$	Marine reflectance	dimensionless
$\rho_{wn}(\lambda)$	Marine reflectance, normalized	dimensionless

1 Introduction

The Sea-Land biogeochemical linkages (Baltic+ SeaLaBio) project was designed to find answers to the following research question:

- Can we quantify the carbon flux from land to sea with Sentinel-3 (S3) OLCI and Sentinel-2 (S2) MSI data in the Baltic Sea region? And if not, what are the main obstacles and potential solutions to be addressed in the future?

With this in mind the overall objective of the project was defined as:

- Develop methods for assessing carbon dynamics and eutrophication in the Baltic Sea through integrated use of **Earth Observation (EO), biogeochemical (BGC) models, and ground-based data**

This requires scientific development in the topics outlined in Figure 1. The generation of information about carbon dynamics and eutrophication from satellite images in the Baltic Sea requires improvements in atmospheric correction and in-water algorithms. Furthermore, the synergistic use of EO and models requires modifications in models and generation of new kind of information from EO.

The work package structure and logic of the study is shown in Figure 2 together with the technical deliverables. The following chapters describe the objectives, actions and results of each work package.

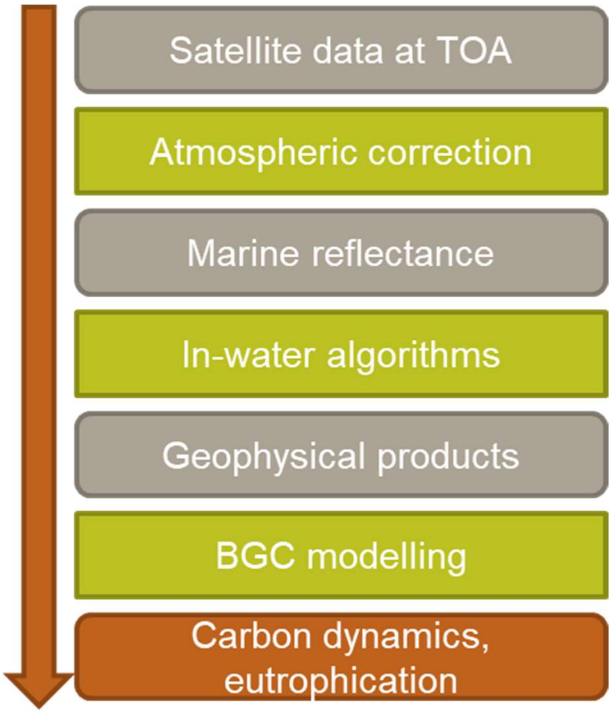


Figure 1. The main processing steps (in green) and the information required (in grey) to generate information about carbon dynamics and eutrophication from satellite data and biogeochemical models.

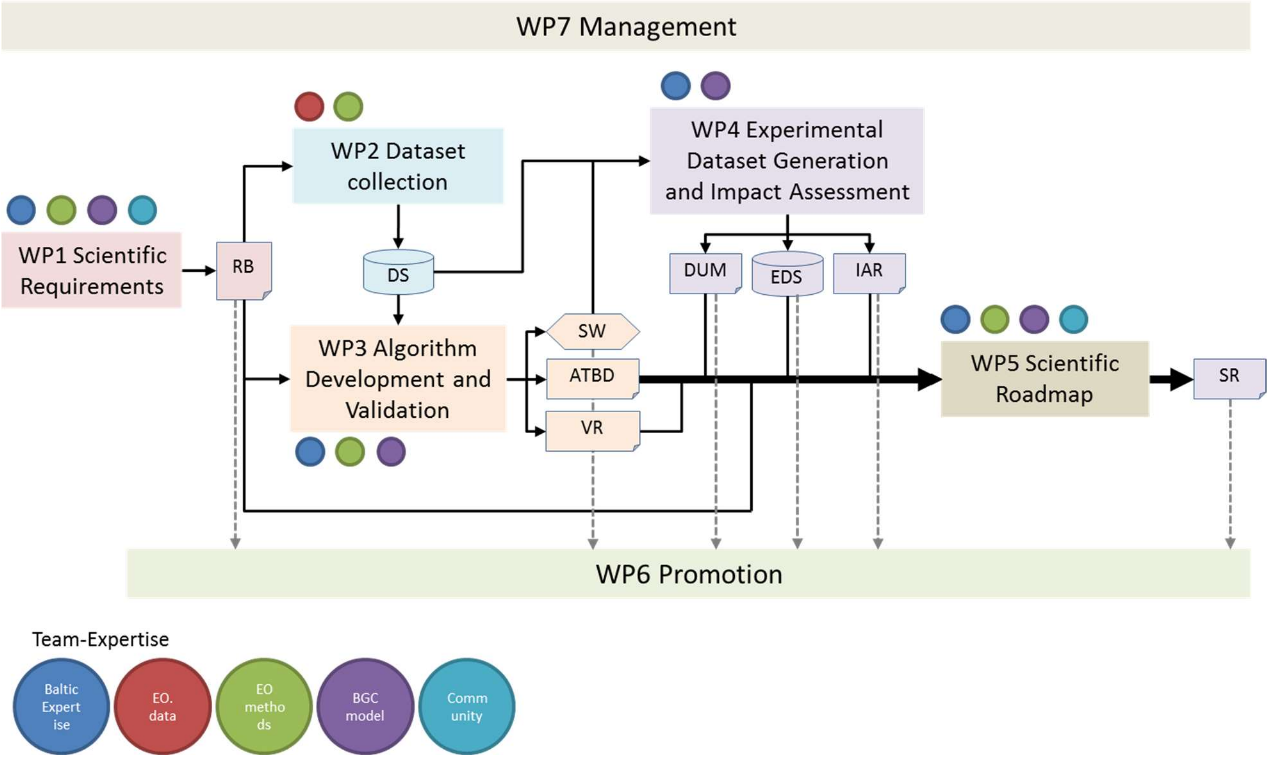


Figure 2. Work logic of the Baltic+ SeaLaBio–project. The deliverables mentioned in the figure are: RB = Requirements Baseline, DS = (Input) Dataset (including Dataset Description), SW = Software, ATBD = Algorithm Theoretical Basis Document, VR = Validation Report, EDS = Experimental Dataset, DUM = Dataset User Manual, IAR = Impact Assessment Report, SR = Scientific Roadmap.

2 WP1 Scientific Requirements

2.1 Objectives

The main objectives of the WP were:

- Review the scientific challenges of the project for the following main topics: Atmospheric correction, in-water retrieval and BGC-models.
- Review available data and related recent studies and perform an initial risk analysis.
- Define the preliminary scientific requirements for and activities to be carried out in WPs 2-6

2.2 Main results

The results are described in detail on the following deliverable:

- **Requirements Baseline** describes the review of scientific challenges, available datasets and related activities, and the preliminary scientific requirements.

Table 1 presents a summary of the preliminary scientific requirements divided into Work Packages. The main goal is to develop methods for monitoring terrestrial DOC fluxes to the Baltic Sea. The study logic is the following:

- Improve methods (atmospheric correction and in-water inversion) that estimate CDOM and other parameters from EO data, especially near river mouths
- Determine the links between TOC, DOC, & CDOM based on literature and existing data
- Utilize river CDOM at test sites as input data in ERGOM in order to improve the model. This gives information about what happens to terrestrial carbon in the Baltic Sea.

Table 1. Preliminary Scientific Requirements of SeaLaBio.

WP	Scientific Requirements
WP 2 Dataset collection	- Ensure that the quality and quantity of in situ data is sufficient for the validation in WP3
WP 3 Algorithm Development and Validation	- Improve atmospheric correction to the level that allows in-water algorithms to provide reasonable concentration estimates for Chl-a, CDOM and other parameters relevant for carbon flux studies in the selected test sites (quantified requirement to be defined during WP3). - Improve in-water algorithms as above concentrating on the carbon fluxes originating from land. - Adapt the ERGOM model to have a finer resolution (1 n.m.) and, therefore, allow for better representation of the coast – open sea CDOM gradient.
WP 4 Experimental Dataset Generation and Impact Assessment	- Data shall be available for time periods as long as possible and cover the vegetation period from March to October
WP 5 Scientific Roadmap	- Based on the results and in consultation with the Scientific Advisory Group and other stakeholders define the goals for further scientific activities after the project (2020-21). - Generate guidelines for ensuring the quality and quantity of in situ data for future EO missions and studies.

3 WP 2 Dataset Collection

3.1 Objectives

The main objectives of the WP were

- Collect in situ and EO data needed for algorithm development, BGC model adaption and impact assessment from various sources.
- Publish the dataset and its description through the project website

3.2 Main results

The results are described in detail in the following deliverable:

- **Dataset Description** describes the EO and in situ data collected during WP2. It also includes instructions where the open access data used in the project can be obtained.

The amount of available in situ data varied a lot depending on the water quality parameters. Figure 3 shows the number of samples in the test dataset for each water quality parameter while Figure 4 shows the locations of the stations. As can be seen there is a lack of data especially about CDOM absorption coefficient (a400, a440, etc.) and DOC (Dissolved Organic Carbon). Furthermore, absorption coefficient data is available only along the Finnish coast and the northern coast of Sweden. This limits the geographical scope of the analysis and should be addressed in future monitoring activities.

Most of the openly available in situ data used in the SeaLaBio can be downloaded as excel files from http://eo.ymparisto.fi/data/water/Baltic_SeaLaBio/.

The EO data used in SeaLaBio is publicly available from the Copernicus services and not replicated here. For downloading the data see instructions in Table 1 of the Dataset Description.

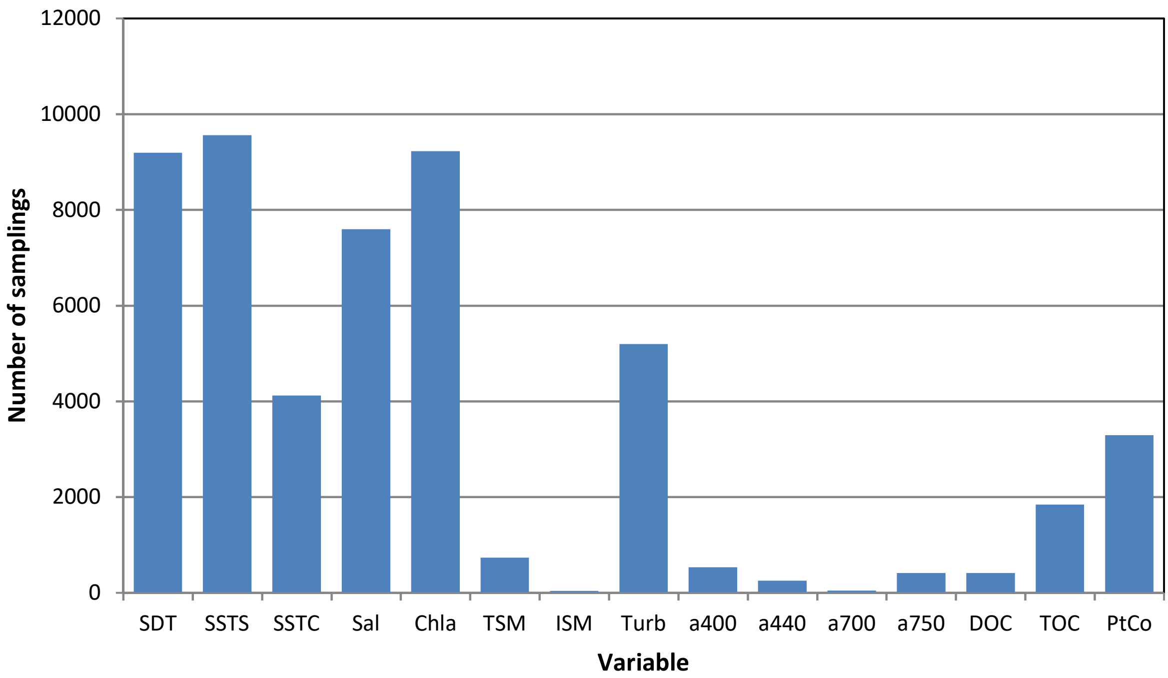


Figure 3. Total number of observations in the SeaLaBio in situ dataset (2015 – 2018, April-October, routine monitoring measurements based on sampling at fixed stations). See the Glossary for details about the parameter names.

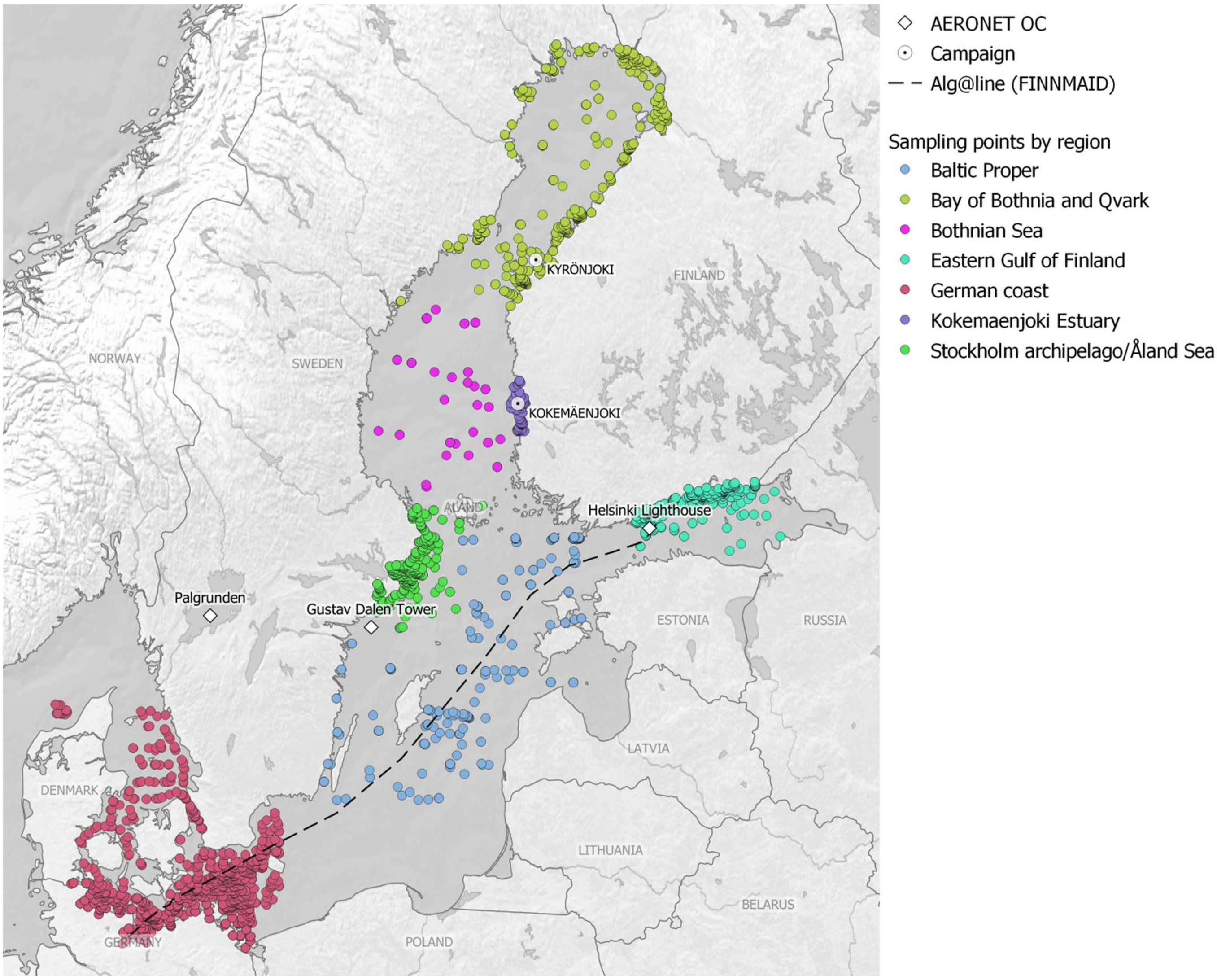


Figure 4. Location of in situ stations included in the SeaLaBio dataset. These stations had at least one measurement of at least one of the SeaLaBio variables.

4 WP 3 Algorithm Development and Validation

4.1 Objectives

The main objectives of the WP were to:

- Develop a new atmospheric correction method (for S2-MSI and S3-OLCI) for the Baltic Sea with utilizes the strengths of POLYMER and C2RCC processors.
- Build a Baltic Sea water model that can be used to develop in-water algorithms that convert atmospherically corrected reflectances into water quality parameters. As a backup, define empirical algorithms.
- Perform modifications to the ERGOM model which improve its spatial resolution and allow aCDOM values to be used as forcing data.
- Validate the EO and model results with in situ data from WP2.
- Implement and test a software prototype of the processor.

4.2 Main results

The results are described in detail on the following deliverables:

- **Algorithm Theoretical Basis Document (ATBD)** describes the scientific developments performed in WP3, including atmospheric correction, in-water algorithms, and model modifications.
- **Validation Report** provides the results of the validation activities of WP3.

For the atmospheric correction (AC) we combined the strengths of the C2RCC and POLYMER processors. The Neural Network approach can aggregate a large knowledge about natural variability (range, covariance) found in the optical properties of water in the Baltic Sea with a dedicated training for this purpose. The POLYMER processors in turn can account for atmospheric affects due to its polynomial modelling. Figure 5 shows an example of the correction in a case of brighter waters and turbid plumes near the estuary of the Kokemäenjoki river. Results for POLYMER and C2RCC are also shown. Comparison between Rayleigh corrected signal, ρ_{Rc}, and the aerosol signal identified by Baltic+ AC, ρ_a and the corrected signal, ρ_w, shows the challenges in decoupling the atmospheric and marine part. Baltic+ AC manages to provide a smooth map of reflectance with realistic amplitude on the whole scenes. All undetected clouds, visible on ρ_{Rc} map are well corrected by the Baltic+ AC and POLYMER: their contribution is set to ρ_a, and the underlying marine reflectance looks realistic compared to the neighboring pixels. On the contrary, these undetected clouds degrade performance of C2RCC, which underestimates ρ_w. This shows that the polynomial model from POLYMER, used in the Baltic+ AC, is robust to such contamination. Baltic+ provides the most contrasted map of reflectance, with relatively low value offshore (purples) while the plume is well captured, contrary to POLYMER.

For in-water inversion a neural network-based method was developed. The NN was trained with a reflectance database simulated with an optical model defined for the Baltic Sea. Several different architectures were tested. However, the NN method was not able to reach the estimation accuracy of the empirical band ratio algorithm using the Baltic AC corrected data.

In order to assess the performance of the full processing chain (AC & in-water algorithm) a matchup analysis with OLCI data was performed. Various reflectance band ratios were tested, and the best correspondences were found with band ratios B8/B6 (665 nm/560 nm) and B11/B6 (709 nm/560 nm). With both ratios there is a clear improvement in correlation compared to the C2RCC results. For further analysis the ratio B8/B6 was selected since B11 still had some uncertainties in the aerosol estimation. Figure 6 shows the corresponding scatter plot. The calibration equation for this case is:

$$a_{CDOM}(400nm) = 4.85 * \left(\frac{\rho_{wn}(665nm)}{\rho_{wn}(560nm)}\right) + 0.65 \quad (1)$$

The AC processor has been made available through the GitHub. A SNAP plug-in has also been created.

The ERGOM model was modified by increasing the spatial resolution from 3 n.m. to 1 n.m. This has the effect of increasing the processing time by a factor 27 (significant demand for additional computing resources). In addition, a salinity based aCDOM estimate is now replaced by a new CDOM state variable, which allows external CDOM values to be used as forcing data.

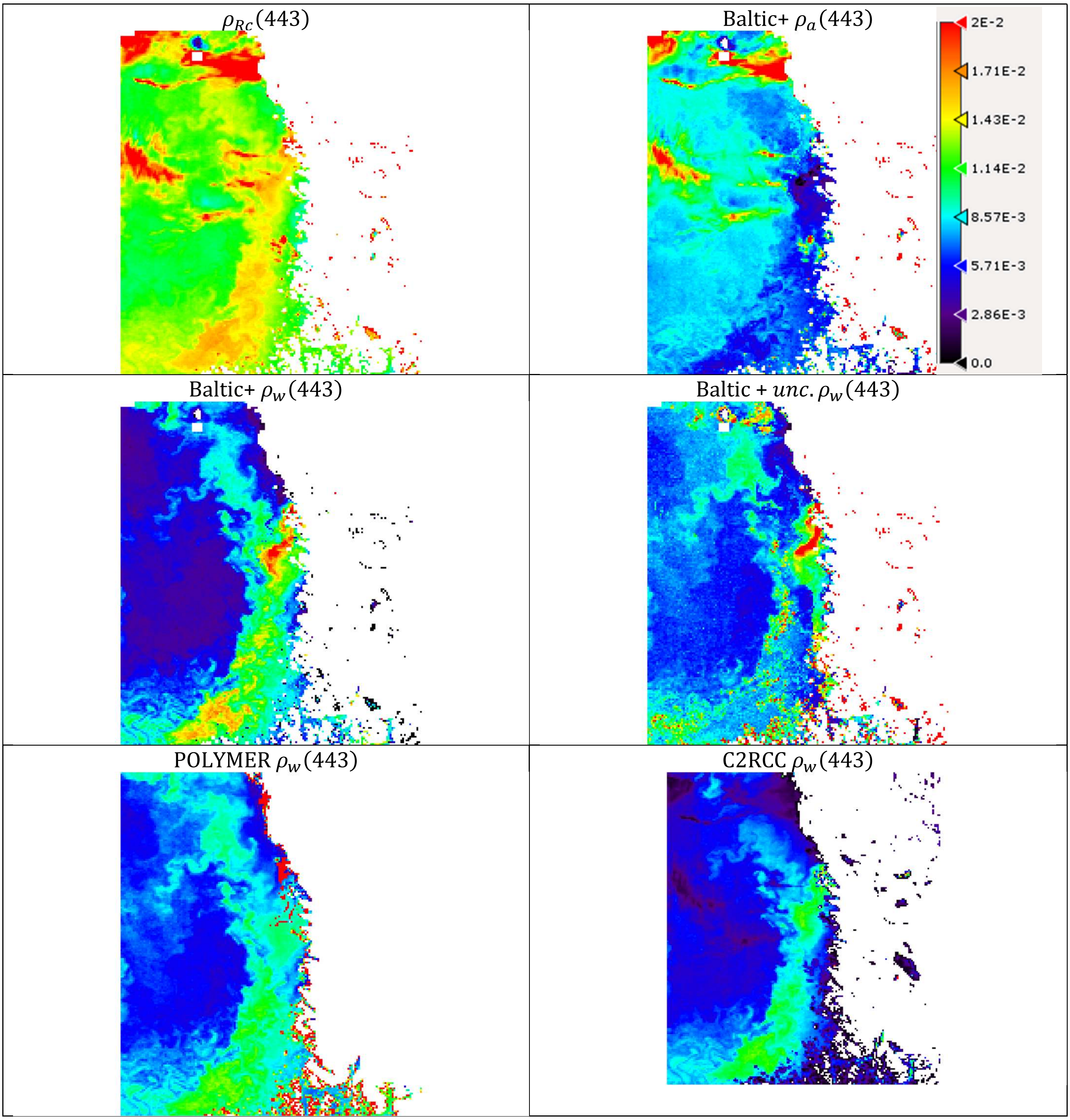


Figure 5. Analysis of Baltic+ AC on the estuary of the Kokemäenjoki river (OLCI-B, 20190415. Same colour scale for ρ_{Rc}, ρ_w and $unc.\rho_w$ (top right colour bar). Band 443 nm.

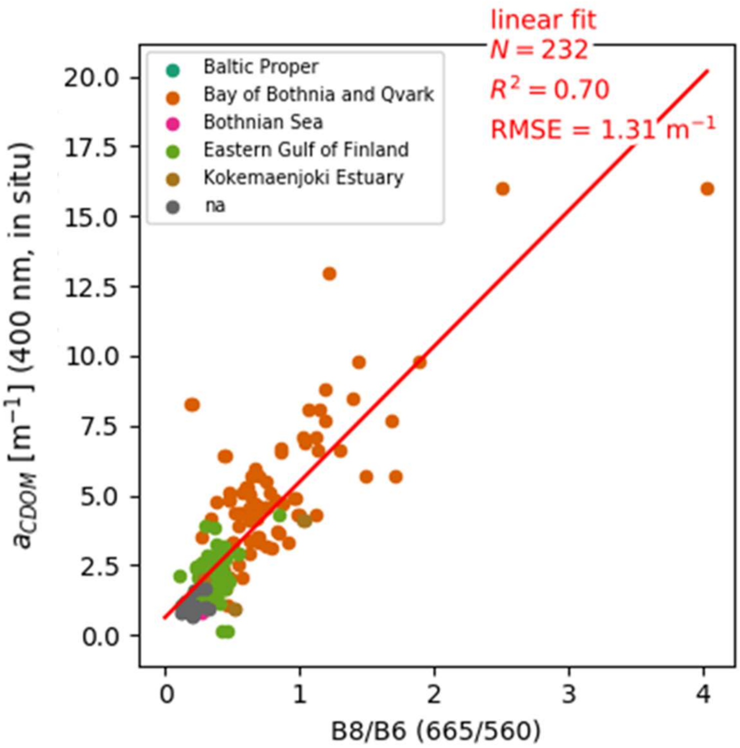


Figure 6. Sentinel-3 & Baltic+ reflectance band ratios vs. in situ aCDOM. Note that the wavelength used in the CDOM absorption coefficient is 400 nm.

5 WP 4 Experimental Dataset Generation and Impact Assessment

5.1 Objectives

The main objectives of the WP were to:

- Generate and publish a dataset of EO based data and model results.
- Compare the results with comparable products from existing services (CMEMS) or other satellite (MODIS, VIIRS), or other algorithms (e.g. OLCI Level 2 products)
- Analyse the further adaptations needed to ERGOM.
- Quantify unknown or poorly known terrestrial CDOM sources.

5.2 Main results

The results are described in detail on the following deliverables:

- **Dataset User Manual** describes the generated and published datasets and the methods to access them.
- **Impact Assessment Report** analyses the results and their relation to the state of the art.

The EO algorithms developed in WP3 were used to generate monthly aCDOM composites for April to September of years 2017-2019. These were then published in the TARKKA service (www.syke.fi/tarkka/en). An example of this is shown in Figure 7a.

The ERGOM model was run with EO based aCDOM values as forcing data. The results show a clear improvement in the CDOM values especially in the coastal areas of the Bay of Bothnia where the aCDOM values are high. Figure 8 shows a comparison of the new values against in situ data from stations along the coast of Finland and Northern Sweden. Figure 9 shows time series plots where the result of the new method can be compared with the salinity-based method and in situ observations. These show strong improvement in the Bay of Bothnia and the Gulf of Finland, while both methods overestimate the values in the south. Figure 10 shows the difference between the old and the new methods and Figure 7b shows an example product in TARKKA.

Baltic Sea countries should report annual loads of TN (and dissolved N), TP (and dissolved P), hazardous substances and organic matter (Total organic carbon (TOC) or Chemical oxygen demand (COD)) from their rivers to the Pollution Load Compilation (PLC) maintained by HELCOM. However, in practice only Sweden, Finland and Estonia report organic matter loads regularly. There is a growing interest of TOC load in the PLC project due to climate change and we analysed how EO could provide a solution to the monitoring problem. By using the EO based aCDOM values derived for ERGOM input locations, river discharge information, and an empirical relationship between aCDOM and TOC, we estimated the TOC loads of the eight largest rivers in the Baltic Sea. These are shown together with the available reported information for 2017-2019 in Figure 11. The PLC only contains data for three rivers. In two of them there is good agreement with EO and in situ-based methods. In the third, the likely reason for the underestimate in the EO values is due to the location of the extraction area, which may not represent well the water coming from the river.

Other datasets of EO-based CDOM were not available in CMEMS or other sources. Thus, these could not be compared to SeaLaBio results.

For data access the following methods have been utilized:

- **TARKKA** (www.syke.fi/tarkka/en) is a public service provided by the Finnish Environment Institute for browsing and viewing SYKE's open satellite data. The map application is designed to display satellite imagery at both high resolution (10 m – 60 m) and moderate resolution (300 m – 1 km) and allows the user to overlay and combine various other datasets with EO products.

- **Data interfaces** (machine to machine) are standardized ways to share data so that a user can access the information without downloading the data as a file in the local environment.

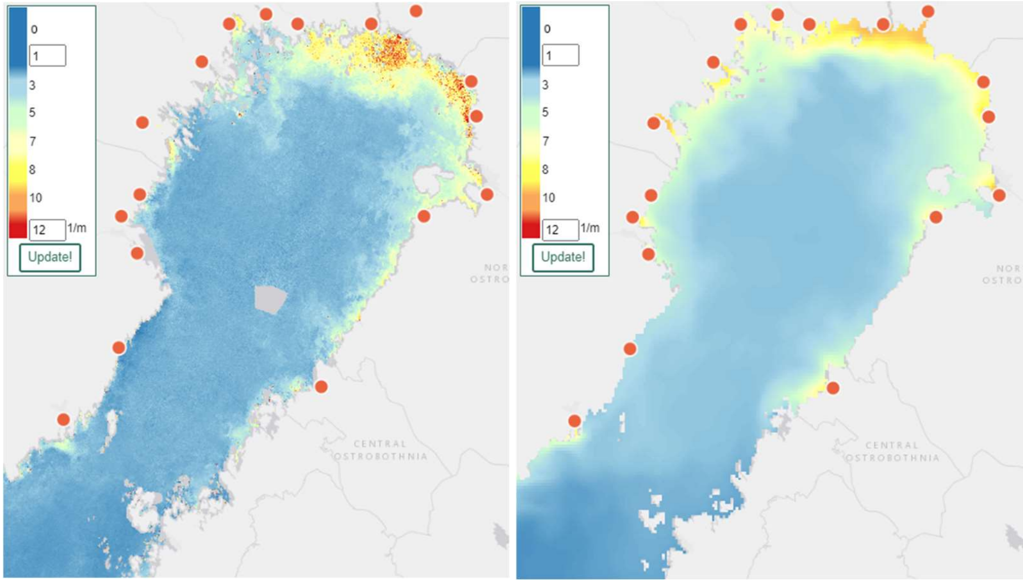
- **SYKE's EO Web Accessible Folder** (EO-WAF) located at eo.ymparisto.fi/data/water/Baltic_SeaLaBio/.

As a summary of the impacts, 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. A band ratio algorithm based on Baltic+ AC results was established and provided better aCDOM values than the other current 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.



(a) (b)

Figure 7. (a) Sentinel-3 OLCI one-month composite of aCDOM (at 400 nm) for May 2019 derived with a band ratio B8/B6 after atmospheric correction with the Baltic+ AC. (b) aCDOM (at 400 nm) simulated with ERGOM for May 2019.

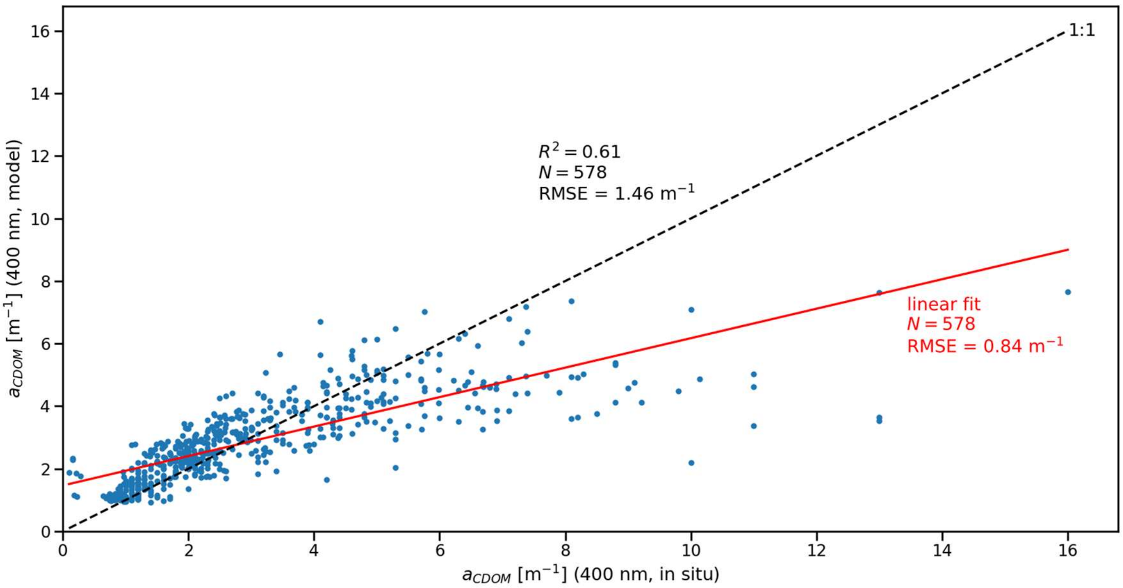


Figure 8. In situ aCDOM vs. ERGOM aCDOM simulated using the 75th percentile EO values as input data at monitoring stations in the Northern Baltic Sea.

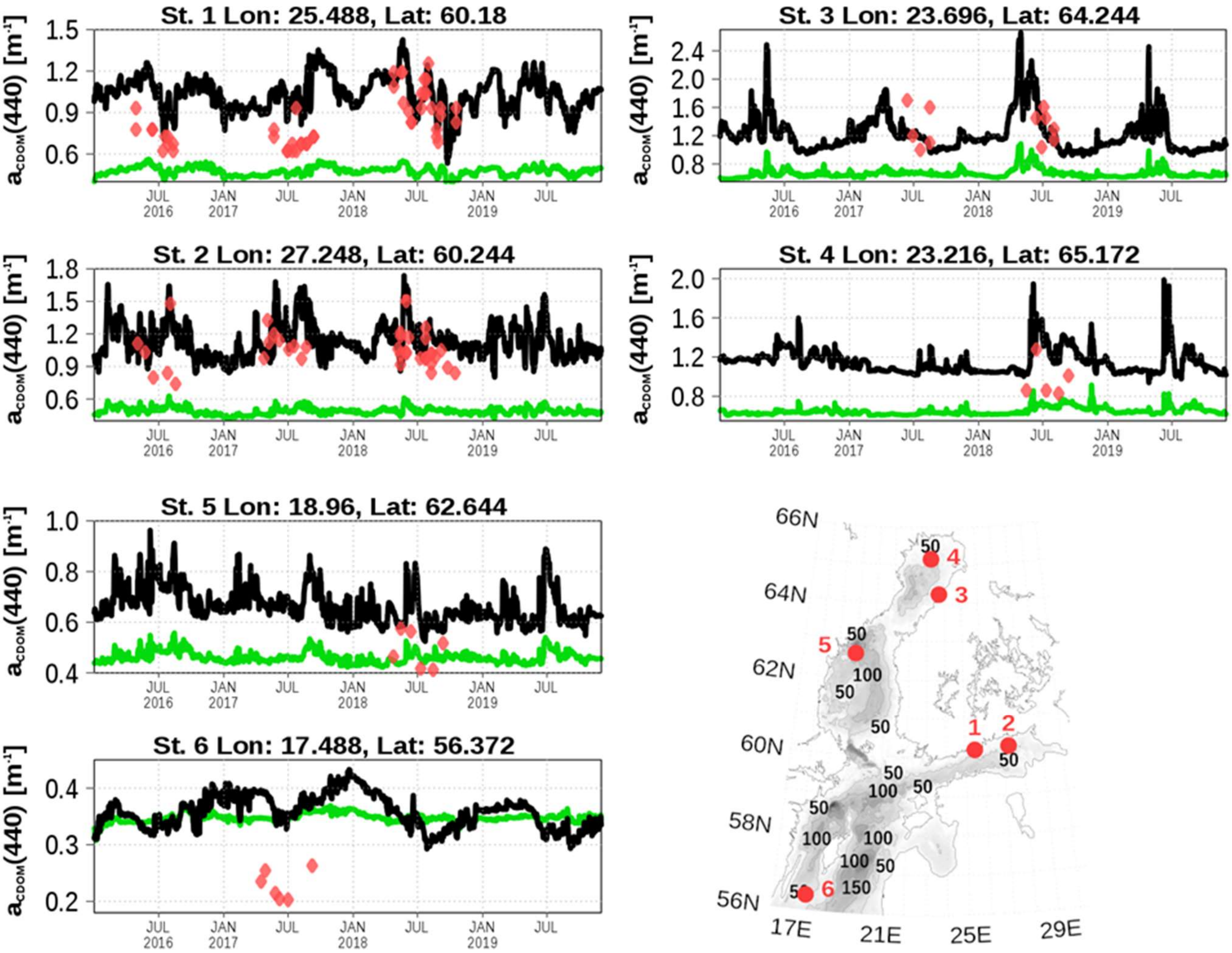


Figure 9. Comparison of EO based method (black) with salt based method (green) and observation (red).

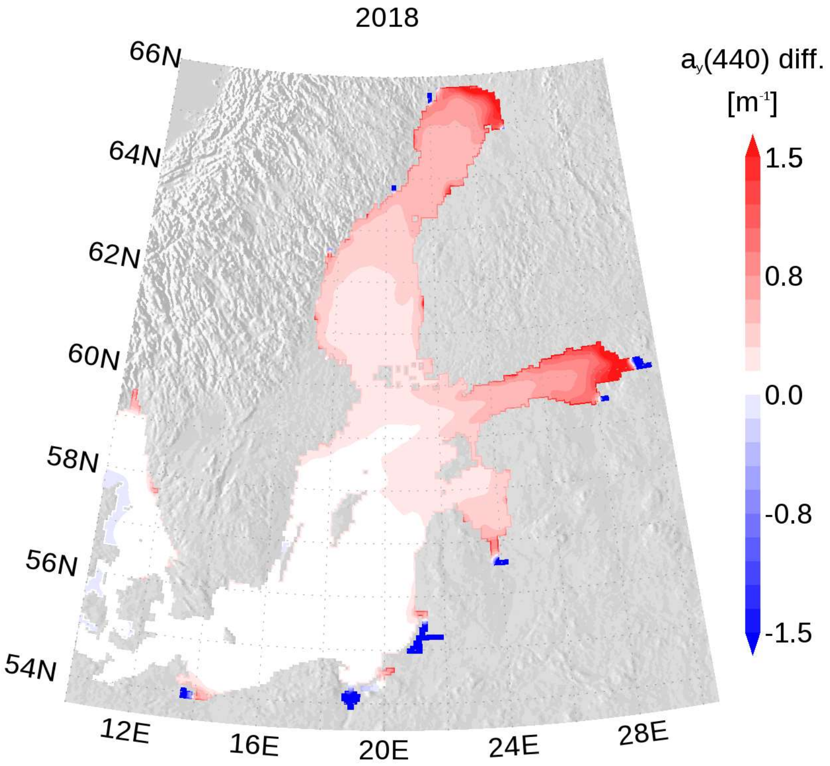


Figure 10. Annual mean differences between the CDOM absorption (at 440 nm) values of two versions of ERGOM ("new" – "old"). "new" is the model with an explicit CDOM variable and "old" the model with CDOM-salinity parametrization.

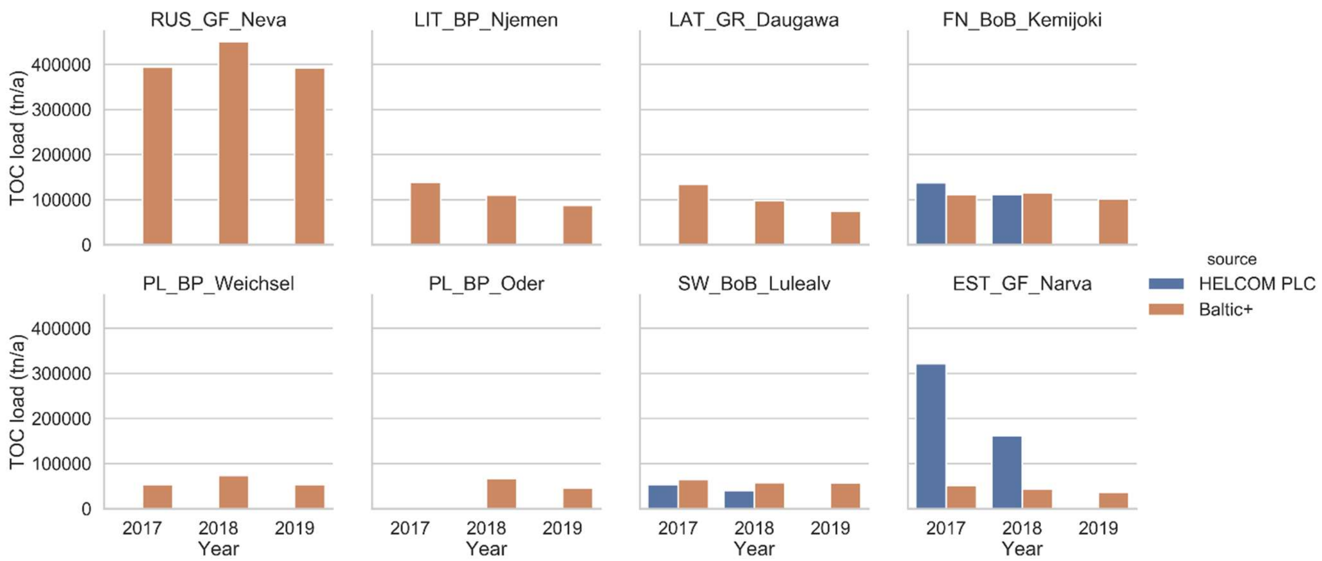


Figure 11. Annual TOC load estimated by the SeaLabio (Baltic+) method and those available in the HELCOM PLC database in eight largest rivers of the Baltic sea (ranking by https://www.worldatlas.com/articles/the-major-rivers-draining-into-the-baltic-sea.html) in 2017-2019.

6 WP 5 Scientific Roadmap

6.1 Objectives

The main objectives of the WP were to:

- Revisit and summarize the main achievements of the Baltic+ SeaLaBio project developments.
- Consolidate the challenges and lessons learnt and communicate the outcome to, and collect feedback from, the Scientific Advisory Board (SAG) and the Baltic Sea community of stakeholders in general.
- Identify next developments steps to make further progress in improving the EO products and biogeochemical modelling to support better carbon cycle understanding.

6.2 Main results

The results are described in detail in the following deliverable:

- **Scientific Roadmap:** Summarizes the results and outlines the next development steps.

The process related to the Scientific Roadmap was started by organizing two User Consultation meetings (telecons):

- June 5, 2020 with focus on the modeling results
- July 1, 2020 with focus on the EO results. Due to technical issues of some participants could not attend on July 1 and a second event with the same content was held on July 3.

The purpose of the meetings was to present the results to a wider audience and gather feedback and input for the Scientific Roadmap. Presentations and minutes were distributed to the attendees and feedback was collected. A first version of the Scientific Roadmap was then compiled and distributed to the SAG members for commenting and approval.

The main scientific advances achieved in the SeaLaBio project were presented in Chapter 5 and also outlined in the Scientific Roadmap. Possible and necessary areas for further improvements were identified and listed. Some of these areas were of more technical in nature, such as:

- Adding more input locations to ERGOM to improve the spatial representability
- Recalibration of ERGOM internally dependent processes after introducing aCDOM as state variable.
- Further develop the data fusion techniques for merging EO, model and in situ data.

In addition, more extensive and dedicated research and developments efforts with respect to carbon cycle analysis and understanding has been identified and listed, such as:

- Investigate Baltic-wide relationships between aCDOM-TOC, aCDOM-DOC, and aCDOM-POC in river outlets
- Analysis of the dynamics of terrestrial organic carbon in marine environments
- Research related to sea-to-atmosphere fluxes (pCO2 estimation)

Finally, the LEGO Baltic Sea Initiative was introduced in the Scientific Roadmap. It stands for the Leveraged use of Earth and Ground Observations for Baltic Sea R&D and puts an emphasis on the need to continue with a more holistic approach for studying, monitoring and managing the Baltic Sea. Spatial, temporal and thematic flexibility of information products is needed in combination with guidance sourced from well documented data and data products, and preferably endorsed by an appointed long-term Baltic panel of experts. Work by such a panel could also include establishment of standards (methods and products) and harmonization of metrics to ensure that appropriate comparisons between member states and regions can be done reliably. Consequently, the LEGO initiative should bring together experts in monitoring and in situ, EO and modelling, as well as, representatives from e.g. HELCOM working groups and projects, to regularly produce new and revised guidelines to support WFD and MSFD and HELCOM Action Plan revision cycles.

In addition to communication of the results, the developed products and processor have been made available to the community for own use, and the operationalization potential has been discussed. A popular science state-of-the-art document has been prepared to inform Baltic Sea monitoring and management organisations about the achievements and possibilities to improve present monitoring programs with EO based products. In addition, Baltic States has been encouraged to support EO activities by including relevant in situ measurements in the national monitoring programs and to push for the establishment and publication of common guidelines for definition of optimal sampling and determination methods for this objective.

7 WP 6 Promotion

7.1 Objectives

The main objectives of the WP were to:

- Design, publish and update project website
- Create a password protected workspace for the project team and ESA
- Generate flyers and social media content (Facebook, Twitter, …)
- Promote the project to the ocean colour community through the IOCCG newsletters (example: http://ioccg.org/2018/01/february-2018/)
- Write a paper to an international peer-reviewed journal
- Participate in relevant scientific conferences and stakeholder events
- Generate a Power Point presentation describing the project – KO+1 (project description and plans) and KO+18 (update including results and achievements).

7.2 Main results

The project website (https://www.syke.fi/projects/BalticSeaLaBio) was published on 2019-03-21. More content has been added whenever new results or other news have become available.

The password protected workspace was launched on 2018-12-10 and it has been in extensive use since. All project deliverables, monthly reports, meeting notes etc. can be found there. Access has been granted to the consortium members, ESA and the Scientific Advisory Group (SAG).

The following paper has been submitted:

- Radiation model for the Baltic Sea with an explicit CDOM state variable: a case study with Model ERGOM (version 1.2), Neumann, T., Koponen, S., Attila, J., Brockmann, C., Kallio, K., Kervinen, K., Mazeran, C., Müller, D., Philipson, P., Thulin, S, Väkevä, S., and Ylöstalo, P., Submitted to Geoscientific Model Development (GMD), 22.9.2020

The project and its results have been presented at the following events:

- Advances in the carbon and eutrophication monitoring of the Baltic Sea with Sentinel satellites, Koponen et al., ESA Living Planet Symposium 2019, Milan, Italy.
- Monitoring of carbon fluxes and eutrophication in the Baltic Sea with Sentinel satellite, Koponen et al., Baltic Sea Science Conference 2019, Stockholm, Sweden.
- Utilization of Earth Observation to support biogeochemical modeling, Koponen et al., 3rd Baltic Earth Conference - Earth system changes and Baltic Sea coasts, 2020, Jastarnia, Hel peninsula, Poland (online conference)
- ESA Baltic+ Sea-Land biogeochemical linkages (Baltic+ SeaLaBio), Koponen et al., ESA Baltic Earth Workshop 2020 (online event)

A presentation at the 6th S3VT meeting was planned but the event was moved from March 2020 to Dec 2020 due to COVID-19. A modified abstract about the project results has been submitted.

The Power Point presentation was created and delivered to ESA on 28 Feb 2019. The updated version was delivered to ESA on 30 Sep. 2020.

8 WP 7 Project management

8.1 Objectives

The main tasks of the WP were:

- Management of administrative, financial and technical elements of the project
- Management of risks table
- Setting-up and interaction with the Scientific Advisory Group (SAG)
- Organizing project meetings
    - Kick-Off, Mid-Term Review, Progress meetings, Monthly Telecons
- Communication of project progress to ESA and stakeholders
- Quality assurance of all deliverables

8.2 Main results

Table 2 shows the planned and actual meeting schedule of the project. In addition to these official review meetings the team held internal telecons at least once per month. The deliverables of the project are shown in Table 3 together with their delivery dates. WP1 and WP2 proceeded with the planned schedule. The development of the atmospheric correction took longer than expected and at the MTR it was decided that the ERGOM testing in WP4 utilizes S2 data processed with C2RCC processor. This allowed the team to proceed with the generation of the model results of the Experimental Dataset while allowing the EO development to continue. There were some delays caused by COVID-19 and in April 2020 it was decided to delay the PM4 until the summer 2020 and the FR to fall 2020.

Table 2. Meetings of the project.

Meeting	Planned Date	Actual date
Kick-Off (KO) TC	KO+0	14-12-2018 (KO+0)
Progress Meeting 1 (PM1) TC	KO+3	21-03-2019 (KO+3)
PM2 TC	KO+6	29-05-2019 (KO+5)
Mid-Term Review (MTR) in Helsinki	KO+8	18-09-2019 (KO+9)
PM3 TC	KO+12	30-01-2020 (KO+13)
PM4 TC	KO+15	02-07-2020 (KO+19)
Final Review (FR)	KO+18	09-10-2020 (KO+22)

Table 3. Deliverables of the project

Deliverable Title	Review Event	Delivery Date to ESA
Requirement Baseline	PM1	03/2019
Dataset	PM2	09/2019
Dataset Description	PM2	09/2019
Algorithm Theoretical Basis Document V1 and V2	MTR (V1) and PM3 (V2)	09/2019 (V1) and 09/2020 (V2)
Product Validation Report V1 and V2	MTR (V1) and PM3 (V2)	09/2019 (V1) and 09/2020 (V2)
Experimental Dataset	PM4	09/2020
Dataset User Manual	PM4	09/2020
Impact Assessment Report	PM4	09/2020
Scientific Roadmap	FR	09/2020
Scientific paper submitted	FR	09/2020
Final Report	FR	09/2020
Executive Summary	FR	09/2020

The Scientific Advisory Group of the project composed of the following individuals:

- Karl Norling, Swedish Agency for Marine and Water Management
- Harri Kuosa, Finnish Environment Institute
- Vivi Fleming, Finnish Environment Institute
- Prof. Anna Rutgersson, Uppsala University
- Hajo Krasemann, Helmholtz-Zentrum Geesthacht
- Lena Kritten, Free University of Berlin
- Juergen Fischer, Free University of Berlin

Harri Kuosa, Vivi Fleming and Hajo Krasemann participated at the MTR in person with the others participated remotely and/or commented the deliverables.