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Contents

Abstract

This document describes the scientific challenges and the preliminary scientific requirements of the SeaLaBio project. Three main topics are addressed: Atmospheric correction, in-water retrieval and BGC-models. We also review available data and related recent studies, and perform an initial risk analysis. Based on the findings the requirements for and activities to be carried out in WPs 2-6 are described.

Glossary

AC	Atmospheric correction
AOT	Aerosol optical thickness
BGC	Bio Geo Chemical
C2RCC	Care 2 Regional Coast Color
CDOM	Coloured Dissolved Organic Matter
Chl a	Chlorophyll a
CMEMS	Copernicus Marine Environment Monitoring Service
CO2	Carbon dioxide
CZCS	Coastal Zone Color Scanner
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
FINDB	Finnish national database
FUB	Free University of Berlin (EO data processor)
EO	Earth Observation
ERGOM	Ecological Regional Ocean Model
HELCOM	Helsinki Commission
HZG	Helmholtz-Zentrum Geesthacht
GHG	Green-house gas
ICES	International Council for the Exploration of the Sea
IOP	Inherent Optical Properties
MERIS	Medium Resolution Imaging Spectrometer
MODIS	Moderate Resolution Imaging Spectroradiometer
MSI	MultiSpectral Instrument
NIR	Near infrared
NN	Neural Network
OLCI	Ocean and Land Color Imager
ONNS	OLCI Neural Network Swarm
POLYMER	POLYnomial based algorithm applied to MERIS
QUID	QUality Information Document
S2	Sentinel-2
S3	Sentinel-3
SAG	Scientific Advisory Group
SHARK	Swedish archive for marine physical-chemical and biological data
SIOCS	Sensor independent method for the retrieval of water quality parameters from Sentinel Satellites and national missions
TOA	Top of Atmosphere
TOC	Total Organic Carbon
TSM	Total Suspended Matter
QAA	Qausi Analytical Algorithm

List of Symbols

Symbol	Definition	Dimension/Unit
λ	Wavelength	nm
$\rho_a(\lambda)$	Aerosol reflectance, including multiple scattering with Rayleigh	dimensionless
$\rho_G(\lambda)$	Sun glint reflectance	dimensionless
$\rho_{ng}(\lambda)$	TOA reflectance corrected for gaseous absorption	dimensionless
ρ_{path}	Path reflectance ($\rho_a + \rho_R$)	dimensionless
$\rho_R(\lambda)$	Rayeigh reflectance (molecular)	dimensionless
$\rho_w(\lambda)$	Marine reflectance	dimensionless
$t(\lambda)$	Total diffuse transmittance, accounting for aerosol and Rayleigh contribution, downward + upward	dimensionless
$T(\lambda)$	Direct transmittance, accounting for aerosol and Rayleigh contribution, downward + upward	dimensionless
$\boldsymbol{x}_a$	Generic notation for the degrees of freedom of the atmospheric correction related to the atmospheric model	dependent on the exact variables
$\boldsymbol{x}_w$	Generic notation for the degrees of freedom of the atmospheric correction related to the marine reflectance model	dependent on the exact variables

1 Introduction

Baltic Sea is a small, shallow, and semi-enclosed sea with high human influence due to the approximately 85 million people live in its drainage basin (HELCOM). As a consequence of the shallow and narrow opening to saline water from the North Sea through the Danish Straits as well as the substantial fresh water inflow of several rivers it is one of the most polluted sea areas in the world and prone to eutrophication. The status of eutrophication and the quality of the water in the Baltic Sea has been under constant concern (e.g. HELCOM, 2007; 2014; 2015, Andersen et al., 2010, 2011, Raateoja and Setälä, 2016). Coastal and adjacent waters, especially the estuaries of the main rivers, are influenced by the drainage basin with nutrient loading, mineral particles and humic substances – all depending on the land use and soil characteristics within the catchment area. The anthropogenic loading from the drainage basin has been continuous, but has intensified along with the industrialization, fertilization and mechanization of agricultural practices (HELCOM 2010, Korpinen et al., 2012, Fleming-Lehtinen et al., 2015). In analyses of long term observation datasets an increased eutrophication has been shown e.g. as elevated nutrient concentrations and vernal as well as summerly phytoplankton blooms (see Figure 1), presence of poorly oxygenated areas (dead zones), and unsatisfactory biodiversity (e.g. Wasmund and Uhlig, 2003, Fleming-Lehtinen et al., 2008, Raateoja et al., 2005, Kahru et al., 1994, Raateoja and Setälä, 2016). The intensive cyanobacteria algae blooms occur typically in July – August, especially in the Gulf of Finland and in the Baltic Proper.

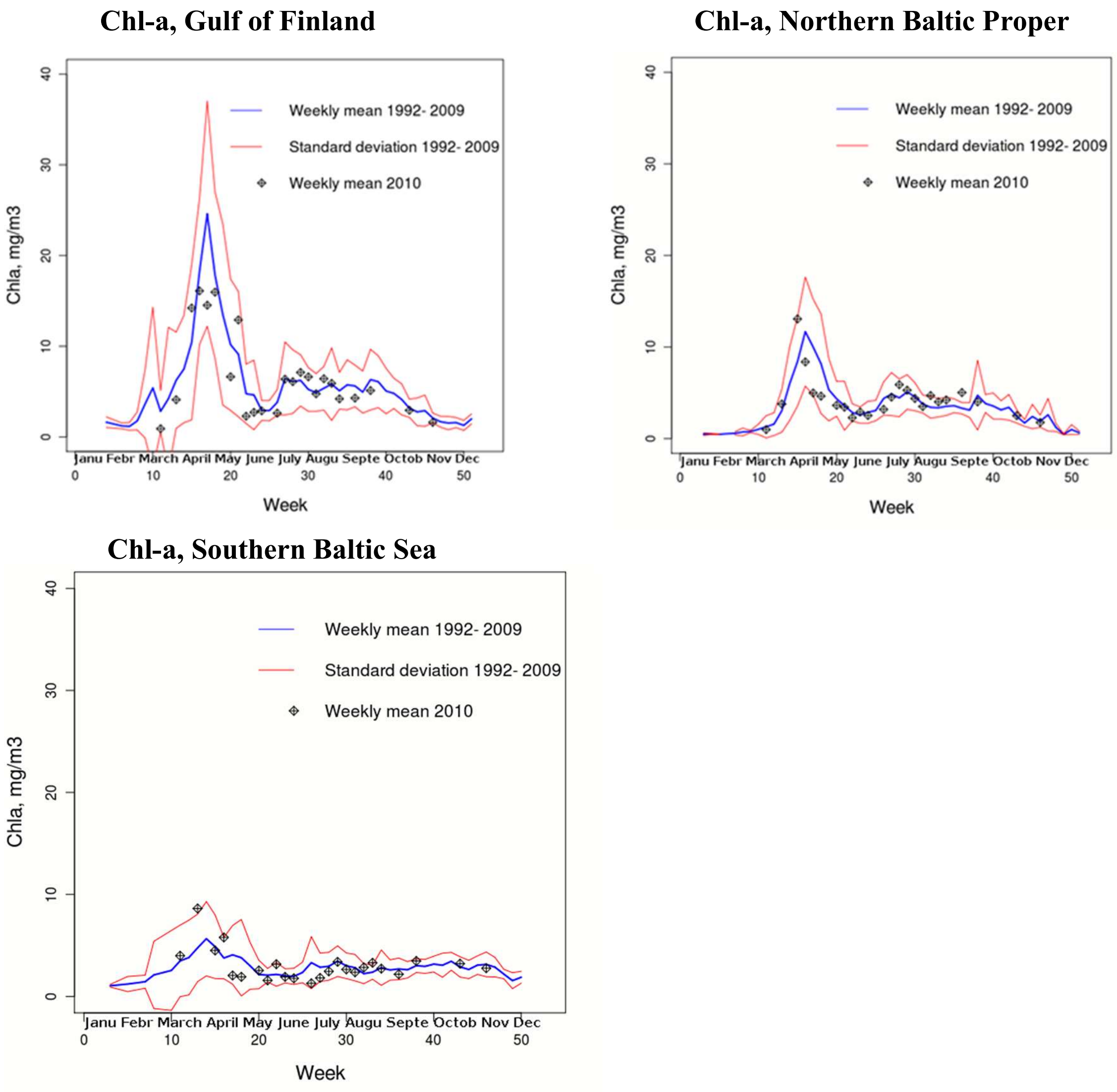


Figure 1. Time series of Chlorophyll-a values based on Alg@line (shipborne flowthrough device) data in three sub-basins of the Baltic Sea. The high values in April and May are caused by spring bloom of phytoplankton.

Rivers transport organic matter from the watersheds to marine environments and thus form a link between terrestrial and oceanic systems (Asmala, 2014). On the Baltic Sea level, the estimated annual total mass of the Total Suspended Matter (TSM) is 4 455 000 t a-1 (tons per year) (Lajczak and Jansson 1993). Some 37% of this material ends up in the central Baltic Sea, i.e. the Baltic Proper. The main sources of suspended matter are the rivers Vistula and Neva, contributing 20% and 12% of the total supply, respectively (Lajczak and Jansson 1993). Soil characteristics and land use (e.g., agriculture and forestry) in the drainage basins of rivers have a large impact on the carbon flux and water quality of coastal areas. The catchment area of the Baltic Sea is characterized by a large percentage of marshes and turf soil, part of which becomes dissolved into the runoff. The runoff is further modified by, for example, the presence of the five largest lakes in Europe – Ladoga, Onega, Saimaa, Peipsi and Vättern– which all lie within the drainage basin of the Baltic Sea (Stålnacke 1996, Rönnberg 2001). The processes and soil affecting the water properties in the lakes and rivers have a strong influence on the coastal waters of the Baltic Sea. Thus, accurate quantification of these riverine fluxes is prerequisite to model the carbon balance of the Baltic Sea, and to determine its role as a sink or a source of atmospheric carbon (Thomas et al., 2010). At present, knowledge of individual river fluxes is severely limited, even with regard to some of the largest contributing rivers, such as the Neva River (Gustafsson et al., 2014).

Within the Baltic Sea area, the concentrations of dissolved organic carbon (DOC) are the highest along the coast of Finland. Studies have been made in this area and carbon river flux data is available. Finnish rivers transport to the Baltic Sea annually nearly one million tons of carbon in the form of organic matter (Räike et al. 2012). The highest DOC concentrations and area specific export were in the rivers with a high percentage of peat in their catchments, and it is well reported that wetlands and peatlands are important contributors to stream organic carbon concentrations (e.g., Hope et al., 1994, Kortelainen et al., 1997, Laudon et al., 2004). From the main 24 rivers, covering 87% of the catchment area of Finland, the average annual load of suspended matter ranges from 4,840 to 120,000 tn/a (Kauppila and Koskiaho, 2003), depending mainly on catchment size and land use. The concentration of humic substances in coastal waters depends on the drainage-area characteristics and river runoff, increasing in the water areas that are close to river mouths (Asmala, 2014). Furthermore, the presence of non-algal suspended matter in the waters of river estuaries is particularly relevant after heavy rains and especially as the snow melts in spring, when concentrations of inorganic particles in the river water can be high.

The cells of all living organisms contain carbon. Thus, the process of eutrophication is linked to the amount of carbon in water. Spatially and temporally extensive monitoring is required for characterizing the current carbon and nutrient fluxes so that further protection measures can be planned and implemented. However, taking the right measures requires a sound understanding of the underlying processes. Continuous pCO_2 measurements in the Baltic Sea reveal a carbon dynamics which cannot be fully explained by nutrient dynamics. During the vegetation period, inorganic carbon is still taken up even when nutrients are depleted. Therefore, the whole carbon cycle is a topic of many research agendas. Figure 2 shows the carbon related processes and fluxes taking place in water. The magnitudes of some of these fluxes can be characterized with EO methods (from the surface layer) in terms of chlorophyll a concentration and absorption by CDOM. Some of the fluxes can be modelled with biogeochemical (BGC) models but currently only at a coarse spatial resolution. Figure 2 describes the EO products and BGC model state variables (in green) that are related to the carbon cycle in surface water layer. The largest component of DOC is the CDOM - although their relationship varies regionally and seasonally (Ylöstalo et al. 2016, Harvey at al., 2015; Stedmon et al., 2000). CDOM can be estimated well via EO methods in the coastal waters (e.g. Attila et al. 2013).

In different coastal waters of the Baltic Sea, the Secchi disk depth varies from an average of 4 – 5 m to low values of 0.6 – 2.5 m in the estuaries and e.g. in the Gulf of Gdansk and the Curonian Lagoon. The Baltic Proper is more transparent, with the Secchi disk depth ranging from 4 m to even 18 m. During the surface-floating cyanobacteria bloom in July – August, the transparency decreases to values between 1.5 m and 3 m (Rönnberg, 2001; Fleming-Lehtinen, 2016). One of the optically most varying areas of the Baltic Sea, the Gulf of Finland, has strong east-westward gradients of salinity, nutrient and coloured dissolved organic matter (CDOM) (Raateoja et al., 2016; Ylöstalo et al., 2016) due to the discharges from the River Neva at the easternmost end of the gulf. It faces the loading from several rivers, most importantly the river Neva, followed by the rivers Narva, Kymijoki and Luga. This leads to a large spatial and temporal variability of optical characteristics of coastal and adjacent waters in the Baltic Sea. For example, in the Finnish and Swedish coastal waters some estuaries have high amounts of CDOM and low concentration of suspended matter (an extreme among Case II waters, Ylöstalo et al. 2016) leading to strong absorption and low reflectance, while other estuaries are strongly impacted by mineral particles and have bright reflectances. An example of this is shown in Figure 3, where suspended matter dominates in river

Kokemäenjoki, whereas the rivers north from Kokemäenjoki bring humic substances to the coastal waters. Examples of corresponding EO time series are near river outlets are shown in Figure 4.

The optical properties of the Baltic Sea have been determined both for the southern parts (Darecki et al., 2003; Kowalczuk et al., 1999, 2000, 2005; 2006; Schwarz et al., 2002) and for the northern and eastern parts (Seppälä et al., 2005; Ylöstalo et al., 2016; Simis et al., 2017). The concentration ranges of Chl-a, CDOM, turbidity and TSM, collected by either published studies or from national databases for different parts of the Baltic Sea are shown in Table 1. As an example, in the Finnish coastal stations the main bulk of Chl-a observations ranges from 0.30 to 23 $\mu g\ l^{-1}$ (5% and 95%) with an average of 7.8 $\mu g\ l^{-1}$. The values of turbidity and $a_{CDOM}(400)$ mostly stay below 12 FNU, and 5 1/m, respectively, although small portion (5%) of the estuary samples represent the extreme conditions that are of special interest in SeaLaBio. Table 2 shows ranges collected by Kratzer & Moore 2018.

The variability of the optical characteristics makes the development of EO methods challenging. The algorithm has to be able to provide reliable results in different circumstances (ranges based on values in Table 1). The increasing gradient of the concentration of humic substances (Ylöstalo et al., 2016) towards the northernmost parts of the Baltic Sea contribute to the signal detected by EO instruments (e.g. Kratzer et al., 2008). Although several studies have determined high uncertainly levels for EO chl-a estimation when using the algorithms designed for global (oceanic) Case I water types, better confidence for water quality estimation has been reached in the Baltic using locally tuned or inversion algorithm approaches (e.g. Darecki et al. 2003; Kratzer et al., 2008; Harvey et al., 2015; Bertran-Abaunza et al., 2014; Alikas et al., 2015; Reinart & Kutser, 2006; Ligi et al., 2017; Pitchard et al., 2016; Attila et al., 2015; Attila et al., 2018).

With all this in mind the overall goal of the SeaLaBio project is to develop methods for assessing carbon dynamics and eutrophication in the Baltic Sea through integrated use of EO, models, and ground-based data. The main research question is: "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? While carbon enters water also from the atmosphere (CO2), the focus of this project is on the carbon fluxes from land. The geographical focus of the project will be on areas where carbon fluxes are large, e.g. estuaries of large rivers (Neva, Kokemäenjoki) and optical characteristics of water cause difficulties for EO algorithms (e.g. Bay of Bothnia).

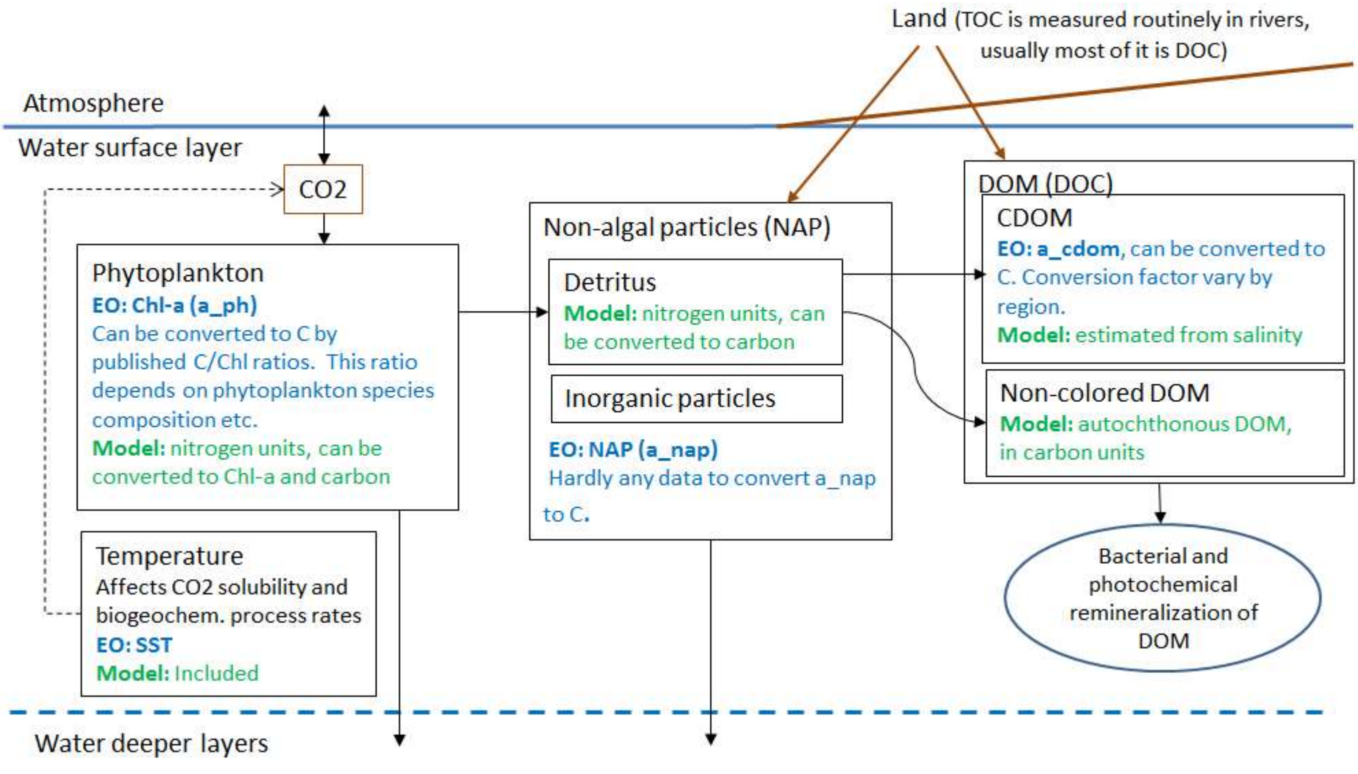


Figure 2. EO products (in blue) and BGC model (Ecological Regional Ocean Model, ERGOM) state variables (in green) that are related to the carbon cycle in surface water layer. TOC: Total Organic Carbon, DOC: Dissolved Organic Carbon, DOM: Dissolved Organic Matter, CDOM: Coloured Dissolved Organic Matter.

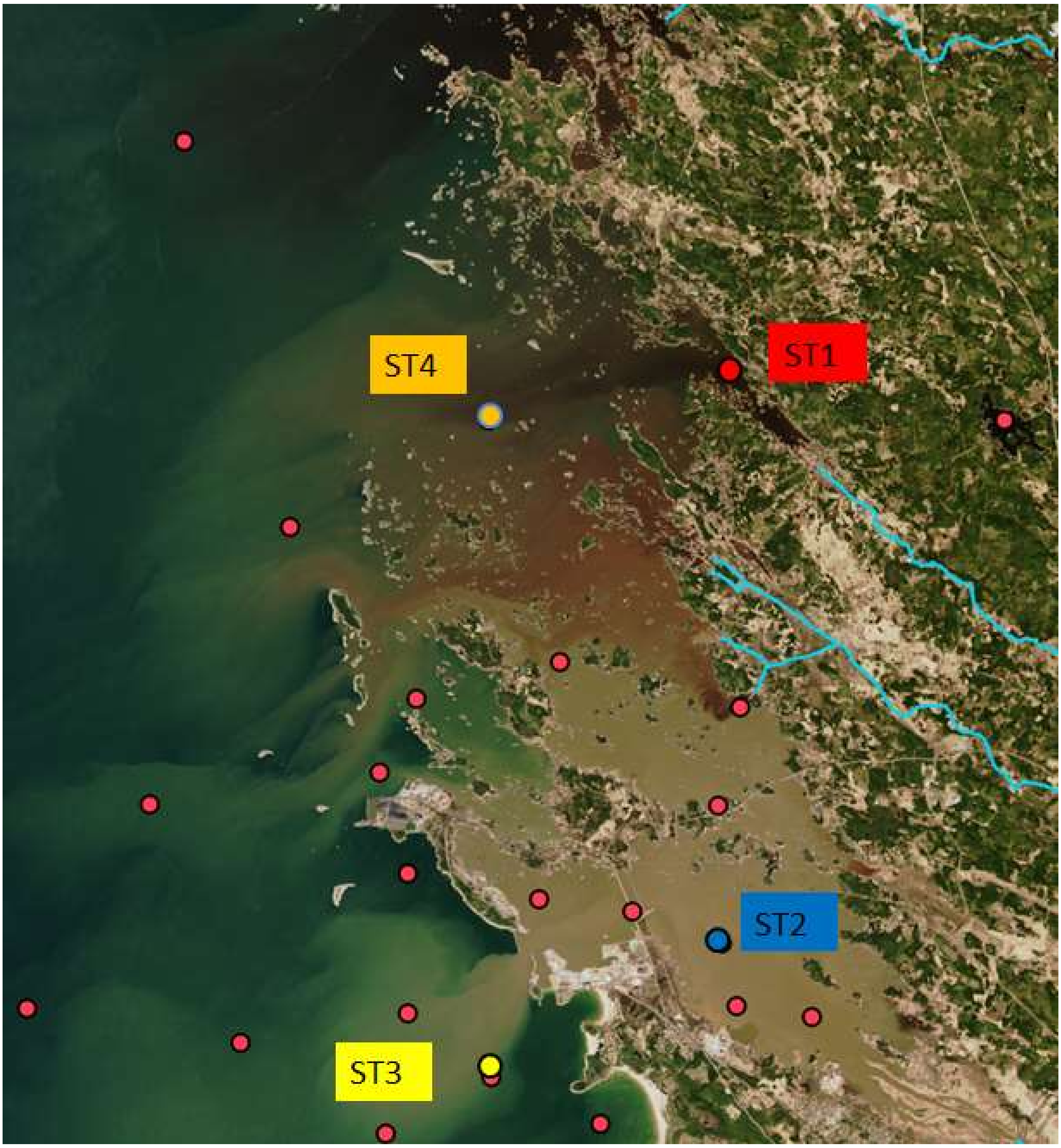


Figure 3. Landsat-8 image (30 m pixels) taken on 14.4.2016 near the town of Pori in the western coast of Finland. The river Kokemäenjoki brings large amounts of suspended terrestrial matter from the south east part of the image (ST2) during the spring time. This is mixed with the clearer water of the open sea (ST3). Small rivers (ST1) bring CDOM rich water making the water darker and brownish.

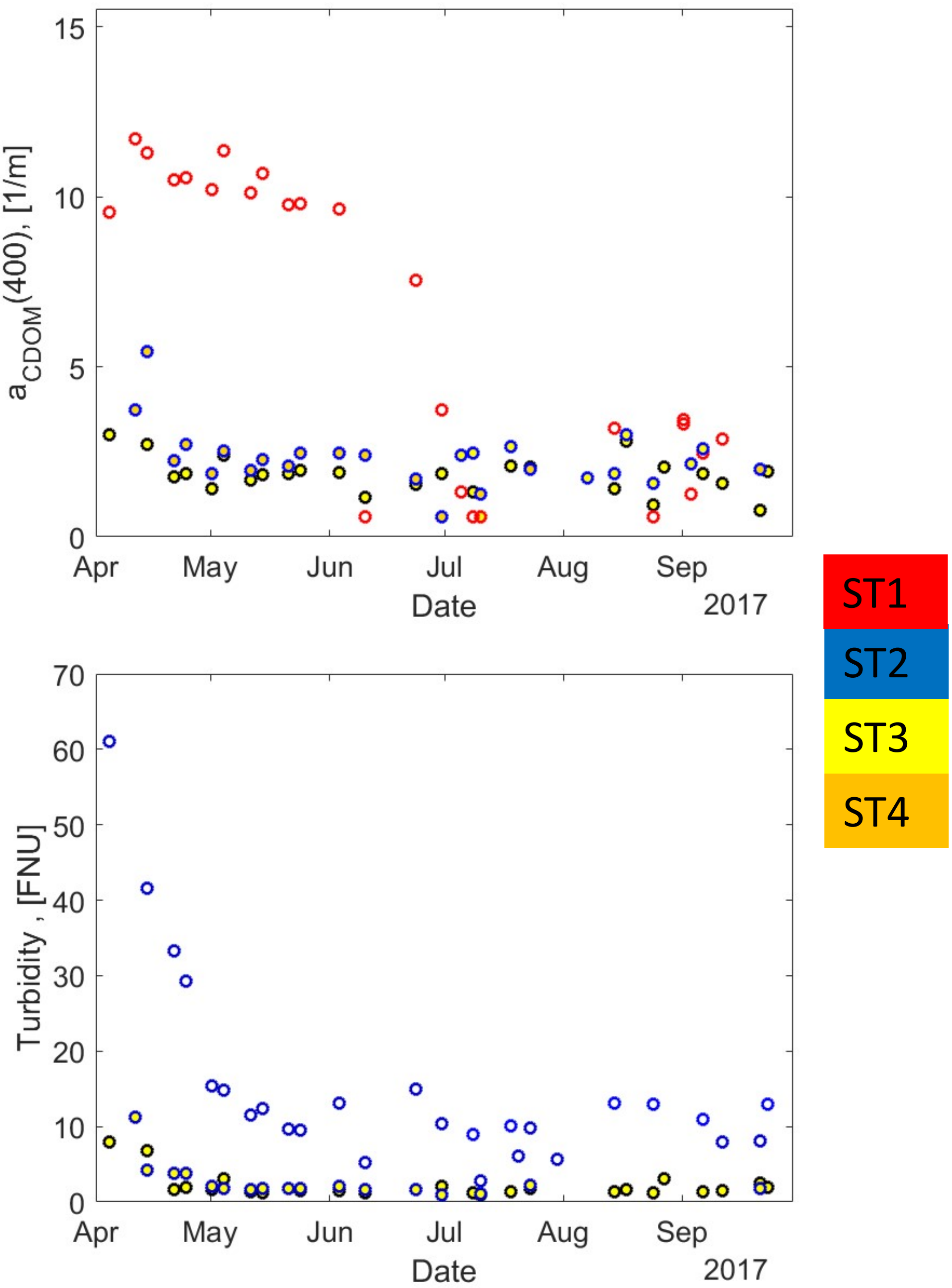


Figure 4. Time series of a_{CDOM}(400nm) and turbidity in four stations indicated in Figure 3. The results are derived from Sentinel 2 and Landsat 8 images.

Table 1. The median, 5th percentile, and 95th percentile values of water quality parameters in the Baltic Sea based on in situ measurements. The locations of the areas are shown in Figure 5. FINDB = Finnish national database, SHARK = Swedish archive for marine physical-chemical and biological data. ICES-dataset and HELCOM 2015: June-September. Ylöstalo et al 2016: April-December.

Area	Chl-a (µg/l) Median (5%-95%)	a_{CDOM}(400nm) (m^{-1}) Median (5%-95%)	Turbidity (FNU) Median (5%-95%)	TSM (mg/l) Median (5%-95%)	Secchi (m)	References
Coast of Bay of Bothnia	3.8 (1.3 – 11, P99: 18, max: 500)	2.8 (1.29 – 8.62, max: 28.6)	1 (0.32 – 3.8, P99:7, max: 89)	3.2 (2.0 – 6.1*	2.2 (0.8 – 6, max: 9)	FINDB & SHARK, INTERREG SEAmBOTH project*
Finnish South-West coast	2.9 (1.1 – 15 P99: 24, max: 79)	1.2 (0.74 – 2.94, max: 8.2)	1.6 (0.51 – 9, P99: 20, max: 1100)	-	2.8 (0.9 – 5.3, max: 11)	FINDB
Finnish coast of GoF	7.9 (2.2 – 30 P99:53.7, max: 270)	1.55 (0.87 – 2.96, max: 7.87)	1.5 (0.4 – 8.9 P99: 27, max: 500)	-	2.2 (0.7 – 5, max: 12)	FINDB
Open assessment areas (Bay of Bothnia, Bothnian Sea, Baltic Proper)	2.5 (0.9 – 4.5)	-	-	-	6.0 (3.9 – 8.2)	HELCOM 2015 **
Open sea (all main basins)	5.2 (2.3 – 20.1)	0.86 (0.51 – 1.67)*	-	2.0 (0.8 – 7.2)	2 – 12 m (min-max)	Simis et al. (2017) Spring included
Open Gulf of Finland	3.51 (0.86 –8.24)	0.97 (0.50 – 1.71)	-	-	5 (3 – 8)	GoF dataset CDOM: Ylöstalo et al. 2016
Neva Bay	5.6 (0.53 –19.12)	2.44 (1.49 – 4.04)	-	-	1.8 (0.9 – 2.6)	GoF dataset, CDOM: Ylöstalo et al. 2016
Stockholm archipelago	1.2 (0.2 – 12)	NA	NA	NA	4.1 (2 – 10)	SHARK
Åland Sea	4.5 (1.8 – 21, P99: 54, max: 332)	0.86 (0.62 – 1.38, max: 2.8)	2.5 (0.52 – 20, P99: 54, max: 800)	-	2 (0.5 – 5, max 12)	FINDB
German coast	3.2 (0.79 – 53)	-	-	-	-	ICES
Schlei	24 (3 – 58)	-	-	-	0.9	ICES

* Calculated from aCDOM(410nm)
** estimated from http://www.helcom.fi/Lists/Publications/BSEP143.pdf

Table 2. A table of optical parameter ranges in various basins of the Baltic Sea (from Kratzer & Moore 2018). CDOM absorption is at 440 nm. SD is Secchi Depth.

Baltic Sea Area	[Chl a] µg L^{-1}	[SPM] g m^{-3}	a_{CDOM} m^{-1}	SD m	References
Arkona Sea	0.3–7.0	0.7–9.0	0.2–0.4	5.0–9.5	[9,10]
Bornholm Sea	0.4–4.0	0.4–5.0	0.2–0.3	2.0–10.5	[9]
Gotland Sea	0.2–4.0	3.0–6.0	0.2–0.4	3.0–10.0	[9]
Pomeranian Bight, Germany	0.4–13.0	0.5–20.0	0.2–0.9	3.0–7.0	[9,11,12]
Gulf of Gdansk Poland	0.4–72.6	0.4–15.7	0.4–4.4	4.5–7.0	[11–13]
SE Baltic Sea, Lithuanian coast	0.6–116.2	1.1–32.0	0.01–2.0	4.0–6.0	[12,14]
Pärnu Bay, Estonia	0.7–10.7	5.0–24.3	0.6–3.7	0.5–4.3	[15,16]
Gulf of Riga, Estonia	2.0–46.0	10.0–24.0	1.5–13.0	3.1–6.9	[10,17,18]
Gulf of Finland	1.2–130	0.8–20.0	0.6–1.2	1.8–4.0	[19,20]
NW Baltic proper	0.4–52.4	0.5–21.7	0.3–4.1	0.7–12.8	[4,8]
Öre Estuary, Bothnian Sea, SE	0.5–96.4	0.2–20.9	0.75–8.8	0.5–6.0	[8]

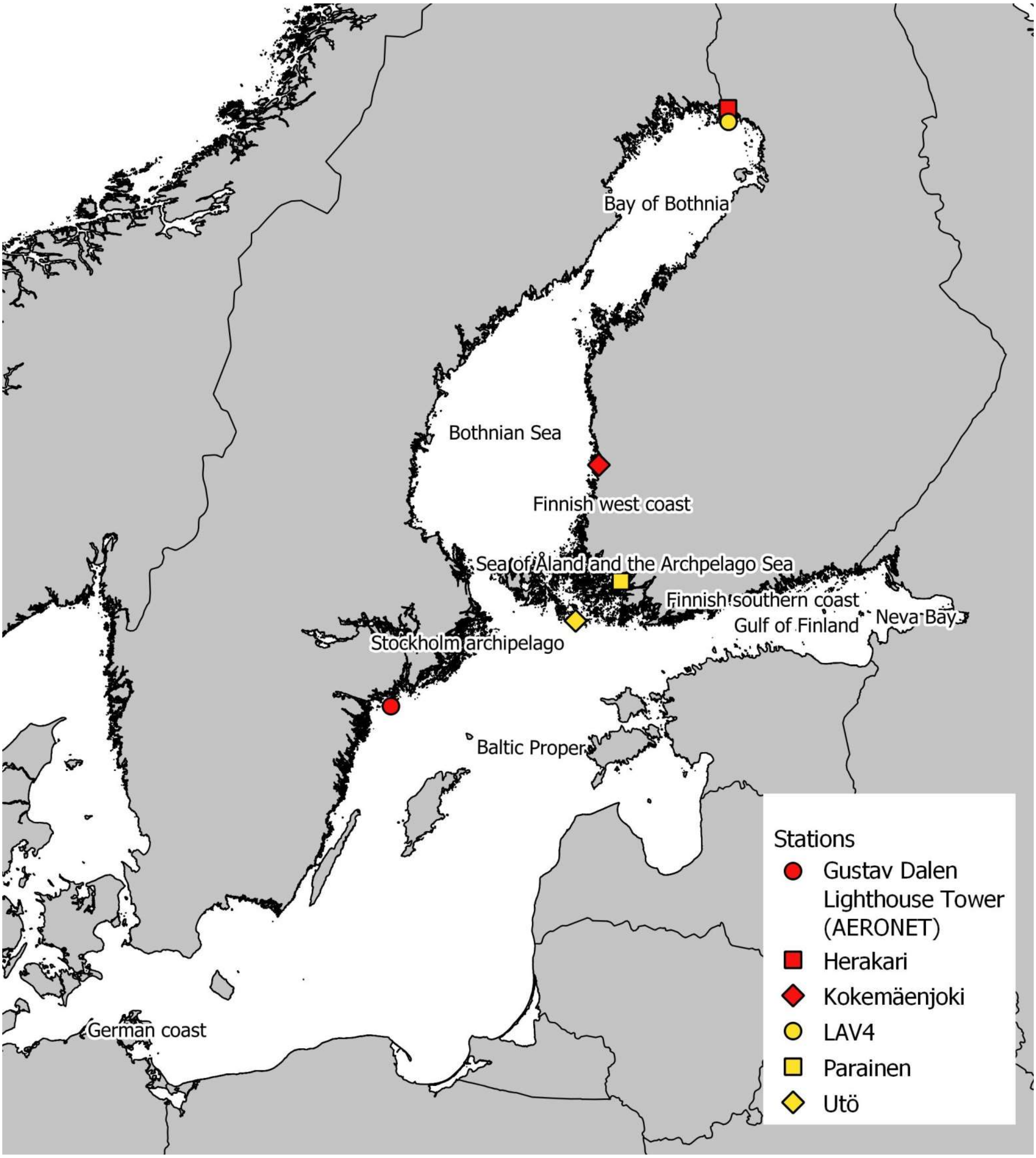


Figure 5. Map of the Baltic Sea and the areas indicated in Table 1. The stations indicated in the map are locations of example cases used in this document.

2 Review of the main scientific challenges

2.1 Review of atmospheric correction challenges over the Baltic Sea

Atmospheric correction (AC) is the first step to estimate water quality from satellite data. The goal is to remove the effects of scattering and absorption by atmospheric molecules and gasses from the signal and to correct for measurement geometry dependent reflection at the water surface. The result of this process is water leaving reflectance. AC is the most critical step: if that fails the estimation of water absorption and scattering is not possible even with a perfect in-water algorithm. In practice, even after many years of ocean colour data available, AC still remains a main issue in optical remote-sensing. The reason is the requirement of a very low error of the AC is the weak contribution of the marine signal to the total TOA signal. This is most amplified in the Baltic area: it is a land enclosed basin with aerosols varying between maritime and rural types of different optical depths, and a very low water signal due to the high CDOM absorption and at times low TSM. Examples of marine spectra encountered in the Baltic are shown on Figure 6, together with a representative spectrum of very clear water (MOBY measurement in the Pacific Ocean). In the blue bands, the marine signal in the Baltic can be easily ten times lower than that over clear waters, and conversely in the Near-Infrared (NIR). Thus, this processing step requires improvement and adaptation over the Baltic where there is currently a problem of data quality (ESA, 2017). The key to success for a good retrieval of the chlorophyll concentration, as required for eutrophication assessment and for CDOM retrieval in the Baltic area (coastal and inland waters) is the atmospheric correction. Both, Chl-a and CDOM retrieval are determined from the water reflectance in the green and blue part of the spectrum which is a real challenge for the AC due to high CDOM absorption and the requirement to retrieve a very small marine reflectance in the visible. Estimation of Chl-a is possible also in red-NIR wavelengths where this problem is not so severe.

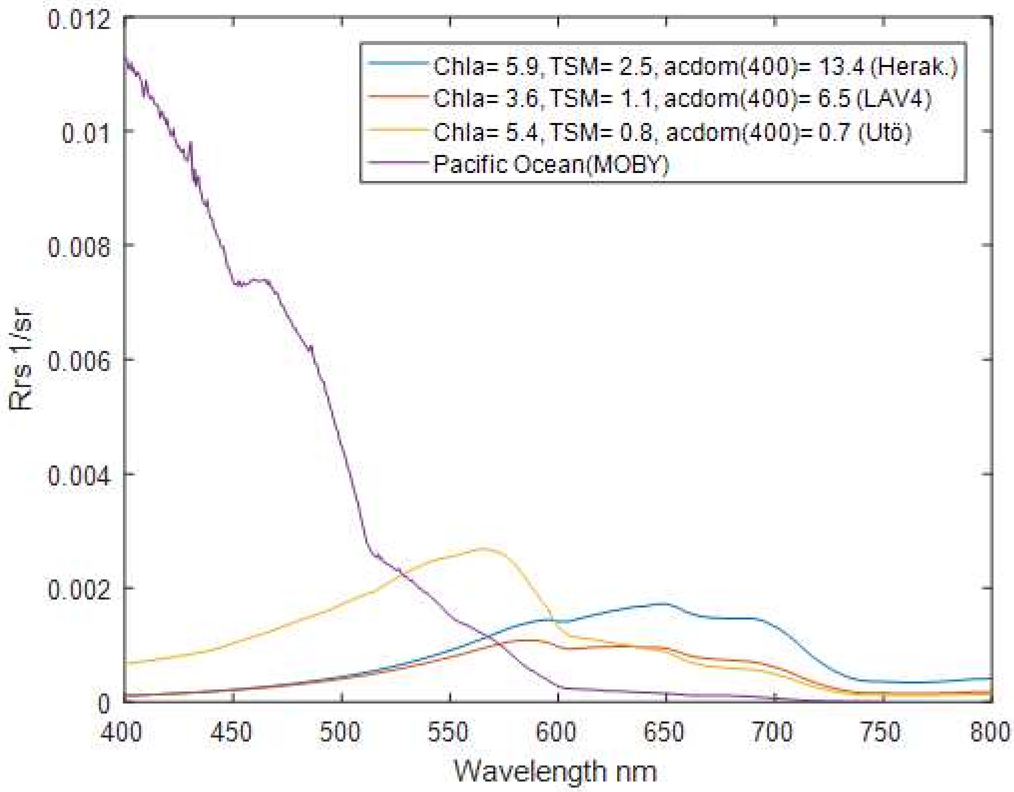


Figure 6. Remote sensing (Rrs) reflectance in three Finnish coastal stations and in Pacific Ocean. The coastal Rrs were simulated with Hydrolight using in situ concentrations measured at stations. The Pacific Ocean Rrs represents very clear water spectrum (Case 1) and was measured with Marine Optical Buoy (MOBY) in November 2012. Acknowledgement of the MOBY data: Ken Voss (University of Miami, USA), Paul DiGiacomo (NOAA/NESDIS). See Figure 5 for the locations of Herak., LAV4 and Utö stations.

All AC methods rely on the physical modelling of the signal at top of atmosphere (TOA):

$$\rho_{ng}(\lambda) = \rho_R(\lambda) + \rho_a(\lambda) + T(\lambda)\rho_G(\lambda) + t(\lambda)\rho_w(\lambda) \tag{1}$$

Where ρ_{ng} is the TOA reflectance already corrected for gaseous absorption, ρ_R is the Rayleigh scattering (known for a given atmospheric pressure), ρ_a is the unknown aerosol reflectance including multiple-scattering with the molecules, ρ_G the sun glint reflectance (generally estimated by statistical model of the surface roughness), T the direct transmittance accounting for aerosol and air molecules, ρ_w the sought marine reflectance (directional, only normalised for illumination) and t the total diffuse+direct transmittance (upward and downward, for Rayleigh and aerosol). The Rayleigh, aerosol and Rayleigh-aerosol multiple-scattering can be gathered in the atmospheric path reflectance ρ_{path}. AC is thus by essence an inverse problem coupling the atmospheric and marine unknowns. Retrieval of ρ_w from the TOA reflectance ρ_{ng}, for one single observation at pixel level, is an ill-posed problem and requires to have prior knowledge or assumptions. It is only in the ideal case of very clear oceanic waters that aerosol can be deduced independently in the NIR, with so-called standard AC (Antoine and Morel, 1999). Over complex waters such as the Baltic Sea, any inversion requires a coupled TOA model that can be written in a generic fashion:

$$\rho_{ng}^{mod}(\lambda) = \rho_R(\lambda) + \rho_a^{mod}(\boldsymbol{x}_a, \lambda) + T(\boldsymbol{x}_a, \lambda)\rho_G(\lambda) + t(\boldsymbol{x}_a, \lambda)\rho_w^{mod}(\boldsymbol{x}_w, \lambda) \tag{2}$$

Where $\boldsymbol{x}_a$ refers to the atmospheric free parameters (classically aerosol optical thickness, AOT, and aerosol type or spectral dependence) and $\boldsymbol{x}_w$ the marine free parameters (typically the Inherent Optical Properties, IOPs, such as CDOM and Chl-a absorption and particulate scattering at a given band). Other parameters chosen to be fixed in the inversion (such as specific IOPs giving spectral shape) are implicit variables of the model. This highlights the need for accurate water modelling in the AC itself, before the in-water inversion.
From the generic formulation of AC by eqs. (1)-(2), we can review the existing approaches and summarise their strengths and weaknesses.

2.1.1 Standard AC

The general principle of atmospheric correction for ocean color sensors was introduced by Gordon and Clark (1981) for the CZCS sensor, then operationalized by Gordon and Wang (1994a) for SeaWiFS, and extended to MERIS by Antoine and Morel (1999), an algorithm still in use today for OLCI. It is based on the black pixel assumption, i.e. negligible effect of marine signal in the near-infrared (NIR) bands, generally true over the open ocean. Over bright waters, the algorithm requires a pre-correction (Bright Pixel Correction; Moore et al., 1999, Bailey et al., 2010) that removes the contribution of scattering particles (essentially sediments). This type of algorithm, referred to as standard or NIR-based AC, consists of five sequential steps:

1. Removal of the potential Sun glint and white-caps perturbing effects by external model and ancillary data about the sea state (Wang and Bailey, 2001; Gordon and Wang, 1994b), in general with simplistic assumption about the direct transmittance $T(\lambda)$;
2. Removal of the contribution of any residual marine signal in the NIR (Bright Pixel Correction).
3. Identification of the unknown aerosol amount (aerosol optical thickness, AOT) and aerosol type (notably aerosol spectral dependence through the Angstrom coefficient) in the NIR. This is achieved by fitting the TOA radiometry at two bands (779 and 865 nm for OLCI) against tabulated radiative transfer modelling (RTM) for pre-determined aerosol models;
4. Propagation of the coupled aerosol-Rayleigh scattering functions, $\rho_R(\lambda) + \rho_a(\lambda)$ and $t(\lambda)$, at all bands λ in the visible domain, through the same RTM for the given aerosol;
5. Correction of the TOA radiometry in the visible to retrieve marine reflectance:

$$\rho_w(\lambda) = \frac{\rho_{ng}(\lambda) - T(\lambda)\rho_G(\lambda) - \rho_R(\lambda) - \rho_a(\lambda)}{t(\lambda)} \tag{3}$$

The interest of this approach is that it does not rely on any modelling assumption in the visible. Conversely, relying only in two bands in the NIR without constraining the model in the visible induces large uncertainties. This problem of uncertainty propagation from NIR to VIS exists even over dark waters (Figure 7): 2% uncertainty in the two NIR bands propagates to a least 5% in the blue, in the best case where errors in the NIR are correlated, and increases to more than 10% or even 20% when errors are weakly correlated.

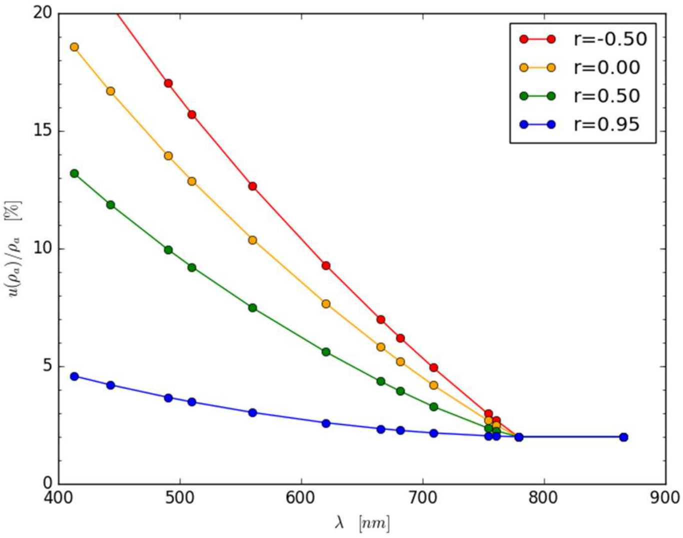


Figure 7 Uncertainty of the extrapolated $\rho_a(\lambda)$ (y-axis in %) as a function of wavelengths (x-axis) in the standard AC when assuming 2% uncertainty in the two NIR bands, with four different correlations (colours).

Figure 8 shows the problem which occurs frequently with the current standard ESA OLCI Level 2 products: the water reflectance becomes negative in the green and blue part of the spectrum, an expression of overestimating the atmospheric path reflectance in a case where the (to be determined) water reflectance is very low. Spectra with negative reflectance cannot be further processed into chlorophyll or CDOM and are lost.

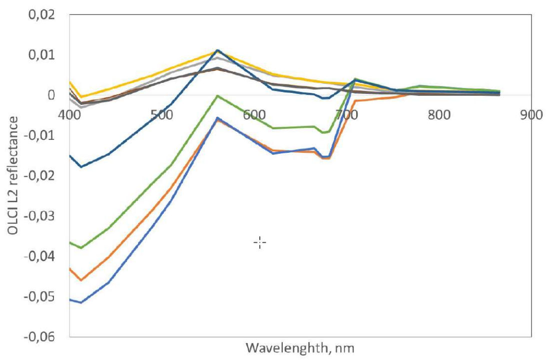


Figure 8. Water leaving reflectance for several stations in the Gulf of Finland; OLCI Image 9.7.2017: many negative reflectances in the green and blue part of the spectrum (all quality flags applied). From Kutser et al. (2018).

Performance assessment on the Baltic (MERIS, relevant for OLCI in the present context.): Mélin et al. (2011), Zibordi et al. (2013), Attila et al. (2013), Qin et al. (2017).

2.1.2 Artificial Neural Network

Artificial neural networks (NN) consist of multiple nonlinear regression derived between the input information (TOA reflectance at all bands, geometry, ancillary data) and the output parameters (typically aerosol and marine IOPs, $\boldsymbol{x}_a$ and $\boldsymbol{x}_w$). The ocean-atmosphere model, ρ_a^{mod} and ρ_w^{mod}, is only involved during the NN training. The application of the NN technique to ocean colour was specifically developed in the MERIS era for dealing with complex waters (Schiller and Doerffer, 1999) and led to various algorithms: the C2R NN by Doerffer and Schiller (2007), the FUB processor by Schroeder et al. (2007), the BOREAL processor by Doerffer and Schiller (2008) until the last version of C2RCC operationally used for OLCI (Brockmann et al., 2016). Recently Fan et al. (2017) have also developed a similar NN technique for MODIS.

Over the Baltic, C2RCC produces better results than the standard AC (Figure 9). However, the comparison with in-situ measured references shows that despite an overall reasonable agreement, the spectra differ in magnitude as well as in important features of the spectral shape. Despite these differences, many image pixels of OLCI over the Baltic Sea can be corrected for the atmosphere and subsequently processed into Chl-a, TSM and CDOM. Thus, the

Copernicus Marine Service has decided to use C2RCC as AC method for its Baltic Sea production, for further processing with the ONNS in-water neural network developed by Hieronymi et al. (2017) (HZG algorithm, Figure 9 and Figure 10).

For Sentinel-2, Toming et al. (2018) have concluded that "C2RCC seems to produce most realistic reflectance spectra" over the Baltic, among five ACs (Sen2Cor, C2RCC, SeaDAS, ACOLITE and iCOR);

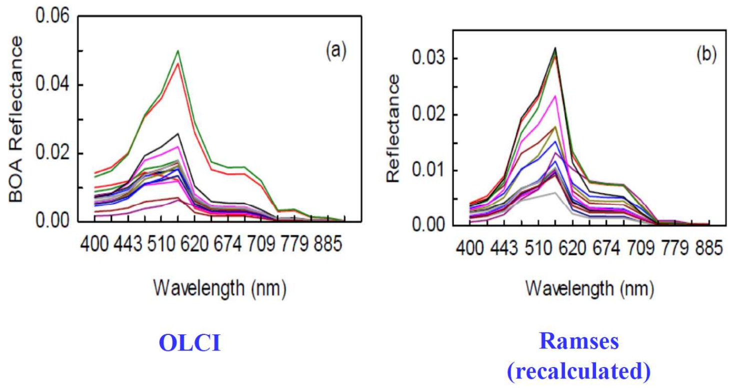


Figure 9. Performance of C2RCC AC and comparison to in-situ measurements. No negative reflectances and similar shape, but still large deviation especially in the blue part of the spectrum. From Kutser et al. (2018).

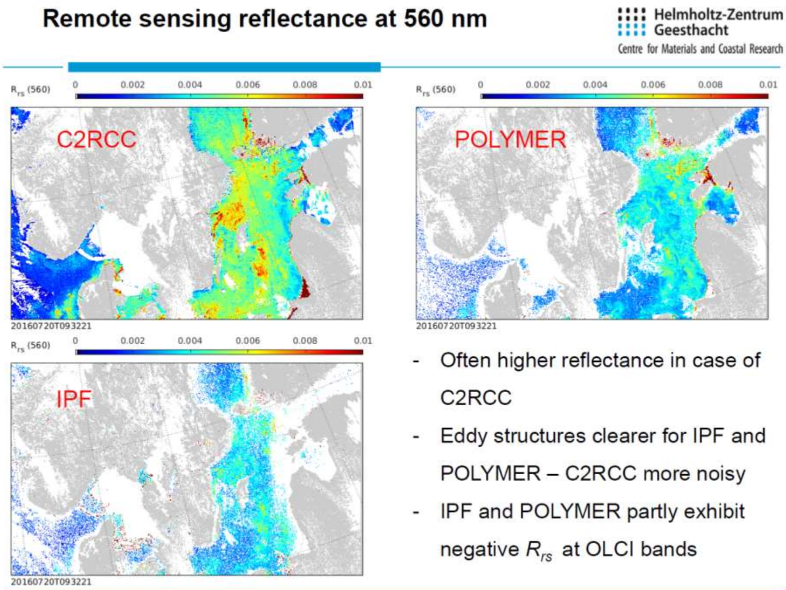


Figure 10. Analysis of different ACs for the Baltic Sea, done by Helmholtz-Zentrum Geesthacht (HZG) in the Copernicus Marine Environment Monitoring Service (CMEMS). The conclusion was that none of them is satisfactory, but CMEMS decided to use C2RCC as input CMEMS in-water processing. From Hieronymi et al. (2018).

2.1.3 Spectral matching AC

This type of AC involves an explicit ocean-atmosphere model during the inversion, contrary to the standard AC. The algorithm is based on spectral optimization over the full spectrum, e.g. Chomko et al. (2003), Kuchinke et al. (2009) and more recently POLYMER (POLYnomial based algorithm applied to MERIS) by Steinmetz et al. (2011). POLYMER is of special interest because it has been selected in the ESA Ocean Colour Climate Change Initiative (OC-CCI) after a detailed round-robin exercise against in situ measurements (Müller et al., 2015) and has experienced successful validation in the Sentinel-3 Validation Team. The atmospheric model uses a polynomial formulation accounting for aerosol, coupling between aerosol and Rayleigh and residual glint:

$$\rho_a(\lambda) = c_o T(\lambda) + c_1 \lambda^{-1} + c_2 \lambda^{-4} \tag{4}$$

This polynomial modelling has various assets against the classical radiative transfer formulation:

- It is not tributary to a discrete set of aerosol models, whose choice is limited and whose optical mixing is not physically justified (Antoine and Morel, 1999; Yan et al., 2002).
- The white term (c_o) is able to correct for residual sun glint reflectance not properly removed by the statistical model.
- It handles correctly high air mass; for this the λ^{-4} term has simply to be replaced by $\rho_R(\lambda)$ (Steinmetz, 2018). This is a key issue for the Baltic region illuminated at large solar zenith angles.
- The shape is also able to integrate the adjacency effects, i.e. scattering by atmosphere of bright targets in the vicinity of the water (Steinmetz, 2018). This is again very relevant for the Baltic because of ice, and current C2RCC failure (Figure 11).

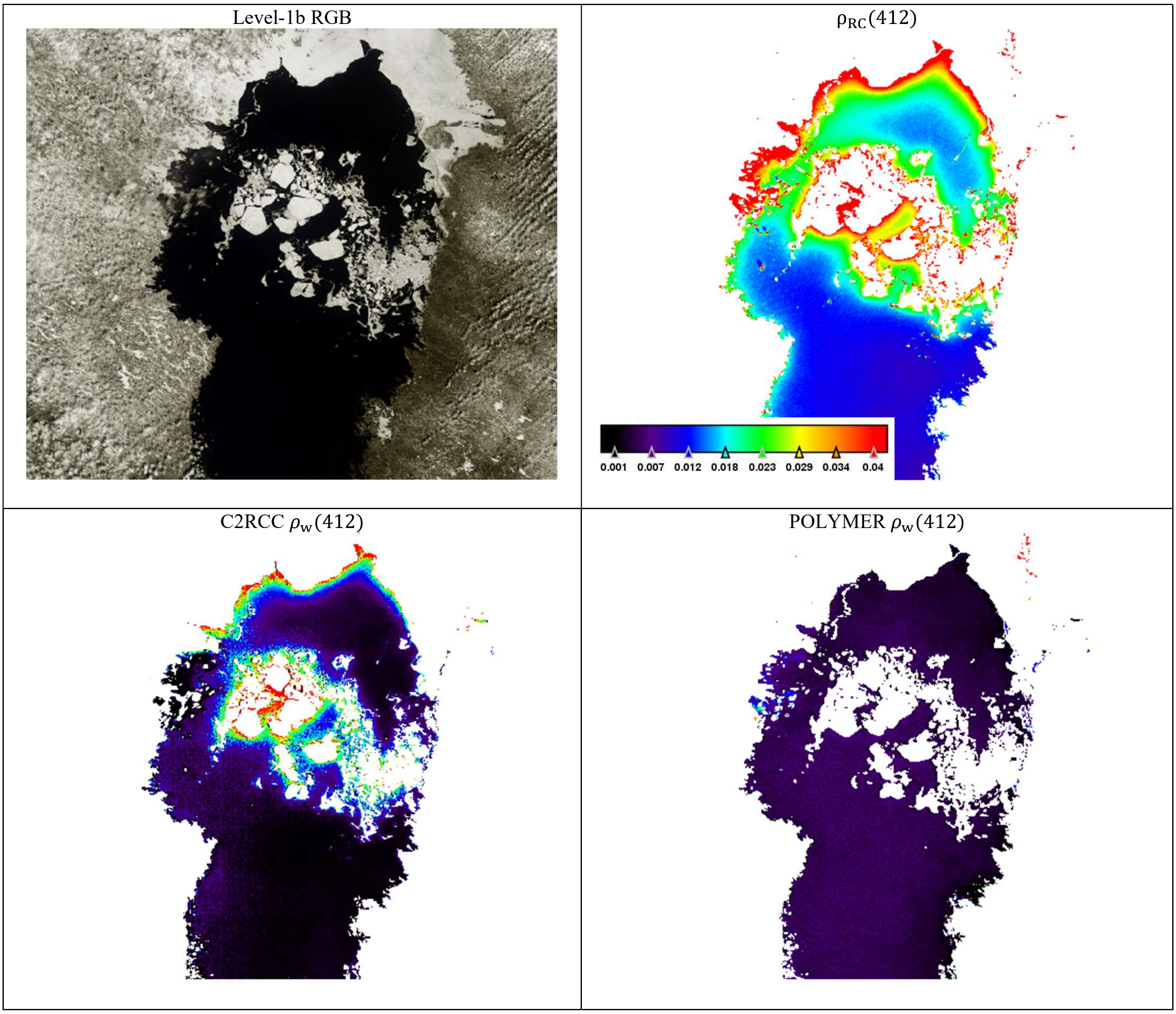
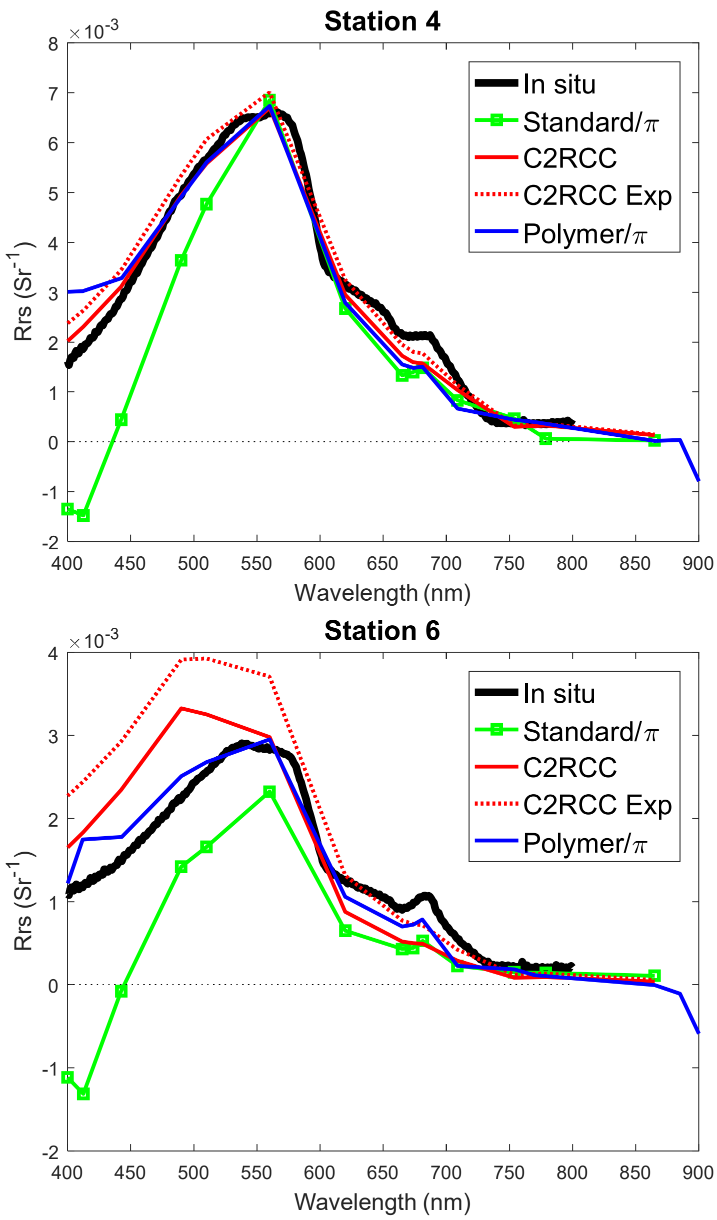


Figure 11. Example of adjacency effects impacting OLCI data in the Baltic Sea (Bay of Bothnia, 01.05.2017). Top left: OLCI Level-1 RGB. Top right: TOA radiometry at 412 nm corrected for Rayleigh scattering only. Bottom: marine reflectance $\rho_w(412)$ retrieved after atmospheric correction, left by C2RCC and right by POLYMER. Same colour scale for ρ_{RC} and ρ_w. Pixels classified as either land, cloud or ice are in white.

The marine reflectance model ρ_w^{mod} embedded in the current version of POLYMER is based on Park and Ruddick (2005) and accounts only for two parameters: chlorophyll concentration and a coefficient related to the backscattering of particles. Importantly, there is no specific modelling for CDOM in the default algorithm.

Validation against field measurements acquired in the southern Finnish coast shows that POLYMER reaches an overall similar reasonable performance than as C2RCC (Figure 12). Qin et al. (2017) have conducted a comprehensive validation of six ACs applied to MERIS data over the central Baltic Sea and have also concluded that POLYMER was overall best performing, followed by the C2RCC. It is however likely that CDOM is artificially compensated by absorption by chlorophyll, what would explain degraded performance in the blue bands. Qin et al. (2017) have concluded on the required improvement of POLYMER in highly absorbing waters, by removing any covariance between chlorophyll and CDOM in the marine model. Unfortunately, adding the CDOM as a third marine inverse parameters (together with the three atmospheric parameters) makes the inversion unstable (F. Steinmetz, personal communication). Other approaches should be investigated for the Baltic Sea.



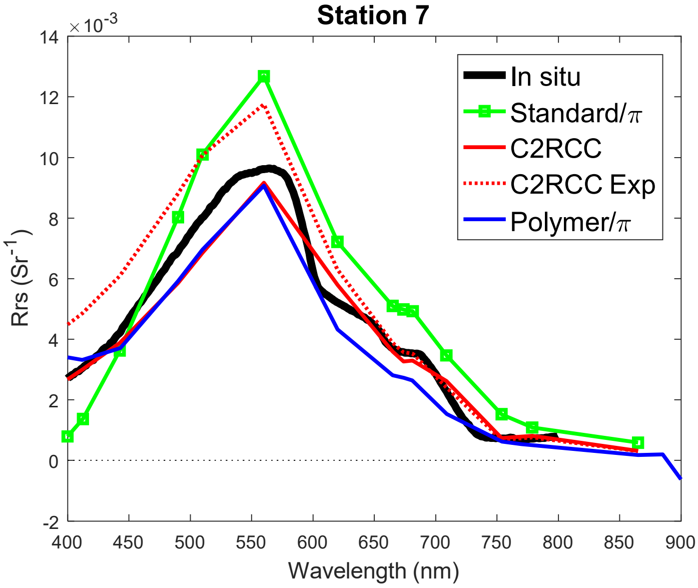


Figure 12. Comparisons of in situ reflectance measured with ASD spectrometer and various EO processors using OLCI data. Measurements were done in Parainen (coast of southern Finland, see Figure 5) on 14.8.2017.

2.1.4 Simple Rayleigh correction

Due to frequent failure of atmospheric correction algorithms in complex waters, it is regularly proposed by data users to simply apply a Rayleigh correction, i.e. to not account for aerosols. Such approach is commonly used in remote-sensing over land for classification purpose, and could be applicable over bright water targets for qualitative application. We emphasized that such approach is not applicable over the Baltic Sea in the present context, due to the very low level of the marine signal. To give order of magnitude, the aerosol reflectance at the Gustav Dalen Lighthouse Tower (located 5 nautical miles off of the Swedish coast in the Baltic Sea) is on average 0.01 at 443 nm, and hardly below 0.005 (Figure 13); this is equivalent in remote-sensing reflectance unit to an average signal of 3.2 10^{-3} sr^{-1} (and not below 1.6 10^{-3} sr^{-1}), hence of very same order of magnitude (and frequently higher) than the marine signal in the blue bands as encountered in the Baltic Sea, see e.g. Figure 6 and Figure 12. A very high accuracy in the aerosol correction is thus required.

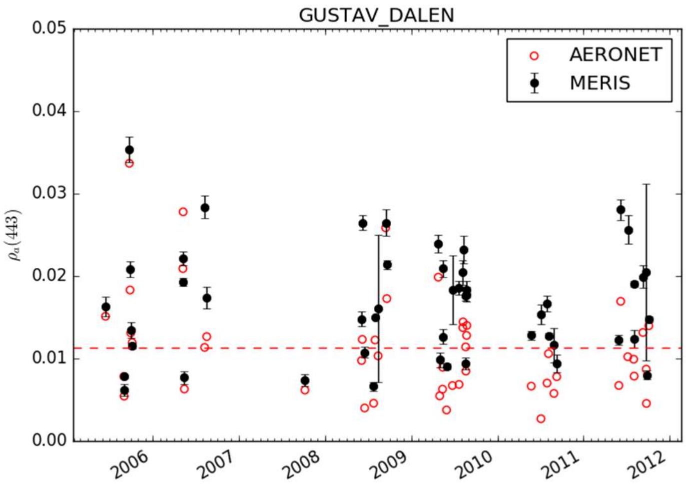


Figure 13. Time-series of aerosol reflectance at 443 nm at the Gustav Dalen Lighthouse Tower (location shown in Figure 5) as measured by the AERONET station (red circles; average dashed line) and retrieved by MERIS 3rd reprocessing (black dots). Note the overestimation of aerosol by the standard AC. From Mazeran and Zagolski, 2017.

2.2 Review in-water retrieval challenges and current approaches

In-water inversion is the second step in the satellite data processing. It converts the water leaving reflectance into information about the absorption and scattering properties of water and the substances suspended or dissolved in it. The absorption and scattering properties can then be converted into concentrations if the conversion factors – which can differ between locations and seasons – are known.

One of the problems in assessing the performance of the in-water retrieval algorithms is that the poor performance (the processed result does not match the in-situ values) can be due to the in-water method itself, or the errors introduced in the atmospheric correction part. Thus, it is not straightforward to make conclusions about the suitability of the algorithm without simultaneously assessing the performance of the AC part.

There are three types of algorithms that perform in-water retrieval:

1. **Empirical algorithms** are based on statistical relationships found between the desired quantity (e.g. Chl a) and one or more spectral bands. By definition, empirical algorithms are restricted to the conditions under which the statistical relationship has been established and thus often limited to certain areas and times (Mathews et al., 2011). Transfer to other conditions requires re-calibration of the algorithm. However, in practice, these algorithms perform very well as long as they are applied in valid conditions. This was shown for the Baltic Sea in Härmä et al. (2001), Koponen et al. (2007), and Ligi et al. (2017). In the scope of the ESA Case 2 Extreme project, Koponen showed excellent correlation using simulated data (Figure 4).
2. **Semi-analytical** algorithms are theoretically more justified and rely on a bio-optical model which is parameterized with ground truth measurements and laboratory analysis of the IOPs and optically active substances in the region of interest (Gordon et al., 1988). In the model, input concentrations are linked to the total absorption and backscattering coefficients through a series of empirical relationships, and water leaving reflectance can then be estimated as a function of the ratio of backscattering to absorption. For the semi-analytical approach, the algorithms are constructed by resampling the output reflectance to the spectral bands of the sensor and then analysing e.g. all possible 2-band ratios with the corresponding input optically active substances. Such algorithms are constructed independently of the actual image data, but are still lacking general applicability to encompass the full complexity and variability of the optical properties of the Baltic Sea. The most prominent example of a semi-analytical method is the QAA model by Lee (2002, 2009), which was validated for arctic waters by Zheng (2014) and re-calibrated for CDOM retrieval by Wang (2017).
3. **Physically based** algorithms such as the in-water NN (Neural Network) of C2RCC are linking the water reflectance ρw to optical properties of the water, the IOPs. These algorithms have the strength that they implicitly contain all the bio-optical variability existing in the nature, and which would be too complex to formalise in an analytical model. In particular, constraints in term of ranges and covariances between the IOPs can be included in the training to force the NN to have a realistic scope. A similar approach was tested in 2015-2017 in the SIOCS processor (Sensor independent method for the retrieval of water quality parameters from Sentinel Satellites and national missions). Instead of training a neural net to approximate a large set of spectra, a spectral database was calculated with a water RT model (Hydrolight) and direct search for a spectrum matching the measured one was performed (Simis et al., 2017). SIOCS showed good results when the spectral database was constructed with a bio-optical model of the Baltic Sea (Kutser et al., 2015).

Each algorithm type has its advantages and disadvantages. For example, empirical algorithms can work very well, but their scope and applicability to larger areas with different characteristics is limited and in the recent years the EO water quality community has concentrated on developing other more widely applicable methods. The project team was not able to find studies where semi-analytical have been used in the Baltic Sea.

Neural network based algorithms have been used more often in the Baltic Sea. Given the current validation results specifically of the OLCI ground segment Case 1 products and the C2RCC, there is a need to better understand the dependency of the NN under certain conditions. As an example, the NN in OLCI ground segment is currently showing a kind of saturation of chlorophyll concentration around Chl-a = 30 mg/m³. Occasionally higher values exist, but overall one can observe that the concentration hardly goes beyond, even where it is known that it should. In a NN approach, it is very difficult to identify the sources for such misbehavior. It can only be done by making experiments with simulated data and analysis of the output of the NN. One example of such analysis is presented in Figure 14 where the standard and experimental C2RCC neural networks are compared for estimation of Chl-a.

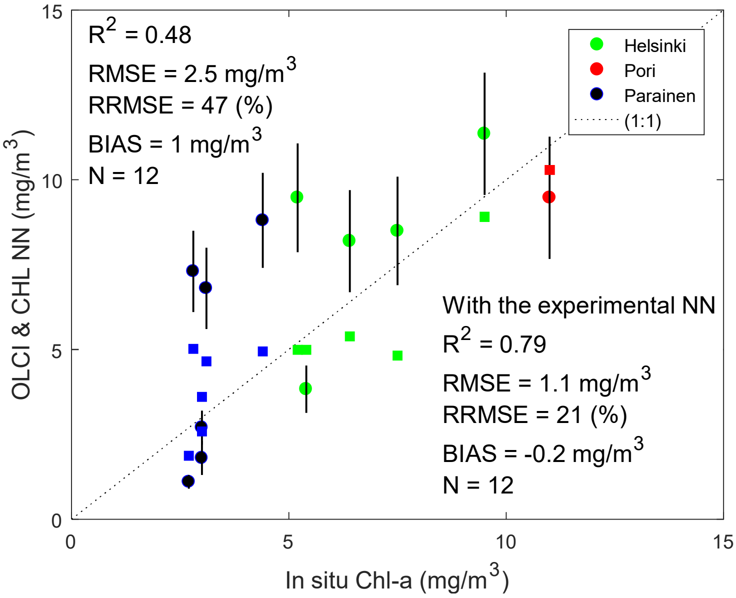
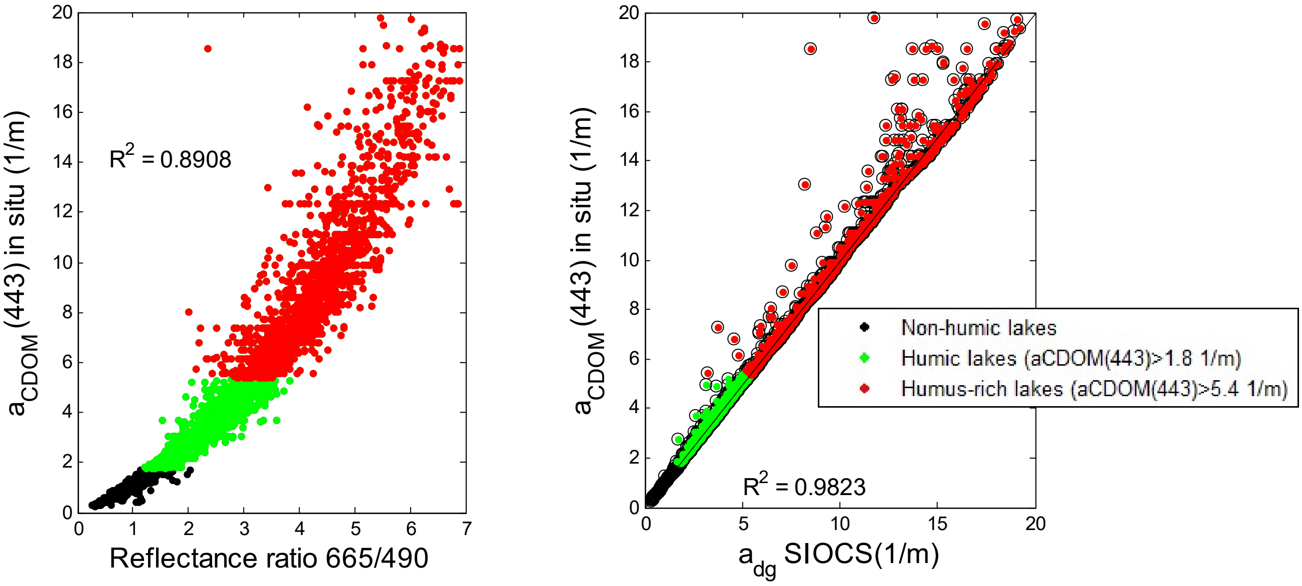


Figure 14. Chl-a estimated in the coastal areas of Finland with the standard C2RCC (circles; top left statistics) and with the experimental NN (squares; bottom right statistics, also known as the Alternate NN). The increase in correlation and the reduction of errors are significant when the experimental version is used. Image presented at Sentinel 3 Validation Team meeting, March 2018 by Sampsa Koponen.

CMEMS is producing operationally chlorophyll concentration and other water parameters for the Baltic Sea from MERIS, MODIS, VIIRS and recently OLCI. The product quality is reported with rather poor quality indicators (CMEMS-OC-QUID, QUality Information Document) e.g. r^2=0.19. The assessment of coastal water bodies is not yet feasible with the Baltic Sea Chl-a products generated by the CMEMS due to its 4 km spatial resolution and its limited accuracy in comparison to in situ data over the Baltic Sea (1 km near real time product correlation r2 = 0.2, Coppini et al. 2013, reprocessed time series (REP), r2 = 0.46, Pichard et al., 2016). In 2018, CMEMS products have been developed further especially by introducing dedicated processing with the ONNS processor for the Baltic Sea (see Figure 6) while the global CMEMS products were aggregated from standard Level 2 products. The quality indicators have slightly improved (r^2=0.25) but are still poor with the Neural Networks-based ONNS (OLCI Neural Network Swarm). The overall non-satisfactory quality of the retrieval may be at least partially due to problems in the AC.

An example of the difference between the results of an empirical and a physically based model can be seen in Figure 15. In both plots the input data has been reflectances simulated with Hydrolight using in situ concentrations of CDOM, Chlorophyll a and TSM/turbidity measured on Finnish lakes (large range in a_{CDOM}). The simple band ratio is able to estimate a_{CDOM} with reasonable accuracy. SIOCS, on the other hand, provides much better estimations. This is due to the algorithms capability to account for variability in Rrs caused by TSM and Chl-a. With measured reflectance data (Figure 16) the SIOCS estimation accuracy remains high although there are some underestimations in the higher concentrations.

Figure 17 shows examples turbidity and CDOM products derived from S2 data with C2RCC and calibrated with in situ data. Figure 18 shows a time series plot and a transect plot, again after calibration with in situ data. In both cases the original processor output follows logically what has been observed in situ, but the magnitude of the signal has not been at the correct level.



(a) (b)

Figure 15 Estimation of aCDOM from simulated Rrs data from Finnish lakes with (a) an empirical band ratio algorithm and (b) with the SIOCS model (physically based method). The number of data points is 5553. Source: GLASS D5.5.

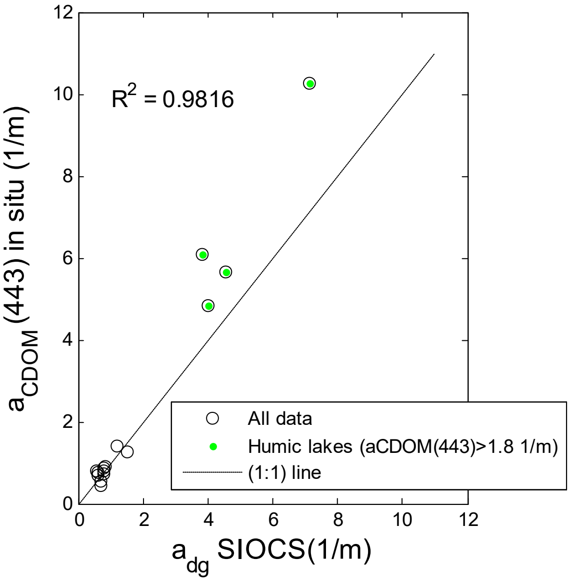


Figure 16. Estimation of aCDOM with SIOCS and measured reflectance data from Finnish lakes. Source: GLASS D5.5.

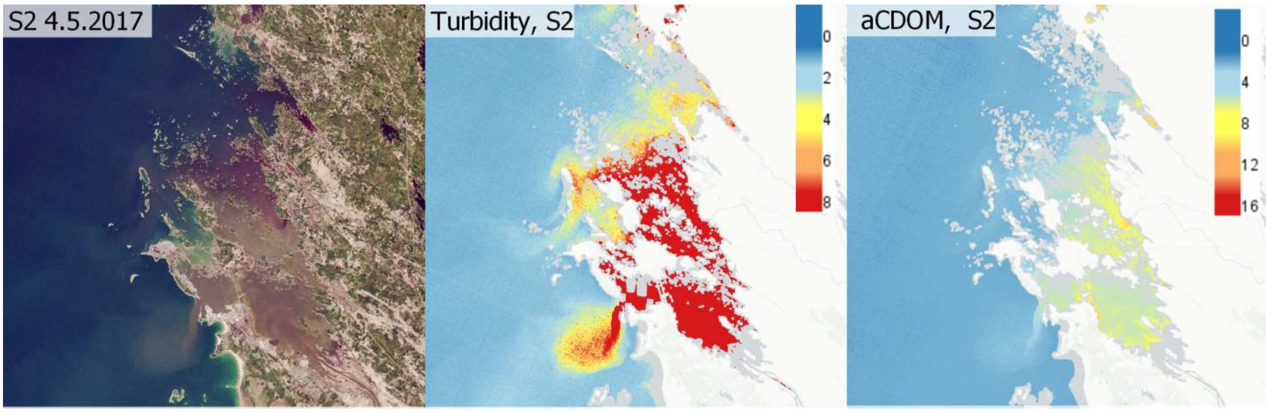


Figure 17. Example S2 true-color image from a river estuary in Finland and corresponding turbidity and CDOM products based on C2RCC, calibrated with local field samples.

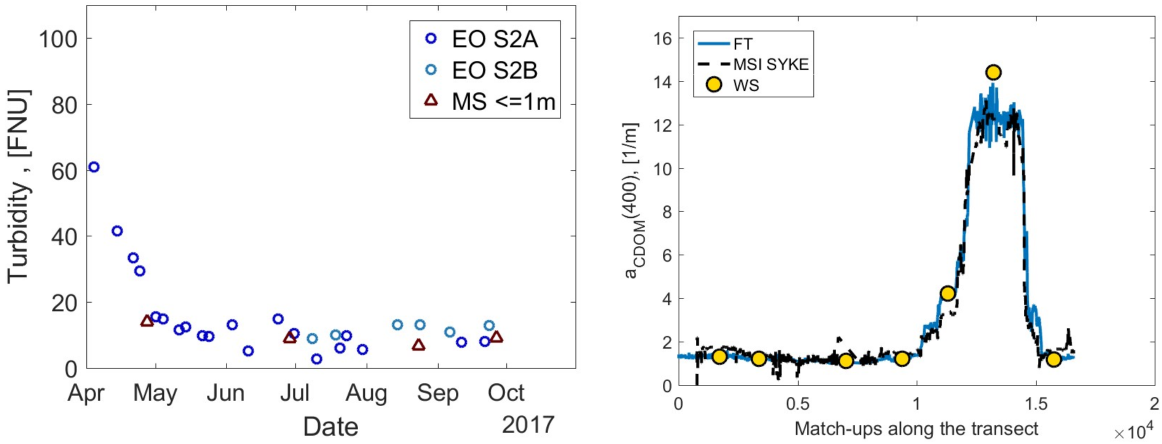


Figure 18. Left: Example of the correspondence between turbidity analysed via water samples and estimated via S2A and S2B (C2RCC-based) at a monitoring station (MS) location nearby the estuary in Figure 17 . Right: Correspondence of the absorption of CDOM as analysed via S2 (C2RCC-based algorithm) and field measured flow-through transect and water samples (WS) on a coastal estuary. In both cases in situ measurements have been used to calibrate the EO results.

2.3 Review BGC model requirements for improvements possible by EO

The data base of dissolved organic carbon compounds in the Baltic Sea is very limited compared to other variables of the ecosystem e.g. nutrients. Especially, calibrating and validating 3D models with in *situ data* is hampered by sparse data. Therefore, the main purpose of EO products for BGC modeling will be constraining the models validity with respect to carbon cycle related variables. In detail, these are surface values of organic carbon compounds (CDOM) and chlorophyll pigments. Figure 19 shows example output products of the ERGOM model.

Owing to the non-linear nature of the system (e.g. filaments, eddies, biogeochemistry), a "one by one" comparison will not be appropriate. In fact, a validation in a statistical sense is preferred. That is, EO products should cover a sufficient time period and number of time steps to derive e.g. monthly mean values. Data should be available for time periods as long as possible and cover the vegetation period from March to October. Preferably, the data will be provided in a commonly used format NetCDF (or HDF).

CDOM concentrations derived from EO data in riverine waters should allow for a quantification of CDOM loads and will support the improvement of boundary conditions for BGC models in the future. In addition, EO data on light attenuation provide useful information for the calibration of radiation models used in BGC modeling.

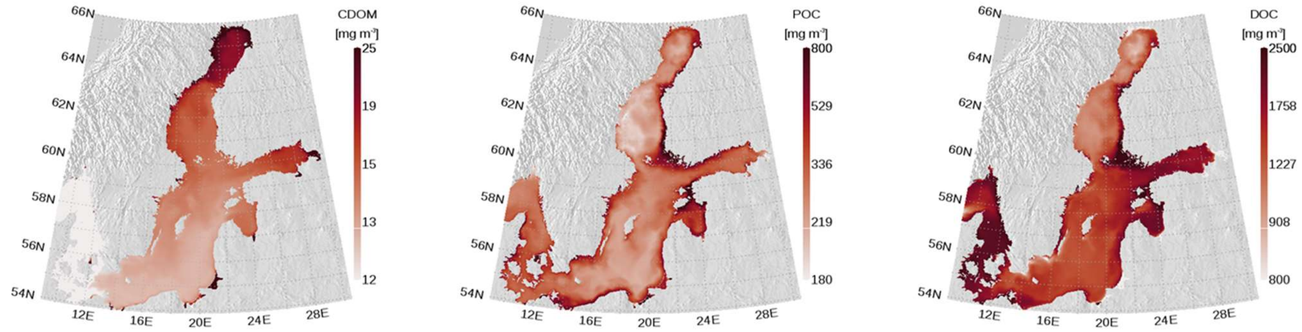


Figure 19. An example of CDOM, POC and DOC output of ERGOM model (August 1985).

2.4 Review requirements for carbon cycle understanding in the Baltic area and land-sea linkages

The flux of carbon into the aquatic systems from the surrounding land areas is currently estimated with river water samples analyzed in a laboratory and water discharge data. This gives information about TOC and DOC (CDOM is not included in routine river monitoring programs) but only at the sampling sites and during the sampling dates. Automated stations are used to measure water discharge continuously in many rivers but to our knowledge automated TOC, DOC and/or CDOM measurements are not available. Thus, this method can miss events where large amounts of carbon flow into the coastal waters during e.g. spring flood or after heavy rains, when the organic carbon concentrations are high.

Baltic Sea countries are supposed to report annual river loadings of organic matter to HELCOM once a year . Organic matter loading can be reported as TOC, DOC or Chemical Oxygen Demand (COD) depending on the routine monitoring program of each river. This reporting, however, does not always happen properly. For example, River Neva TOC loading was last time reported to HELCOM for 2012 (Räike, personal communication 2019).

EO can provide improved spatial and temporal coverage but only about turbidity/TSM and the colored component of dissolved carbon, i.e., CDOM. Since it is only one part of DOC there is also need for a method that can quantify DOC from CDOM values. DOC/aCDOM ratios have been published in a few river estuaries in the Baltic sea (e.g. Harvey et al. 2015, Ylöstalo et al. 2016) and for the open Baltic Sea (Simis et al. 2017). Furthermore, in order to estimate TOC, one needs to know the TOC/DOC ratio. In the boreal rivers flowing to the Baltic Sea most of TOC is in dissolved form (DOC) (e.g. Heikkinen 1989, Mattsson et al. 2005). Heikkinen (1989) reported that DOC represents on average 90% of the TOC transported to the Gulf of Bothnia by the river Kiiminkijoki in northern Finland. Mattsson et al. (2005) studied the DOC/TOC ratio in fifteen rivers in Finland during one year and concluded that 95% of TOC was on average in dissolved form. In Lake Ladoga, located in Neva river catchment, the DOC proportion was on average 93% (Ostapenia et al. 2009), which is in agreement with Ylöstalo's (unpublished) measurements in Neva Bay.

The other source of carbon to aquatic systems is the atmosphere. CO_2 is the most important anthropogenic greenhouse gas (GHG) and plays a key role in climate and climate change related research and analysis. Atmospheric CO_2 concentrations depend on anthropogenic emissions but also on the response of the other spheres to enhanced concentrations, and processes in and over the ocean are therefore of large importance for the atmospheric CO_2 budget. The feed-back of the oceans is a key question since they most likely take up about 40% of the anthropogenic GHG emissions. Oceanic uptake of carbon dioxide also has a potentially large impact on biogeochemistry of the oceans and the marine ecosystems since increased oceanic uptake generates an acidification of the oceans. Climate focused research programs have expressed a need for global air-sea flux estimates with high temporal and spatial resolution. Surface concentrations of CO_2 are important for a number of reasons and EO data has a unique possibility to provide horizontally distributed information to support the estimations. There is however no generally applicable remote sensing based algorithm to derive surface concentration of carbon dioxide (usually expressed in terms of partial pressure, pCO_2). Several studies have identified and utilized the strong correlation between pCO_2 and temperature that exists in many oceanic regions to interpolate pCO_2 measurements in time and space (e.g. Stephens, 1995 and Olsen, 2004). In high-latitude oceans, as the Baltic Sea, other processes such as biological production/respiration and ocean stratification have a larger effect on pCO_2 (Chierici et al. 2009; Omstedt 2009; Parard et al., 2015). In addition, recent research and attempts to generate pCO_2 maps from MODIS standard products indicated that different pCO_2 models are necessary also for the different Baltic Sea basins (Parard et al., 2015, 2016 and 2017). However, according to several studies (e.g. Darecki and Stramski, 2004) the quality of the MODIS standard products in an optically complex water basin like the Baltic Sea is relatively low. EO based products of chlorophyll-a, coloured dissolved organic matter (CDOM) and sea surface temperature are important parameters that potentially can be estimated with higher quality and higher resolution from Envisat MERIS/AATSR and Sentinel-3 OLCI/SLSTR instruments. The conclusion is that high-quality EO products, based on MERIS, AATSR, OLCI and SLSTR instruments, are required in order to improve pCO_2 analysis, models and estimations in the Baltic Sea.

In addition, salinity has been identified as a critical parameter for biogeochemistry of oceans and developing a remote sensing salinity product for the Baltic Sea would be beneficial for many applications as well as to improve the pCO_2 algorithm significantly. However, there is presently no EO based salinity product of sufficient quality and resolution for the Baltic Sea.

3 Survey of available data and related projects

3.1 EO data

SYKE currently collects all S2 and S3 data from the Baltic Sea area to the databases of the Finnish National Satellite Data Centre in Sodankylä. The data is placed also to the FinCal massive parallel processing system for convenient processing.

3.2 In situ data

Table 3 shows a summary of the data sources available for the validation. Figure 20 shows the locations of the ICES data and the Alg@line transects. Further in situ data will be collected during 2019. Thus, we estimate that the amount of data is sufficient for the validation activities planned within the SeaLaBio project.

Table 3. In situ data available for validation of EO methods.

Source	Description	Data policy	Responsible SeaLaBio partner
Finnish coastal monitoring stations	Simultaneous Chl-a, turbidity, CDOM absorption and Secchi disk depth measurements (bottle samples) are performed throughout the open water period/season. Intensive measurement stations throughout the coastal waters, including the eastern parts of the Gulf of Finland and northern parts of the Gulf of Bothnia. The northern part of Gulf of Bothnia has three intensive monitoring stations (sampling twice a month) and 11 other stations (sampling three times during summer). The laboratory determinations also included total and dissolved organic carbon, and total phosphorous and nitrogen. Sampling dates adjusted to S2 overpasses in 2016-2018.	Publicly available	SYKE
Alg@line ferrybox data	Flow-through data and laboratory analysed bottle samples from two ships	Publicly available	SYKE
Campaign data	Bottle samples, flow-through transects from three campaigns, and reflectance measurements with concurrent S2 and/or S3 data		SYKE
Rflex	Reflectance measurement system on-board Alg@line ships in (2015-2016)	Publicly available	SYKE
Swedish national coastal monitoring stations	Water quality data (surface samples + hose) from Swedish national coastal monitoring stations. Turbidity and CDOM measurements have been added to the national program in some regions from 2018 in order to meet the request for necessary reference data for EO developments.	Publicly available	BG
Swedish regional and local monitoring data	Water quality data from programs funded by the coastal Societies for water conservation and different local recipient control programs.	Publicly available or on request	BG
Marine buoy data	Water quality data from three TechWorks Marine buoys that are located in the coastal zone on the east coast of Sweden. The buoys deliver high frequency data of temperature, salinity, chlorophyll, acidity and turbidity at surface and salinity, acid and temperature in the water profile. Funded by the Swedish Research Council and hosted by Umeå, Linné and Stockholms University.	Publicly available	BG
Campaign data	Collected in the Bothnian Bay 2018, within the framework of the INTERREG Nord SEAmBOTH project. BG and SYKE are collaborative partners in SEAmBOTH.	Publicly available (SWE) or on request	BG
NorSOOP ferrybox	Water quality data Norwegian Ships of Opportunity Program for marine and atmospheric research	Publicly available	BG
German national	Germany operates a network of monitoring stations in its		BC

coastal monitoring stations	Baltic Sea waters. The data are quality controlled and stored in the national marine environmental database (MUDAB) and also and entirely reported to the ICES database[1] (International Co International Council for the Exploration of the Sea, Denmark). At ICES also monitoring data from other Baltic states are collected and BC will extract all relevant from the ICES database.		
ICES database	The International Council for the Exploration of the Sea (ICES) is an intergovernmental marine science organization, meeting societal needs for impartial evidence on the state and sustainable use of our seas and oceans. The ICES Data Centre provides marine data services to ICES member countries, expert groups, world data centres, regional seas conventions. Baltic Sea data is available. Early data is already available beginning of 1900, the latest data is currently from 2017. The database is updated regularly.	Publicly available	SYKE
AERONET-OC	Two AERONET -OC stations that collect reflectance data exist(ed) in the Baltic Sea: Gustav Dahlen Tower, 5 nautical miles off of the Swedish coast (PI G. Zibordi), and Helsinki Lighthouse, Gulf of Finland approximately 15 nautical miles off the Finnish coast (PI G. Zibordi). From the summer 2019 onwards the system at Helsinki Lighthouse will include an updated version of the device that has bands matching S3-OLCI.	Publicly available	SYKE

[1] ICES Dataset on Ocean Hydrography. The International Council for the Exploration of the Sea, Copenhagen. 2014

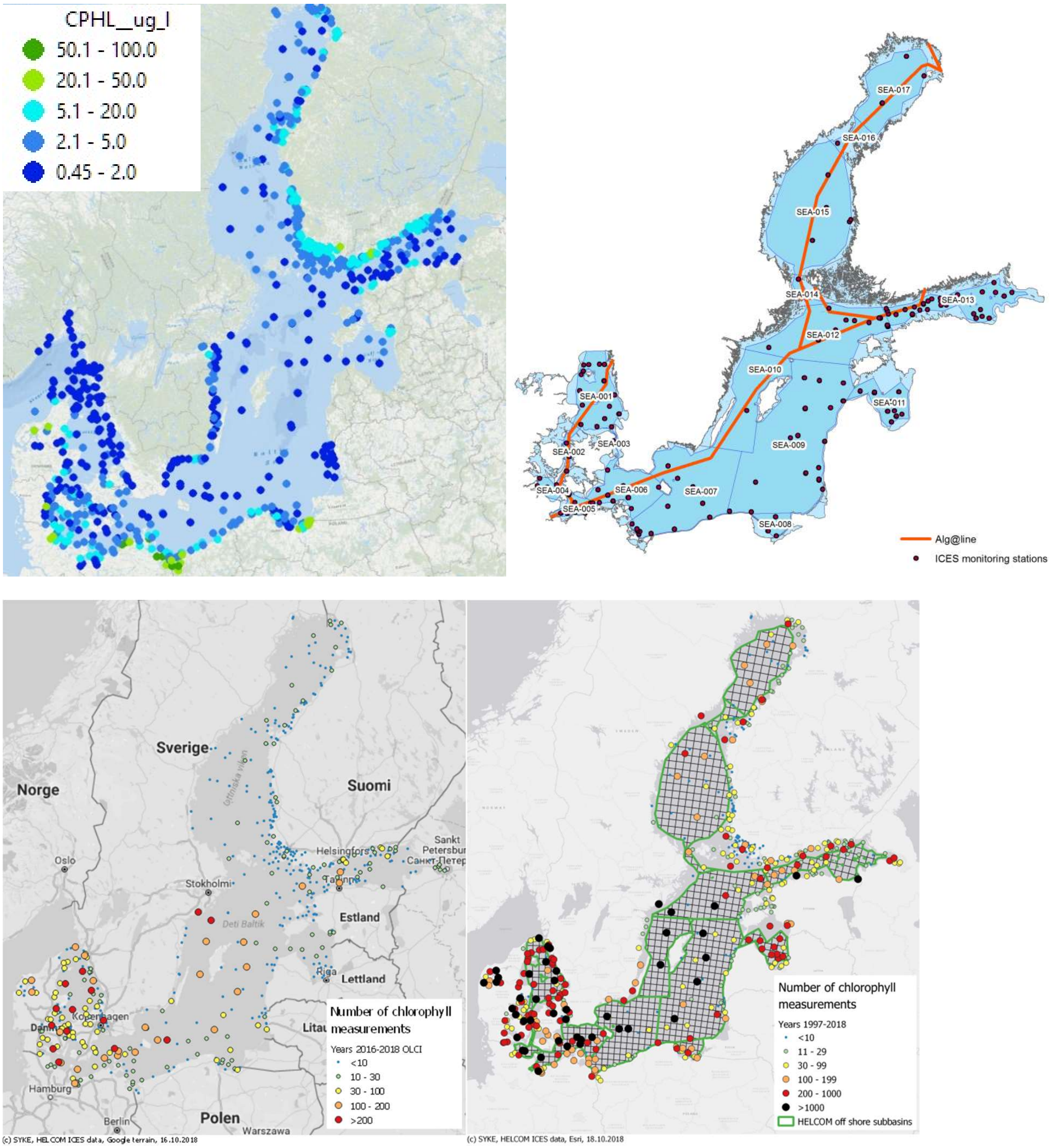


Figure 20. Top-Left: Distribution of chlorophyll values in the Baltic Sea, according to the measurements available from the ICES data base (acquired in 2016 and 2017). Top-Right: Alg@line transects (in 2016, the northernmost line not operating currently). Rflex reflectance measurements have been collected in 2015-2016 in both lines crossing the Baltic Proper. Bottom-Left: The number of chlorophyll measurements in the ICES database from different areas. Bottom-Right: Stations with long term observation series on water quality variation.

3.3 Survey of relevant past projects

Here we review past project that have results that could benefit the SeaLaBio project. We limit the scope to studies completed during 2017 or 2018.

Project name	**Case2Extreme**
Start and end date	05/2015-04/2017
Consortium	BC, HZG, RBINS, HYGEOS, PML
Website	http://www.seom.esa.int/page_project014.php
Project description and goals	The project studied and advanced the retrieval of water reflectance, IOPs and concentrations from ocean colour data of extreme absorbing and extreme scattering Case 2 waters. The algorithms have been developed for MERIS historical data and Sentinel 3 OLCI sensors.
SeaLaBio partners within the project consortium and their role	BC: project lead, algorithm development, validation and dissemination (C2RCC), software development (C2RCC operator) HYGEOS: algorithm development and validation (POLYMER) SYKE: advisory board
Benefit to SeaLaBio	One of the test areas was the Baltic Sea for extreme absorbing waters. The algorithms were further developed for absorbing waters and limitations were demonstrated. Optical models have been improved. The current C2RCC version has gained better performance by the C2X project.

Project name	**HIGHROC**
Start and end date	01.01.2014 – 31.12.2017
Consortium	Royal Belgian Institute of Natural Sciences (RBINS), Université Pierre et Marie Curie – Paris 6, (UPMC), Laboratoire Océanographique de Villefranche (LOV), Norsk Instituut for Vannforskning (NIVA), Brockmann Consult GMBH (BC), Vlaamse Instelling voor Technologish Onderzoek NV (VITO), Centre for Environment Fisheries and Aquaculture Science (CEFAS), University of Hull (UHULL)
Website	http://www.highroc.eu/
Project description and goals	The HIGHROC (HIGH spatial and temporal Resolution Ocean Colour) project will carry out the research and development necessary for the next generation coastal water products and services from ocean colour space-borne data by giving an order of magnitude improvement in both temporal and spatial resolution. These improvements will both open up new application areas for remote sensing, such as the assessment/monitoring of environmental impacts from dredging and offshore construction, and will strengthening existing applications, such as the assessment and monitoring of water quality in the context of the European Union Water Framework and Marine Strategy Framework Directives.
SeaLaBio partners within the project consortium and their role	Development and implementation of pre-processing algorithms for S3Plus sensors • Development and operation of S3Plus sensors processing chain • Development of a Multi-Sensor Processor • Validation of numerous water quality algorithms • User requirement studies and design of services • Business model and potential setup for core and downstream services
Benefit to SeaLaBio	SeaLaBio will benefit from the expertise gained in the processing development and algorithm implementation.

Project name	**SIOCS and SIOCS-II**
Start and end date	06/2012-09/2014 (SIOCS) 10/2015-06/2017 (SIOCS-II)
Consortium	BC, FUB (Freie Universität Berlin)
Website	-
Project description and goals	SIOCS stands for "Sensor independent method for the retrieval of water quality parameters from Sentinel Satellites and national missions." Within the SIOCS project was t a sensor independent processor for the retrieval of water quality parameters from Earth Observation data has been developed. The algorithms are based on the inversion of water reflectances. The work has been performed in 3 modules: Development of the method, software implementation and interaction with users. The SIOCS framework has been used successfully with a dedicated LUT provided by SYKE and has been integrated in the workflows of the FerryScope project.
SeaLaBio partners within the project consortium and their role	BC: project lead, software development (SIOCS framework, SIOCS operator), validation, user interaction
Benefit to SeaLaBio	The SIOCS framework provides the opportunity to run learning algorithms on own spectral LUTs for retrieving water quality parameters.

Project name	**BONUS FerryScope**
Start and end date	07/2014 – 06/2016
Consortium	BC, SYKE, EMI
Website	https://www.bonusportal.org/projects/innovation_2014-2017/ferryscope
Project description and goals	BONUS FERRYSCOPE built an integrated system of optical measurements from ferries and satellites. This serves monitoring, research, and resale of marine spatial information through improved quality of spatial biogeochemical products, and by providing the tools to harvest and analyze the observation data in near real-time. The project had three cornerstones: (1) State-of-the-art optical instrumentation were placed on ferries in the Baltic Sea, to complement existing ferry-based observations with reference measurements of water-leaving radiance. These were delivered to satellite imagery processors in near real-time. (2) A data harvesting, assimilation, and analysis engine was developed, allowing significant reduction of uncertainties in remotely sensed imagery of the optically complex Baltic Sea. (3) Biogeochemical dynamics including phytoplankton bloom diagnostics were developed, harnessing the power of on-the-fly time series analysis and feedback to in situ observation and water sampling efforts.
SeaLaBio partners within the project consortium and their role	BC: Overall coordination, implementation of processing chain, service operation, validation SYKE: Development and implementation of RFLEX devices
Benefit to SeaLaBio	RFLEX data from the Baltic Sea is available from years 2015-2016

Project name	**HELCOM EUTRO-OPER**
Start and end date	2014 – 2015 (EUTRO OPER EXTENDED project was established in 2016
Consortium	Representatives from HELCOM participating countries
Website	http://www.helcom.fi/helcom-at-work/projects/completed-projects/eutro-oper
Project description and goals	The two-year project on 'Making HELCOM Eutrophication assessments operational (HELCOM EUTRO-OPER)' was finalized in 2015. During this time, the project developed an operationalized work flow for updating the eutrophication indicators and assessment. Four out of the five existing HELCOM CORE indicators of eutrophication were included into the process algorithms. EUTRO-OPER developed six PRECORE or candidate indicators of eutrophication. Of these, the e.g. cyanobacterial bloom and

	indicator could be updated to CORE status in time for be included to the HOLAS II. The EUTRO-OPER project piloted the production of assessment products through efficient data flow processes. During the project, the entire assessment process, from monitoring and data aggregation to assessment calculation, was defined and documented, together with the protocols as well as responsibilities of QA/QC guidance and review. The project continued to improve the quality of the existing eutrophication status core indicators through enabling use of remote sensing and ship-of-opportunity data.
SeaLaBio partners within the project consortium and their role	SYKE participated by providing EO chl-a products and validation for test assessment tool and for the manuals. SAG member Vivi Fleming-Lehtinen was the project Manager in HELCOM Secretariat during EUTRO-OPER
Benefit to SeaLaBio	Expertise on how HELCOM assessment tools can be complemented with EO derived statistics.

3.4 Interaction with ongoing projects and initiatives

Here we analyze currently ongoing projects and other activities related to EO and monitoring of the Baltic Sea. In addition to analyzing the benefits of these projects to SeaLaBio, we examine how the other projects can benefit from SeaLaBio.

Project name	**H2020 EOMORES**
Start and end date	11/2016-11/2019
Consortium	Water Insight (NL), Deltares (NL), National Research Council of Italy (Italy), SYKE (FI), Tartu Observatory (EE), Klaipeda University (LT), University of Stirling (GB), Plymouth Marine Laboratory (GB), Evenflow (BE)
Website	eomores-h2020.eu
Project description and goals	Excerpt from the EOMORES website: "EOMORES is a European innovation project aiming to develop commercial services for monitoring the quality of inland and coastal water bodies, using data from Earth Observation satellites and in situ sensors to measure, model and forecast water quality parameters."
SeaLaBio partners within the project consortium and their role	SYKE: Responsible for providing EO services for Finnish lakes and coastal areas (i.e. the Baltic Sea). SYKE has also conducted measurement campaigns and performed validation.
Benefit to SeaLaBio	Access to campaign data for validation. This includes reflectance measurements with a WISP spectrometer.
Benefit to EOMORES	EOMORES will end in November 2019 and its benefits from SeaLaBio will be limited. If the new algorithms developed in SeaLaBio are ready to be tested before end of September 2019 and perform better than the currently used algorithms, they can be used in service provision.

Project name	**Interreg SEAmBOTH**
Start and end date	X/2018-X/2019
Consortium	Metsähallitus, SYKE, Centre for Economic Development, Transport and the Environment in Northern Ostrobothnia and Lapland, GTK, County Administrative Board of Norrbotten, SGU (BG as a subcontractor)
Website	seamboth.com
Project description and goals	The main goal of the project is to help ensure the conservation of the biological diversity, habitats, ecosystems and the ecosystem services existing within the Bothnian Bay. One method used to reach this goal is data collection through in situ and EO methods.
SeaLaBio partners within the project consortium	SYKE and BG are partners in this project and their role is to test and develop EO methods that provide useful data for the assessment of the status of the area

and their role	
Benefit to SeaLaBio	Bothnian Bay is in the northernmost area of the Baltic Sea and the water in the region is characterized by high concentrations of CDOM. Thus, it is an ideal test area for SeaLaBio. SeaLaBio will have access to most of the in situ data collected in SEAmBOTH
Benefit to SEAmBOTH	The EO part of SEAmBOTH will end in spring 2019 and thus the benefit from SeaLaBio to SEAmBOTH will be limited.

Project name	**Copernicus OC-CMEMS System Evolution and Implementation**
Start and end date	09/2018 - 04/2021
Consortium	CNR, HZG, SYKE
Website	http://marine.copernicus.eu/about-us/about-producers/oc-tac/
Project description and goals	The overall goal is to improve the quality of CMEMS OC products in the Baltic Sea for MERIS, MODIS and OLCI lifetime.
SeaLaBio partners within the project consortium and their role	SYKE: Validation of the quality of the data CMEMS provides for the Baltic Sea and to offer guidance on how to improve the products.
Benefit to SeaLaBio	Direct contact with CMEMS production organizations. RFLEX data.
Benefit to OC-CMEMS	Improved EO algorithms for the Baltic Sea

Project name	**Carbon monitoring of the Baltic Sea using remote sensing**
Start and end date	06/2018-06/2021
Consortium	Uppsala University (UU), Brockmann Geomatics (BG), University of Liege (UL) and University of Exeter (UE)
Website	https://www.rymdstyrelsen.se/forskning/beviljade-bidrag/utlysning-2017-rfak/monitorering-av-ostersjons-kolcykel-med-hjalp-av-fjarranalys/
Project description and goals	By combining methods developed by the group at Uppsala Universit earlier research projects, and introducing new in-situ data from the EU project INTEGRAL (Integrated carboN and TracE Gas monitoRing for the bALtic sea), using products from new EO sensors (e.g. Sentinels) and a new open-source software toolbox for air-sea exchange calculations (FluxEngine developed in a ESA-SOLAS program), the goal is to develop Baltic Sea specific remote sensing based methods and products for surface water pCO_2 and CO_2 exchange between water and atmosphere. Coastal retrievals will be possible and of a high enough quality to be used for estimating the net carbon emission-uptake for the Baltic Sea basin to support Baltic Sea ICOS contributions, policy and Baltic Sea research.
SeaLaBio partners within the project consortium and their role	UU: Prof. Anna Rutgersson (SAG) BG: Sentinel-3 data production and validation
Benefit to SeaLaBio	Scientific advice and understanding of atmosphere-sea carbon cycle.
Benefit to CarbMonBS	CarbMonBS will benefit from the expertise gained in the processing development and algorithm validation.

Project name	**Bonus Blue Baltic Integral**
Start and end date	July 2017 to June 2020
Consortium	University of Uppsala, UU (SE), Finnish Meteorological Institute, FMI (FI), Institute of Oceanology of the Polish Academy of Sciences, IOPAN (PL), Tallinn University of Technology, Department of Marine Systems, TTU (EE), GEOMAR Helmholtz Centre for Ocean Research Kiel, GEOMAR (DE), Swedish Metrological and Hydrological Institute, SMHI (SE), University of Exeter, Centre for Geography, Environment and Society, UNEXE (UK), Leibniz-Institute for Baltic Sea Research Warnemünde, IOW (DE).

Website	https://www.io-warnemuende.de/project/194/integral.html, https://www.bonusportal.org/projects/blue_baltic_2017-2020/integral
Project description and goals	BONUS INTEGRAL seeks to demonstrate and exploit the potential added value of the marine stations of ICOS and similar instrumentation for the ecosystem state monitoring of the Baltic Sea as an important contribution to a state-of-the-art improved HELCOM monitoring. In direct response to the requirements of the European Marine Strategy Framework Directive, BONUS INTEGRAL will provide new approaches for the monitoring of marine eutrophication and acidification, and explore the integrated greenhouse gas flux as a potential new indicator for the good environmental status of the Baltic Sea. Within BONUS INTEGRAL, the carbon system implementation in an existing high resolution, physical-biogeochemical model will be scrutinized and improved, and the model results will be evaluated against observations of the carbon system (and other variables). This approach is based on the strong, scientifically underpinned belief that the cycling of carbon is the key variable of marine biogeochemistry, is linking the effects of eutrophication and deoxygenation, and determines the magnitude of coastal acidification.
SeaLaBio partners within the project consortium and their role	IOW: Coordination, field work, modeling
Benefit to SeaLaBio	Field work in INTEGRAL will strengthen the process understanding for the carbon cycle in the Baltic Sea.
Benefit to INTEGRAL	SeaLabBio will provide additional data of the Baltic Sea carbon cycle which are not available in INTEGRAL.

Project name	**H2020 DataCube Service for Copernicus (DCS4COP)**
Start and end date	01.01.2017 – 30.11.2020
Consortium	Royal Belgian Institute of Natural Sciences (RBINS), Université Pierre et Marie Curie – Paris 6, (UPMC), Laboratoire Océanographique de Villefranche (LOV), Norsk Institutt for Vannforskning (NIVA), Brockmann Consult GMBH (BC), Vlaamse Instelling voor Technologish Onderzoek NV (VITO), Centre for Environment Fisheries and Aquaculture Science (CEFAS), University of Hull (UHULL), Starlab.
Website	http://dcs4cop.eu/
Project description and goals	DCS4COP addresses the challenges of handling big data volumes, integrating data streams from different sources and generating high-quality information from the novel sensors of the Sentinel satellite series by implementing the Copernicus Water DataCube Service as a first application. This new service model (EODataBee) will integrate Sentinel data, Copernicus Service data and user supplied data in a DataCube system that allows for tailor-made integration of data and information services into the users' business environment.
SeaLaBio partners within the project consortium and their role	BC: project coordinator; processing chain development and (NRT) running for MODIS, VIIRS, OLCI. data cube generation and maintenance
Benefit to SeaLaBio	Knowhow gained on software technologies and data layers developed within DCS4COP may be beneficial background knowledge for SeaLabio.
Benefit to DCS4COP	Implementation of the improved algorithms in the DSC4COP processing chains for improved/new data layers generation and service offer.

Project name	**H2020 CyanoAlert**
Start and end date	11/2016 to 02/2020
Consortium	Brockmann Geomatics (BG), Brockmann Consult (BC), Odermatt & Brockmann (O&B), InfoBaltic - The Information Office for the Baltic Sea (IB), Danube Delta National Institute for Research and Development (INCDDD), National Institute of Health (ISS)
Website	http://www.cyanoalert.com/
Project description and goals	CyanoAlert (funded by the European Commission under Horizon 2020 EO-1-2016 "Downstream Applications") will be a global service for environmental authorities and the commercial sector, concerned by health risks and quality of water resources. The project makes use of the wealth of information provided by Copernicus to deliver a fully automated application for assessing toxin-producing cyanobacteria blooms in water resources globally. The service foresees a dual system that provides user-specific information for monitoring and reporting purposes to paying customers, and a free and open information service for the general public.
SeaLaBio partners within the project consortium and their role	BG: coordinator; algorithm development and product validation BC: algorithm implementation and product validation; processing chain development and (NRT) running for OLCI and S2; data cube generation and maintenance.
Benefit to SeaLaBio	SeaLaBio will benefit from the expertise gained in the processing development and algorithm implementation.
Benefit to CyanoAlert	The post-project CyanoAlert service can benefit from the expertise gained in the processing development and algorithm validation.

Project name	**BONUS SEAM: Towards streamlined Baltic Sea environmental assessment and monitoring**
Start and end date	
Consortium	University of Gothenburg, DTU, TTU, SYKE, IOW
Website	www.bonusportal.org/projects/synthesis_(2018-2020)/seam
Project description and goals	HELCOM and ICES organize a long-established coordination of monitoring in the Baltic Sea. It supports regular comprehensive environmental assessments and regular advice for fisheries management. European and Baltic Sea policy for the marine environment now presents demands for a variety of information on progress towards a good environmental status and the sustainability of ecosystem services. A key challenge is to ensure that monitoring activity serves the widest range of needs in a streamlined way. New innovations for data collection and interpretation may also offer possibilities for further refining approaches to provide an increased return of information on investments in monitoring. The overall objective of the BONUS SEAM project is to elaborate a concept and proposal for a revised monitoring system for the Baltic Sea. The project will develop a proposal for a revised monitoring system for the Baltic Sea, which will communicate to, and test, with key policy and technical stakeholders, including those authorities in charge of the monitoring nationally, to ensure that there is a close fit with possible implementation routes.
SeaLaBio partners within the project consortium and their role	SYKE: Provision of information on the State-of-the-art EO methods for monitoring of Baltic Sea IOW:
Benefit to SeaLaBio	Contacts to users. Promotion of the developed methods.
Benefit to BONUS SEAM	Latest EO methods can be utilized in the planned monitoring system

Project name	**BONUS FUMARI: Future Marine Assessment and Monitoring of the Baltic Sea**
Start and end date	
Consortium	SYKE, UDE, SLU, HH, SMHI
Website	http://www.syke.fi/projects/bonusfumari
Project description and goals	The aim is to make a proposal for a renewed monitoring system of the Baltic Sea marine environment. This will require a thorough review of the gaps between the monitoring requirements set in the international legislation and the existing monitoring and data management. BONUS FUMARI will also explore the possibilities that novel monitoring methods can offer to address the shortcomings in the existing monitoring system. The recommendations aim to enhance the spatial coverage, comparability, sensitivity and cost effectiveness of Baltic Sea monitoring. The monitoring requirements are based on a wide range of international and European legislation, directives and policies. This can create overlapping and sometimes even divergent demands for the monitoring. Evaluating the current policy implementation with a gap analysis is necessary to define the synergies between various directives and to achieve their common goal of sustainable marine ecosystem management.
SeaLaBio partners within the project consortium and their role	SYKE: Provision of information on the State-of-the-art EO methods for monitoring of Baltic Sea
Benefit to SeaLaBio	Contacts to users. Promotion of the developed methods
Benefit to BONUS FUMARI	Latest EO methods can be utilized in the analysis

Activity name	**HELCOM In-Eutrophication group**
Start and end date	On-going working group of helcom
Consortium	Representatives from HELCOM participating countries
Website	http://www.helcom.fi/helcom-at-work/groups/state-and-conservation/in-eutrophication
Project description and goals	The HELCOM intersessional network on eutrophication serves as a discussion platform and operational group producing eutrophication assessments under the HELCOM State and Conservation group. The main aim of the work of the group is to develop and produce eutrophication indicators. The group works intersessionally between the meetings of the State and Conservation working group meetings. The nominated national experts regularly meet via online meetings.
SeaLaBio partners within the project consortium and their role	Chair of HELCOM intersessional network on eutrophication Ms. Vivi Fleming-Lehtinen is SeaLaBio SAG member
Benefit to SeaLaBio	Expert comments from the chair of the In-Eutrophication group
Benefit to In-Eutrophication group	Information exchange between the project and the group especially on the development of SeaLaBio

Activity name	**Baltic Earth**
Start and end date	Ongoing activity since 2013
Consortium	Individuals from various organizations from the Baltic Sea area
Website	https://www.baltic.earth
Project description and goals	Baltic Earth strives to achieve an improved Earth System understanding of the Baltic Sea region as the basis for science-based management in the face of climatic, environmental and human impact in the region. Baltic Earth brings together a broad international research community around core scientific issues identified as fundamental to informing societal efforts to achieve sustainability in the region. These “Grand Challenges” are tackled through joint research efforts, workshops, conferences and capacity building events accompanied by a continuous process of synthesis of the current state of knowledge. Communication with stakeholders and research funders

	aims to ensure impact and relevance of the research. Baltic Earth targets the atmosphere, land and marine environment of the Baltic Sea, its drainage basin and nearby areas with relevance for the Baltic Sea region The "Grand Challenges" point to hot topics in Baltic Sea research and are the basis for the Baltic Earth science plan (https://www.baltic.earth/material/Baltic_Earth_Science_Plan_2017.pdf). Of particular interest for SeaLaBio is Grand Challenge #2: "Land-Sea biogeochemical linkages in the Baltic Sea region" (https://www.baltic.earth/organisation/bewg_biogeoch/index.html).
SeaLaBio partners within the project consortium and their role	The current chairman is from IOW
Benefit to SeaLaBio	Contacts to users. Promotion of the developed methods. SeaLaBio will be included in the project list of Baltic Earth
Benefit to Baltic Earth	Improved monitoring methods for the Baltic Sea

Project name	**VESISEN 2**
Start and end date	08/2018 – 06/2018
Consortium	SYKE
Website	https://www.syke.fi/Projects/VESISEN
Project description and goals	VESISEN 2 provides EO water quality products for the water body classification of the Water Framework Directive. Data is provided via EO-database and STATUS-interface to users. Algorithm development and validation. Linkages between turbidity and phosphorus. VESISEN 2 is a follow-up project of VESISEN that generated EO-algorithms and validation for Finnish coastal waters to estimate chl-a, turbidity, Secchi disk depth and a_{CDOM}.
SeaLaBio partners within the project consortium and their role	SYKE: Produces and validates all EO products via https://syke.fi/TARKKA/en and develops STATUS-interface for EO-data.
Benefit to SeaLaBio	In situ data, algorithm development. Interface for EO-data distribution. User contacts.
Benefit to VESISEN 2	The project will end before SeaLaBio can provide improved EO methods

Activity name	**EUMETSAT IOP study**
Start and end date	12/2017 - 03/2019
Consortium	Laboratoire d'Océanologie et de Géosciences (LOG), Laboratoire d'Océanographie de Villefranche-sur-Mer (LOV), ACRI-ST
Website	-
Project description and goals	The project aims at developing community reviewed state-of-the-art Inherent Optical Properties (IOPs) products from the OLCI instrument. This study is expected to handle fundamental modelling of IOPs and marine reflectance, particularly through the NASA GIOP framework.
SeaLaBio partners within the project consortium and their role	Hubert Loisel (LOG) is part of the Scientific Advisory Group
Benefit to SeaLaBio	Expertise on the IOP and marine reflectance modelling, ideally with any dedicated model for the Baltic
Benefit to EUMETSAT IOP study	The project will end before SeaLaBio can provide improved EO method

Activity name	**EUMETSAT BPC study**
Start and end date	06/2018 - 04/2019
Consortium	SOLVO, HYGEOS, HZG
Website	https://www.eumetsat.int/website/home/Data/ScienceActivities/ScienceStudies/OceanColourBrightPixelCorrection/index.html
Project description and goals	The capability of ocean colour sensors to provide accurate water-leaving reflectances over high chlorophyll and complex waters, in particular sediment-dominated, relies on accurate and robust Ocean Colour Bright Pixel Correction (OC-BPC). This algorithm removes water-leaving signal in the near infrared (NIR) range of the spectrum in waters where such signal is not negligible, and provides smooth transition to clear oligotrophic waters. Complex waters cover most of global coastal and inland regimes, thus OC-BPC is critical to meeting ocean colour mission requirements and to many applications and data services. The purpose of this study is scientific review and development of the OC-BPC. The correction is being developed for the Copernicus Sentinel-3/OLCI Level-2 products and exploits the capabilities of the OLCI instrument. The goals of the study are to: • Review the current state-of-the-art in OC-BPC developments and evaluate impact on the quality of OLCI ocean colour products. • Propose an OC-BPC solution that is accurate, robust, unambiguous and uses OLCI extended spectral capabilities. • Prototype the selected OC-BPC solution for OLCI. • Validate the OC-BPC prototype to ensure the quality of OLCI ocean colour products. • Provide independent scientific feedback.
SeaLaBio partners within the project consortium and their role	SOLVO: prime contractor and scientific development HYGEOS: software development
Benefit to SeaLaBio	Lessons-learnt about IOPs modelling in the NIR and inverse method. Validation of alternative atmospheric correction for OLCI in the Baltic Sea.
Benefit to EUMETSAT BPC study	The project will end before SeaLaBio can provide improved EO method

4 Consolidated risk analysis

The project has the ambition to advance the current state of the art in three important scientific themes, which have to be addressed in sequential order and in rather short duration of 18 months. Although the work on one theme can start before the previous has been finally completed, a final conclusion and algorithm definition can only be performed after the previous step has been consolidated. In order to not jeopardise the whole project it is therefore important to stop algorithm development at a certain point in time even and proceed with the next step. In practice this may mean that certain aspects cannot be tackled, or successfully concluded. With this constraint in mind the risks associated to each main step are described below:

1) Atmospheric correction for the Baltic Sea, for S2 and S3

The objective of this critical step is to provide sufficiently accurate surface reflectances for the next step. This has proven challenging in the past and the main risk here is that despite the new developments, sufficient accuracy is not reached in all situations. For example, the AC may succeed in improved performance due to algorithmic revision described above, but will not find a solution for the adjacency effect. Likewise, the algorithm may work for a majority of cases but fails for example in extremely CDOM rich locations. Then we will stop the development but define a flag to indicate potential adjacency effect or other failure and increase the uncertainty for these pixels.

2) In-water retrievals for the Baltic Sea (highly absorbing waters), for S2 and S3

In addition to accurate atmospheric correction successful in-water retrieval requires sufficient information about the Specific Inherent Optical Properties (SIOPs) of water in the target areas. Thus, the quantity and quality of available in-situ data is a critical issue. We may find in-water algorithms dependent on region or time, but do not succeed in due time to find an optical water type classification to merge and blend the different algorithms. Then, we will stick to a regional algorithm selection at the costs of visible jumps in images, but still best product quality per pixel which is most important for subsequent BGC modelling.

SIOPs have been studied in the Baltic Sea by various research groups (Analysis of **other potential risks:**

Plenty of S2 and S3 images are already available from the Baltic Sea and due to the redundancy of satellites in orbit the availability of EO data is not a risk for the project.

We will follow the progress of themes and the associated risks as part of WP7 Management in form of a risks table.

Table 4). Open sea areas have been covered pretty well, at least in summer. In coastal waters SIOPs probably vary more than in the open sea. SIOP surveys are particularly scarce in those coastal waters and river estuaries where CPSs are influenced by river water. SIOPs can vary due to the share of river water in coastal waters. Moreover, SIOPs in river water can vary due to differences in the land use and soil type of the river basins. For example, different mineral particles (clay vs fine sand) probably have characteristic specific scattering properties. To our knowledge the available SIOPs in the Baltic Sea have not been compared systematically. We will do such a comparison of the key SIOPs (e.g. bp* and aph*) as part of WP2.

EO can provide only the colored component of DOC. The proportion of CDOM from DOC can vary in space and time. Thus, similarly to the previous paragraph on SIOPs, this variability has to be accounted for in the production.

3) Modelling of biogeochemical linkages land-sea

The planned improvements for the model include increase in resolution from 3 nm to 1 nm. Compared to EO data this is still quite coarse and there is a risk that land-sea links in coastal areas will not be visible enough in the model results. This must be addressed in the test area selection by including areas where gradients are present in open sea areas as well.

Analysis of other potential risks:

Plenty of S2 and S3 images are already available from the Baltic Sea and due to the redundancy of satellites in orbit the availability of EO data is not a risk for the project.

We will follow the progress of themes and the associated risks as part of WP7 Management in form of a risks table.

Table 4. SIOP data available from the Baltic Sea and from lakes of its drainage basin.

Area	Water type	Season	Reference
NW Baltic Proper	Coast and open sea	Summer	Kratzer & Moore (2018)
Southern coast of Finland	Coast	Summer	Not published (SYKE)
Gulf of Bothnia (Swedish side)	Coast and open sea	Spring and summer	Not published (SeamBoth, Kratzer)
Open Baltic sea (all basins)	Open sea	Spring	Simis et al. 2017
		Summer	Simis et al. 2017
Southern Baltic sea	Coast and open sea	Spring and summer	Several publications (IOPAN)*
Southern Baltic sea	Coast	Summer	Babin et al. (2003)
Finnish lakes	Lake	Spring and summer	Kallio (2005), Ylöstalo et al. (2014)

* Kowalczuk (1999, 2002), Darecki et al. (2003), Kowalczuk et al. (2005)

5 Consolidation of preliminary scientific requirements

5.1 Added value of the work to be carried out with respect to existing activities

5.1.1 Atmospheric correction

The existing requirement on OLCI is defined as 5. 10^{-4} uncertainty in absolute value for the marine reflectance over open waters (Donlon, 2011), and is achievable for standard AC over such waters. This number corresponds to 1.6 10^{-4} in sr^{-1}, what seems to be relevant over the Baltic Sea too, in view of retrieving the proper order of magnitude of the signal. However, this requirement over the Baltic Sea needs much more robust AC due to the complexity of the signal over the full spectrum.

The pros and cons of the approaches reviewed in section 2.1 are summarised in Table 5. This overview shows that the two types of ACs, spectral optimization and NN, are very complementary, and there is an added value to combine both and benefit from the each strength's. Since C2RCC and POLYMER are currently the best performing methods for Sentinel 2 and Sentinel 3, they will constitute the starting points for the development of a dedicated Baltic Atmospheric Correction. As pointed out before, without solving the AC problem –especially for the critical areas in the Northern and Eastern Baltic Sea, all subsequent improvements of in-water retrieval and BGC modelling would be wasted.

Table 5. Pros and cons of ACs

	Explicit modelling, spectral optimization (e.g. POLYMER)	Artificial NN (e.g. C2RCC)
Strength	Straightforward access to the modelling in the Level-2 processor for checking and improvement, and study of convergence Relevant formalism for propagating uncertainty of the path reflectance to marine reflectance	Include large knowledge of natural variability; deals with physical constraint (e.g. covariance in the IOPs) Fast computation (after training) Existing uncertainty formalism for the IOPs (e.g. uncertainty NN of C2RCC)
Weakness	Limited to a given marine model; in practice limited number of inversed IOP (e.g. no CDOM in POLYMER) and no constraint in the IOPs Potentially costly inversion	Difficult understanding of the behavior with a single end-to-end NN (e.g. failure due to ambiguity in the model) Need to train the NN after any change in the modelling

5.1.2 In water processing

As explained in Chapter 2.2, empirical, semi-analytical and full spectrum inversion performed by neural networks, are common approaches for development of water quality retrieval algorithms. Empirical algorithms are usually not sufficiently general to be valid in a variety of contexts, but can perform very well in the environment they were developed for. Compared to empirical algorithms, semi-analytical algorithms are not dependent on actual image data, but are most likely not flexible enough to encompass the full complexity and variability of the optical properties of the Baltic Sea. Compared to the empirical and semi-analytical approaches, the NN will account for a larger complexity in the spectral impact by the optically active substances on the available bands. The availability of high quality reference data for development and validation of algorithms is a limitation, as well as, the range of available training data.

On the basis of good water reflectances from the previous step, we will test different empirical algorithms which have been developed by the partners, as well as the full spectrum neural net inversion by C2RCC, and Chlorophyll which is derived as part of the POLYMER algorithm. The C2RCC neural net will be trained with a dedicated regional Baltic Water model. We will use IOPs and concentrations available within the team to characterise this regional water model, and to validate the different algorithms. We will include in our analysis a test if an optical water type characterisation and subsequent sub-basin or pixel specific algorithm selection improves the results.

One important factor for the carbon cycle understanding is the separation of Chlorophyll and CDOM from the EO signal. Another is separating Phytoplankton and Cyanobacteria in the in water retrieval. For cyanobacteria estimation we test the MPH algorithm (Pitarch et al. 2017). It is currently re-calibrated for lakes and also for the Baltic in the scope of the CyanoAlert project. It works well with concentrations above 10 µg/l and is using the red/rededge bands. For Chl –a it uses bands 681, 709, and 753 nm. For the differentiation of cyanobacteria and phytoplankton it uses the absorption at 620 nm.

In Chapter 2.2 we showed validation results of current processors against in situ data. The correspondence was good after the EO result was calibrated with in situ data. The requirements here is that the processor can provide good estimates of turbidity, CDOM and Chl-a without calibration based on local data.

The validation will be based on comparisons of surface reflectances and water parameters (IOPs, Chl concentration, CDOM absorption, TSM concentration and related parameters) with high quality in-situ measured reference data. We will use these comparisons to validate not only our retrievals but also the associated uncertainties we estimate. The validation results will be shown as traditional statistics and scatter plots but also as time series plots and transect plots (examples shown in Figure 21 and Figure 22)

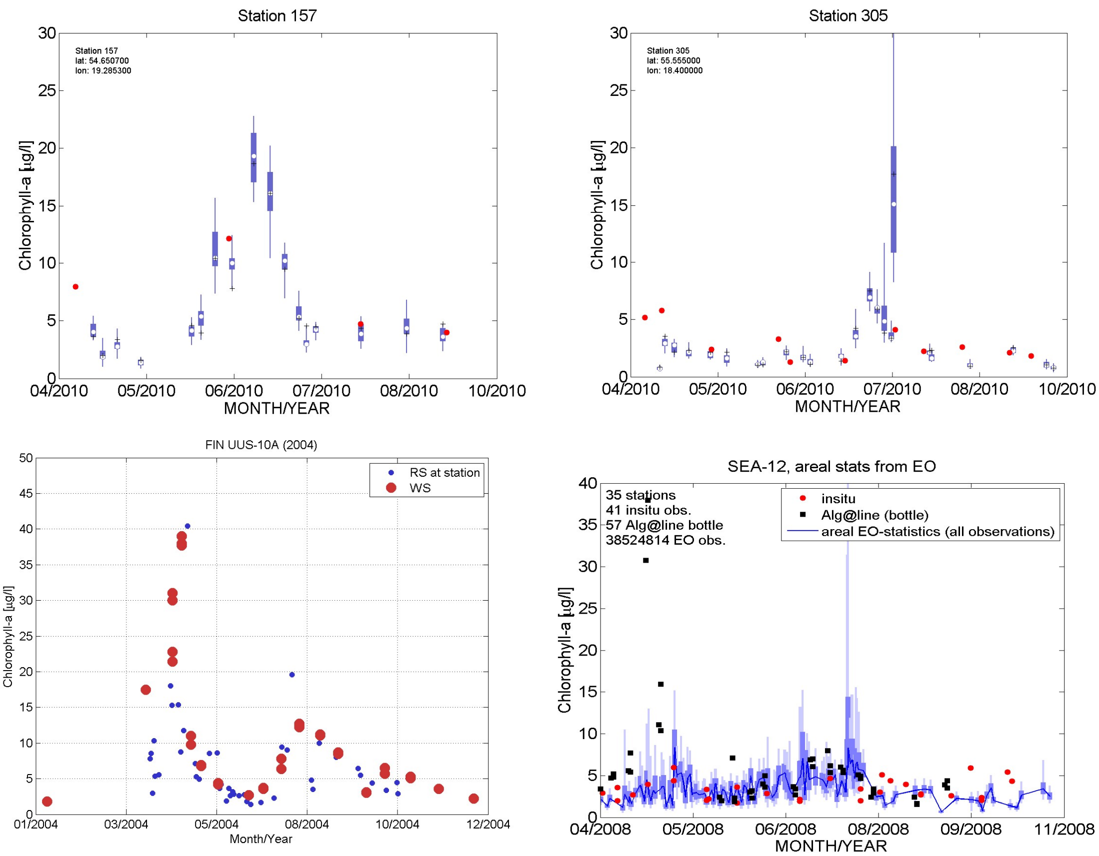


Figure 21. Examples of validation accomplished on ICES stations and HELCOM assessment areas for MERIS timeline (HELCOM EUTRO-OPER, 2015).

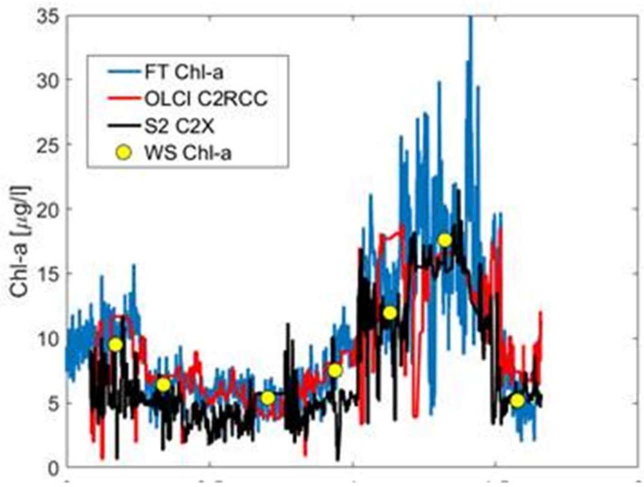


Figure 22. Initial experiments of using s3 OLCI and S2 MSI for determining Chl-a concentrations along a flow-through transect in an estuary (Helsinki, Finland). The data are processed using C2RCC-based approach (C2RCC and C2X-processors).

S2 & S3 Synergy

A synergistic use of the **spectral measurements** is difficult due to the differences in overpass time in combination with water as a rapidly changing object, and due to differences in spatial scales and viewing geometry. We will thus focus on exploring synergy on **product level**, i.e. IOPs, Chl-a, TSM etc. Figure 22 shows an example of the behavior of S2 and S3 Chl-a products along a transect of in situ measurements. Another approach is to merge the products during a temporal compositing step. A temporal window of one week should give input for a L3 product, and even when cloud coverage is taken into account a certain amount of values will be obtained at basin level. During our analysis we will make a trade-off analysis between length of the aggregation window and uncertainty introduced by the natural variability and systematic change of the quantity during that period.

If the purpose of an analysis is to study a time series at a certain point location or small area, e.g. river runoff into the sea, Sentinel 2 will be the best choice due its spatial resolution, but the time series can be gap-filled by data from Sentinel 3.

The benefit of Sentinel 2 and Sentinel 3 in combination with BGC model for the purpose of investigating land-sea interactions is the complementarity of spatial scales. Eutrophication status in the coastal waters will be assessed by Sentinel 3 data, while the high spatial resolution of Sentinel 2 allows studying river estuaries, and mixing zone of different water masses can be identified in Sentinel 2 images if the water types differ in their optical properties, e.g. due to high CDOM or TSM concentration in river waters.

5.1.3 BGC model

The added value is a data set supporting model validation and parameter calibration. A unique specific is the spatial and temporal coverage of EO products. Owing to the high spatial resolution, CDOM concentrations in rivers can be estimated and loads quantified. Attenuation coefficients derived directly from EO data provide constrains for the light climate used in BGC models. SeaLaBio is a pilot study on how EO products can be made useable for carbon cycle modeling.

5.2 Selection of test areas

The selection of test areas was based on covering different geographical areas and water quality characteristics (areas where large errors are reported in atmospheric correction and in-water processing), and on the availability of in situ data. The selected areas are shown in Table 6.

Table 6. Test areas selected for the SeaLaBio project.

Area name	Reasoning	Partner(s) responsible
Bay of Bothnia	High CDOM concentrations cause problems for AC. Availability of in situ data is good. Gradient of CDOM also in open sea areas.	SYKE, BG
Kokemäenjoki river estuary	Complex area: One large river discharging suspended solids and smaller rivers bringing CDOM rich water to the area	SYKE
Eastern Gulf of Finland (Neva river)	Largest river in the Baltic Sea bringing large amounts of suspended and dissolved matter into the Gulf of Finland. Not much data available so the need for better monitoring is great.	SYKE
Archipelago of Stockholm and Åland Sea	Archipelagic areas with many and small islands and islets. Turbid waters with influence from land and inland waters.	BG, SYKE
ICES Stations German part of Baltic Sea	ICES collection of in-situ measurements for match-up and time series analysis. (could be easily extended to whole Baltic Sea when using full collection)	BC
Bights along German Baltic Sea	Förde and Bights along the German Baltic Sea. Adjacency effect can be well tested in relatively straight, but small bights; Greifswalder Bodden as large, but rather closed system	BC
Schlei	The Schlei has brackish water, has a bad ecological status, is highly contaminated with nutrients and heavy metals, high chl a concentration; investigation of resolvable water bodies (spatial resolution)	BC
Open sea area of Baltic Proper	A reference case area with not much terrestrial influence	SYKE

5.3 Analysis of technical and scientific constraints

The technical and scientific constraints are closely related to the risks in atmospheric correction, in-water retrieval and modelling of biogeochemical land-sea linkages (described in Chapter 4). Due to the sequential flow of data and processing, failures in atmospheric correction constrain in-water retrieval and so forth. It has been shown that within the Baltic Sea area EO methods have been able to provide reasonable results in many cases while in others they have failed. Advances in the atmospheric correction are expected to not only improve the results in successful cases but also to improve the coverage towards more extreme cases. The magnitude of the improvements – and possible constraints – cannot be assessed until the algorithm modifications described in earlier chapters are implemented and tested.

5.4 Summary of Preliminary Scientific Requirements

Table 7 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.

Concerning the atmospheric correction, a quantified requirement on the accuracy of the marine reflectance over complex waters does not - to our knowledge - exist in the literature and will be investigated during the study, as part of WP3. The only requirement existing to date for ocean colour radiometry was historically derived for Case-1 waters: starting from the requirement to discriminate 10 classes of chlorophyll values within each of the 3 decades between 0.03 and 30 mg/m^3, and given a blue-to-green band ratio algorithm, Antoine and Morel (1999) have found that atmospheric correction errors over the open ocean must be maintained within ±1-2 10^{-3} at 443 nm, within ±5 10^{-4} at 490 nm, and within ±2 10^{-4} at 560 nm, which has become an OLCI mission requirement (Donlon, 2011). We will conduct a similar methodology with the in-water inverse methods considered over the Baltic (empirical algorithms and neural networks). This can be handled through sensitivity study: starting from reference spectra characterizing reference sets of IOPs, how much error is acceptable on the radiometry (both absolute and spectrally variable biases) so that the inversed IOPs remain within the required range of accuracy? Compared to the Case-1 situation where by definition all particles and dissolved material are supposed to co-vary with one unique parameter (chlorophyll), an additional challenge over the Baltic is that the various IOPs are independent and requires a multi-dimensional sensitivity study.

Regarding the in-water parameters, Table 8 shows the expanded uncertainty of laboratory analyses in Finnish water laboratories. Sorensen et al. (2010) found that the accuracy of the laboratory analyses for Chl-a varies between 10 to 25% for the HPLC and from 5 to 25% for the spectrophotometric determination. Our preliminary goal is to reach similar uncertainties with EO products. This will be further defined during WP3.

Table 7. 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.

Table 8. Expanded uncertainty (95% confidence level) of in-water parameter determinations reported by Finnish water laboratories (based on 1-4 laboratories) and recommended for water laboratories in Finland (Näykki & Väisänen 2016).

Parameter	Finnish laboratories	Recommendation for laboratories
Chl-a	15 – 40% (for Chl-a >2 g/l)	< 20% (Chl-a >2 μg/l)
TSM	20%	< 20% (TSM >3 mg/l)
Turbidity	10 – 20%	< 20% (Turb > 1 FNU)
acdom(400)	10%	-

5.5 Consultation with the Scientific Advisory Group (SAG)

A Scientific Advisory Group (SAG) has been established for the project. Its role will be to:

- Review the Requirement Baseline (RB) document and participate to or provide comments before the Progress Meeting 1 on March 21 2019
    - The comments received from SAG members have been used to improve the content of this second version of the document
- Review ATBDs and Product Validation Report and participate (remotely or in person or by providing comments by email) to the Mid Term Review (July 2-3, 2019 in Helsinki,)
- Iterate the Scientific Roadmap with the team during spring 2020
- Participate in the Final Review (remotely or in person, or through email comments prior to the meeting), current plan: May 27, 2020

The members of the group are:

- Karl Norling, Senior Analyst, Environmental Monitoring, Science Affairs Department, Swedish Agency for Marine and Water Management
- Harri Kuosa Finnish Environment Institute
- Vivi Fleming-Lehtinen 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

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