

DOCTORAL THESIS

Processes Influencing Coastal
Water Quality in the Eastern
Baltic Sea as Observed from
Remote Sensing Data

Age Aavaste

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Declaration:

Hereby I declare that this doctoral thesis, my original investigation and achievement, submitted for the doctoral degree at Tallinn University of Technology has not been submitted for doctoral or equivalent academic degree.

Age Aavaste

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**Kaugseire andmetest hinnatud
rannikuvee kvaliteeti mõjutavad protsessid
Läänemere idaosas**

AGE AAVASTE



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List of Publications

The list of author's publications, on the basis of which the thesis has been prepared:

- I Aavaste, A., Sipelgas, L., Uiboupin, R., Uudeberg, K., 2021. **Impact of Thermohaline Conditions on Vertical Variability of Optical Properties in the Gulf of Finland (Baltic Sea): Implications for Water Quality Remote Sensing.** *Frontiers in Marine Science*, 8, 674065. DOI: 10.3389/fmars.2021.674065
- II Toming, K., Kutser, T., Uiboupin, R., Arikas, A., Vahter, K., Paavel, B., 2017. **Mapping Water Quality Parameters with Sentinel-3 Ocean and Land Colour Instrument Imagery in the Baltic Sea.** *Remote Sensing*, 9(10), 1070. DOI: 10.3390/rs9101070
- III Uudeberg, K., Aavaste, A., Kõks, K.-L., Ansper, A., Uusõue, M., Kangro, K., Ansko, I., Ligi, M., Toming, K., Reinart, A., 2020. **Optical Water Type Guided Approach to Estimate Optical Water Quality Parameters.** *Remote Sensing*, 12(6), 931. DOI: 10.3390/rs12060931.
- IV Sipelgas, L., Uiboupin, R., Arikas, A., Siitam, L., 2018. **Water quality near Estonian harbours in the Baltic Sea as observed from entire MERIS full resolution archive.** *Marine Pollution Bulletin*, 126, 565–574. DOI: 10.1016/j.marpolbul.2017.09.058.
- V Sipelgas, L., Aavaste, A., Uiboupin, R., 2021. **Mapping Flood Extent and Frequency from Sentinel-1 Imagery during the Extremely Warm Winter of 2020 in Boreal Floodplains and Forests.** *Remote Sensing*, 13(23), 4949. DOI: 10.3390/rs13234949.

Author's Contribution to the Publications

The author's contributions to the papers included in this thesis are:

- I The author participated in field measurements, processed and analysed *in situ* data, downloaded and processed remote sensing data, and prepared the manuscript.
- II The author participated in the fieldwork, carried out the laboratory analysis of data collected on board the R/V Salme, and contributed to manuscript writing.
- III The author participated in field measurements in the Gulf of Finland, processed and analysed the *in situ* data from the Gulf of Finland (Chl-*a*, TSM, RAMSES), made a partial contribution to the search for published algorithms on water quality parameters, and contributed to the manuscript writing.
- IV The author was responsible for processing the remote sensing data and contributed to the manuscript writing.
- V The author processed Sentinel-1 and Sentinel-2 data, participated in water mapping fieldwork using a drone, evaluated the accuracy of open-water mapping, and contributed to the manuscript writing.

Abbreviations

AOPs	apparent optical properties
ASAR	Advanced Synthetic Aperture Radar
C2R	Case II Regional processor
C2RCC	Case 2 Regional CoastColour processor
CDOM	coloured dissolved organic matter
CHIME	Copernicus Hyperspectral Imaging Mission for the Environment
Chl- <i>a</i>	chlorophyll- <i>a</i>
CTD	conductivity, temperature and depth
CZCS	Coastal Zone Color Scanner
DOM	dissolved organic matter
ERS	European Remote Sensing satellite
EW	Extended Wide swath mode
FR	full resolution
FUV	flooding under vegetation
GRD	Ground Range Detected
HH	horizontal transmit and horizontal receive polarization
HS	hydrological station
HV	horizontal transmit and vertical receive polarization
IOPs	inherent optical properties
IW	Interferometric Wide swath mode
L1	Level-1
L2	Level-2
MAE	mean absolute error
MAPE	mean absolute percentage error
MERIS	Medium Resolution Imaging Spectrometer
MNDWI	modified normalized difference water index
MODIS	Moderate Resolution Imaging Spectroradiometer
MSI	Multispectral Instrument
NIR	near-infrared
NN	neural network
OCI	Ocean Color Instrument
OLCI	Ocean and Land Colour Instrument
OLI	Operational Land Imager
OSCs	optically significant constituents
OWF	open-water flooding
OWT	optical water type
PACE	Plankton, Aerosol, Cloud, ocean Ecosystem
PAR	photosynthetically active radiation
PRISMA	PRecursore IperSpettrale della Missione Applicativa

RMSE	root mean square error
RMSLE	root mean square logarithmic error
ROI	region of interest
SAR	synthetic aperture radar
SD	standard deviation
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SLSTR	Sea and Land Surface Temperature Radiometer
SPIM	suspended particulate inorganic matter
SPOM	suspended particulate organic matter
SST	sea surface temperature
TIRS	Thermal Infrared Sensor
TSM	total suspended matter
VH	vertical transmit and horizontal receive polarization
VIIRS	Visible Infrared Imaging Radiometer Suite

Symbols

λ	wavelength
$a(\lambda)$	spectral absorption coefficient
$a_{\text{CDOM}}(\lambda)$	spectral absorption coefficient of coloured dissolved organic matter
$a_{\text{CDOM}}(442)$	spectral absorption coefficient of coloured dissolved organic matter at 442 nm
$b(\lambda)$	spectral scattering coefficient
$b_b(\lambda)$	spectral backscattering coefficient
$c(\lambda)$	spectral attenuation coefficient
$E_d(0^+, \lambda)$	spectral downwelling irradiance just above the water surface
$E_u(\lambda)$	spectral upwelling irradiance
$K_d(\lambda)$	spectral diffuse attenuation coefficient for downwelling irradiance
$L_{\text{sky}}(\lambda)$	spectral sky radiance
$L_t(\lambda)$	total spectral radiance
$L_u(\lambda)$	spectral upwelling radiance
$L_w(\lambda)$	spectral water-leaving radiance
$R(\lambda)$	spectral water-leaving reflectance
$R_{\text{rs}}(\lambda)$	spectral remote sensing reflectance
$z_{90}(\lambda)$	optical depth from which 90% of the water-leaving signal originates
ρ	air-sea interface reflection coefficient
R	correlation coefficient
R^2	coefficient of determination
p	statistical significance level
B3	Sentinel-2 MSI green band used in the modified normalized difference water index
B11	Sentinel-2 MSI shortwave infrared band used in the modified normalized difference water index

Introduction

1.1 Environmental Drivers of Coastal Water Quality in the Baltic Sea

Coastal water quality in the Baltic Sea is shaped by physical forcing, biogeochemical processes and human activities that modify the concentration, composition and vertical distribution of optically significant constituents (OSCs). The main OSCs affecting the optical signal in Baltic Sea coastal waters are coloured dissolved organic matter (CDOM), total suspended matter (TSM) and phytoplankton. The optical contribution of phytoplankton is mainly associated with its pigments, particularly chlorophyll-*a* (Chl-*a*). These constituents determine the absorption, scattering and attenuation of light, water transparency and the spectral shape of the water-leaving signal measured by optical remote sensing sensors (Kowalczuk et al., 2006; Alikas and Kratzer, 2017; Kratzer and Moore, 2018; Kangro et al., 2026). Their effects are particularly important in the eastern Baltic Sea, where shallow coastal areas, semi-enclosed bays, riverine input, sediment resuspension and seasonal stratification create strong optical heterogeneity (Sipelgas et al., 2004; Paavel et al., 2011; Rahn et al., 2023).

The Baltic Sea is a shallow, semi-enclosed brackish sea with restricted water exchange through the Danish Straits and a drainage basin much larger than the sea itself. The large freshwater surplus creates strong horizontal salinity gradients and contributes to density stratification, while local coastal conditions modify basin-scale gradients through river discharge, bathymetry, wind-driven circulation and residence time (Leppäranta and Myrberg, 2009; Lehmann et al., 2022; Meier et al., 2022). In shallow coastal waters, these processes determine whether land-derived material is retained near the coast, mixed within the water column or transported offshore (Carstensen et al., 2020; Vigouroux et al., 2021; Friedland et al., 2025).

1.1.1 Riverine Forcing

Riverine input transports freshwater, nutrients, suspended particles and dissolved organic matter to Baltic Sea coastal waters (Kowalczuk et al., 2006; Humborg et al., 2007; Kuliński et al., 2022; Friedland et al., 2025). CDOM, the optically active fraction of dissolved organic matter, absorbs light strongly in the ultraviolet and blue spectral regions and links terrestrial organic matter export directly to the optical properties of coastal waters (Kowalczuk et al., 2006; Harvey et al., 2015; Voss et al., 2021). Suspended particles introduced by rivers, coastal erosion and resuspension mainly affect scattering and turbidity (Kyryliuk and Kratzer, 2019; Kratzer et al., 2020), while nutrient inputs may later modify phytoplankton biomass (Kuliński et al., 2022; Berthold et al., 2025).

The spatial and temporal expression of riverine influence depends on discharge, wind forcing, coastal circulation and the background density field. River plumes can therefore form strong gradients in salinity, CDOM, TSM and nutrients near river mouths and semi-enclosed bays, but their extent and persistence vary with hydrodynamic conditions (Lips et al., 2016; Soosaar et al., 2016; Friedland et al., 2025). Seasonal runoff and flood events can intensify this influence by producing short-term pulses of land-derived material (Ylöstalo et al., 2016; Voynova et al., 2017; Friedland et al., 2025). The optical response is not necessarily synchronous for all parameters: CDOM absorption and TSM-related scattering may respond rapidly to riverine export, whereas phytoplankton biomass can change later if nutrient inputs stimulate growth (Kowalczuk et al., 2006; Ylöstalo et al., 2016; Seidel et al., 2017; Voss et al., 2021; Friedland et al., 2025).

1.1.2 Phytoplankton Seasonality and Optical Complexity

Nutrient enrichment affects coastal water quality mainly through phytoplankton production, organic matter cycling and changes in water transparency. In the Baltic Sea, phytoplankton seasonality is pronounced, with optically different bloom phases during the productive season (Conley et al., 2009; Kuliński et al., 2022; HELCOM, 2023). Spring blooms are commonly dominated by diatoms and dinoflagellates, while summer conditions often include cyanobacteria, especially under warm and stratified conditions (Simis et al., 2017; Rahn et al., 2023). These seasonal changes affect pigment absorption, particle scattering and the spectral characteristics used in satellite-based retrievals (Brando et al., 2021; Ansper-Toomsalu et al., 2024; Rahn et al., 2026).

The optical complexity of Baltic Sea waters arises because CDOM, suspended particles and phytoplankton biomass vary partly independently. High CDOM absorption suppresses the blue part of the spectrum, while particles and phytoplankton affect the green, red and near-infrared (NIR) regions through scattering and pigment absorption (Darecki and Stramski, 2004; Kowalczyk et al., 2006; Kratzer and Moore, 2018). Similar reflectance spectra may therefore correspond to different combinations of OSCs. This ambiguity limits the transferability of standard open-ocean remote sensing algorithms and requires regionally evaluated or water-type-specific approaches (Odermatt et al., 2012; Moore et al., 2014; Paper III).

1.1.3 Physical Processes: Coastal Upwelling

Wind-induced coastal upwelling can rapidly modify the surface layer by bringing colder subsurface water into the upper water column. The immediate signal is usually a decrease in sea surface temperature (SST), but upwelling also changes salinity, nutrient availability and the near-surface distribution of OSCs (Myrberg and Andrejev, 2003; Vahtera et al., 2005; Uiboupin et al., 2012; Dabuleviciene et al., 2020; Skudra et al., 2023). In optical remote sensing, this is important because the water-leaving signal measured by the satellite sensor is controlled by the properties of the surface optical layer. Upwelling can therefore alter the optical signal through water-mass displacement before any later biological response becomes visible.

A Baltic Sea-wide analysis of SST data for 2002–2020 identified 19 recurrent coastal upwelling zones, with zone lengths of 50–370 km and widths of 10–54 km. The strongest seasonality occurred from May to October, with monthly occurrence locally reaching up to 30% in September and October (Zhang et al., 2022).

1.1.4 Physical Processes: Sediment Dynamics

Shallow coastal waters are also affected by sediment resuspension. Wind waves, currents and vessel-induced mixing can increase suspended matter concentrations and turbidity, especially where fine bottom sediments are available and the water is shallow (Kutser et al., 2007; Suursaar et al., 2009; Kyrlyuk and Kratzer, 2019). Harbour-related activities, including dredging, sediment disposal, port construction and vessel traffic, can intensify these effects by disturbing bottom sediments and increasing particle concentrations. However, the attribution of harbour-related turbidity is complicated because natural resuspension and seasonal variability may produce signals comparable to direct anthropogenic disturbance (Kutser et al., 2007; Raag et al., 2014; Doxaran et al., 2026).

The optical effect of suspended matter also depends on particle composition. Mineral particles generally increase scattering and the magnitude of water-leaving reflectance,

whereas organic particles may contribute more to absorption in the blue and blue-green spectral regions (Babin et al., 2003; Kyriliuk and Kratzer, 2019; Kratzer et al., 2020; Doxaran et al., 2026). This distinction is relevant near harbours and river mouths, where turbidity and CDOM may increase for different reasons. TSM mainly reflects particle-related processes, whereas CDOM is more closely associated with dissolved organic matter and riverine influence (Kowalczyk et al., 2006; Harvey et al., 2015; Kyriliuk and Kratzer, 2019).

1.2 Satellite Remote Sensing in Water Quality Monitoring

Satellite remote sensing is used in water quality monitoring to resolve near-surface spatial variability that discrete sampling captures only locally. *In situ* measurements provide direct biogeochemical and optical observations at sampling locations, whereas satellite data show how near-surface conditions vary over larger water areas. In the Baltic Sea, satellite data have been used to assess Chl-*a*, cyanobacterial blooms, CDOM, TSM, turbidity and Secchi depth (Darecki and Stramski, 2004; Kutser et al., 2006; Attila et al., 2013; Alikas and Kratzer, 2017; Ligi et al., 2017; Kratzer and Moore, 2018; Brando et al., 2021; Soomets et al., 2022; Rahn et al., 2023; González Vilas et al., 2024; Ansper-Toomsalu et al., 2024; Attila et al., 2025). In all these applications, the target signal is spectral water-leaving radiance or reflectance, from which near-surface water quality conditions are derived.

Optical remote sensing of water quality is based on the measurement of solar radiation that has penetrated the water column, interacted with water and its OSCs, and returned through the water surface towards the sensor (Figure 1). The resulting water-leaving radiance and reflectance are governed by absorption and scattering processes caused by pure water, CDOM, phytoplankton pigments and suspended particles (Mobley, 1994; Kirk, 2011; IOCCG, 2018). The radiance measured at the sensor includes atmospheric and surface contributions, which must be removed before water quality parameters can be retrieved. Its interpretation is limited by the upper optical depth of the water column and by uncertainties related to atmospheric correction, surface conditions and the bio-optical properties of the water (IOCCG, 2000; Mobley et al., 2016).

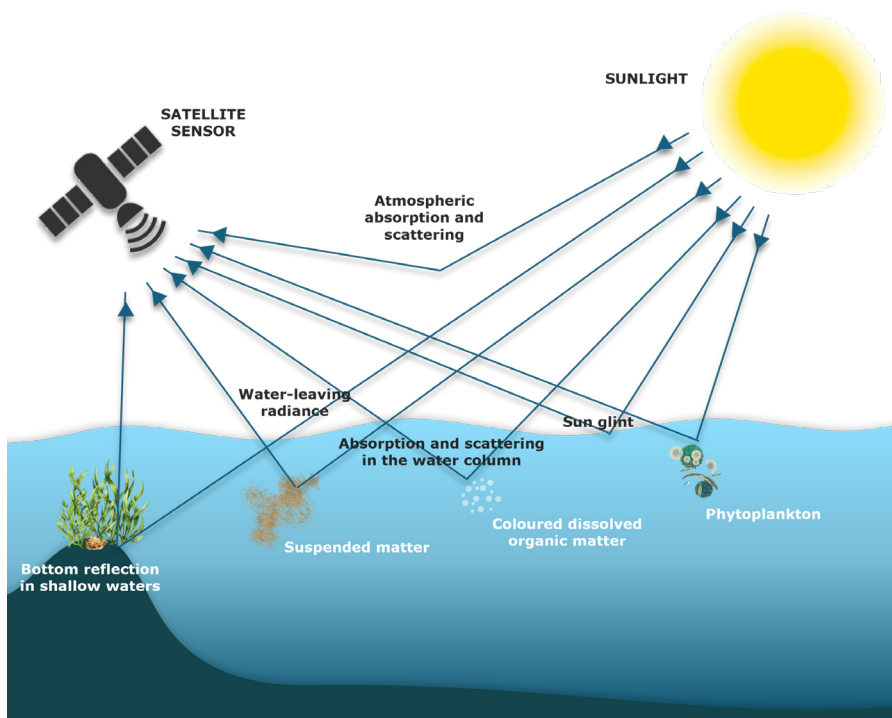


Figure 1. Formation of the optical signal measured by a satellite sensor over water.

The Baltic Sea is challenging for optical remote sensing because the water-leaving signal is weak and spectrally complex. High CDOM absorption reduces water-leaving reflectance in the blue spectral region, while phytoplankton and suspended particles vary strongly in space and time (Darecki and Stramski, 2004; Kowalczyk et al., 2006; Simis et al., 2017; Kratzer and Moore, 2018). Low sun angles, seasonal bloom dynamics, cyanobacterial accumulations and adjacency effects in coastal areas further increase retrieval uncertainty (Soomets et al., 2022; Paper II). These conditions require atmospheric correction and retrieval algorithms to be evaluated specifically for Baltic Sea coastal waters (Soomets et al., 2022; González Vilas et al., 2024; Ansper-Toomsalu et al., 2024; Paper II).

Satellite-based water-colour monitoring is based on multispectral sensors that differ in spatial resolution, spectral coverage and mission period. Long-term records include observations from the Coastal Zone Color Scanner (CZCS) on Nimbus-7, the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) on OrbView-2, the Moderate Resolution Imaging Spectroradiometer (MODIS) on Terra and Aqua, and the Visible Infrared Imaging Radiometer Suite (VIIRS) on Suomi NPP and NOAA-20/21 (Groom et al., 2019; Müller et al., 2026). For Baltic Sea applications, the Medium Resolution Imaging Spectrometer (MERIS) on Envisat and the Ocean and Land Colour Instrument (OLCI) on Sentinel-3 are important medium-resolution sensors. Their spectral configuration is suitable for optically complex waters. MERIS supports historical analyses for 2002–2012, whereas Sentinel-3 OLCI continues comparable observations with 21 spectral bands and 300 m spatial resolution (Donlon et al., 2012; Brando et al., 2021; Soomets et al., 2022; Paper II).

The Multispectral Instrument (MSI) onboard Sentinel-2 and the Operational Land Imager (OLI) on Landsat 8 and Landsat 9 provide finer spatial resolution than OLCI, which is useful for narrow coastal zones and small water bodies. However, their spectral band configuration was not optimised for ocean colour retrieval, unlike dedicated ocean colour sensors (Drusch et al., 2012; Warren et al., 2019; Pahlevan et al., 2020; Soomets et al., 2020; Ansper-Toomsalu et al., 2024; Müller et al., 2026). Hyperspectral missions, including PRISMA (PRecursore IperSpettrale della Missione Applicativa), the Ocean Color Instrument (OCI) on NASA's Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission and the planned Copernicus Hyperspectral Imaging Mission for the Environment (CHIME), provide finer spectral sampling for optically complex waters, where CDOM, phytoplankton pigments and suspended particles have overlapping spectral effects (Bresciani et al., 2022; Dierssen et al., 2023; Werther et al., 2025; Xu et al., 2026). Geostationary ocean colour sensors provide high-frequency observations that are valuable for dynamic coastal waters, but current systems do not provide operational coverage for the Baltic Sea region (Portela et al., 2024).

Optical sensors provide information on water colour (the spectral signal shaped by OSCs). However, process-based interpretation of coastal water quality may also require information from complementary sensor types, including thermal infrared and radar observations. Thermal infrared sensors, such as the Moderate Resolution Imaging Spectroradiometer (MODIS) onboard Terra and Aqua, the Sea and Land Surface Temperature Radiometer (SLSTR) onboard Sentinel-3 and the Thermal Infrared Sensor (TIRS) onboard Landsat 8 and Landsat 9, retrieve SST from emitted thermal radiance. Satellite-derived SST represents the sea-surface skin layer rather than bulk water temperature. SST fields can be used to detect large-scale thermal patterns, coastal upwelling, fronts and mesoscale variability (Donlon et al., 2002; Donlon et al., 2012; Uiboupin and Laanemets, 2015; Bradtke, 2021; Beauchamp et al., 2025; Paper I).

Radar remote sensing provides information independent of water colour and light conditions. Synthetic Aperture Radar (SAR) is an active microwave imaging technique that records backscattered energy, which depends on sensor wavelength, polarization, incidence angle and target properties. Over open water, the return is primarily controlled by wind-generated capillary and short gravity waves, whereas land, ice and vegetated floodplain surfaces are also affected by dielectric and structural contrasts (Hasselmann et al., 1985; Ulaby et al., 1986; Plant, 1990; Rikka et al., 2018). SAR observations from missions such as ERS-1/2, Envisat Advanced Synthetic Aperture Radar (ASAR), RADARSAT, TerraSAR-X/TanDEM-X and Sentinel-1 have been used to detect wind and wave patterns, sea ice, surface films, oil spills and inundation (Voormansik et al., 2014; Rikka et al., 2017; Rikka et al., 2018; Paper V; Hasimoto-Beltran et al., 2023; Eriksson et al., 2025; Vidjajev et al., 2025). The ability of SAR to acquire data independently of daylight and cloud cover makes it suitable for flood mapping in boreal regions, where optical observations are often limited during flood events (Paper V; Portalés-Julià et al., 2025).

1.3 Optical Basis of Water Quality Remote Sensing

Understanding the optical properties of natural waters is fundamental for accurately interpreting remote sensing data and assessing water quality. These optical properties are classified into two main categories: inherent optical properties (IOPs) and apparent optical properties (AOPs) (Preisendorfer, 1976; Mobley, 1994; Kirk, 2011).

IOPs depend only on the aquatic medium and its constituents. These properties influence how light is absorbed and scattered within the water, independent of external factors such as the angle of incoming light. The absorption coefficient $a(\lambda)$ describes the rate at which light diminishes as it passes through a medium due to absorption, whereas the scattering coefficient $b(\lambda)$ quantifies the rate of reduction in light intensity due to scattering processes (Preisendorfer, 1976; Dera, 1992; Kirk, 2011). These properties are fundamental in determining the beam attenuation coefficient $c(\lambda)$, which represents the total loss of light intensity as a result of both absorption and scattering (Mobley, 1994; Kirk, 2011):

$$c(\lambda) = a(\lambda) + b(\lambda). \quad (1)$$

The coefficients $a(\lambda)$, $b(\lambda)$ and $c(\lambda)$ are expressed in m^{-1} and vary as a function of wavelength. Their magnitude and spectral shape are determined by pure water and by OSCs, including phytoplankton pigments, TSM and CDOM (Prieur and Sathyendranath, 1981; Mobley, 1994; Babin et al., 2003; Kirk, 2011). The bulk IOPs of natural waters can be expressed using an additive formulation, where the total coefficient is represented as the sum of contributions from pure water and individual OSCs. The contribution of each constituent depends on its concentration and constituent-specific optical properties (Prieur and Sathyendranath, 1981; Arst, 2003; Kirk, 2011). For instance, the total absorption coefficient can be expressed as:

$$a(\lambda) = a_w(\lambda) + \sum_i a_i^* C_i. \quad (2)$$

where a_w is the absorption coefficient of pure water, a_i^* is a specific absorption coefficient of the i -th constituent, and C_i is the concentration of the i -th constituent. Similar additive expressions apply to the scattering and attenuation coefficients, although it is important to note that CDOM typically does not contribute to scattering (Mobley, 1994).

The additive formulation does not mean that constituent concentrations can be retrieved by a fixed universal conversion. The specific absorption and scattering coefficients of phytoplankton and suspended particles vary with pigment composition, cell size, particle size distribution, refractive index and mineral or organic composition (Bricaud et al., 1995; Babin et al., 2003; Stramski et al., 2004; Kirk, 2011). Phytoplankton affects absorption mainly through chlorophyll- a (Chl- a) and accessory pigments, with Chl- a absorption maxima around 440 nm and 675 nm, while chlorophyll- b , chlorophyll- c , carotenoids and phycobiliproteins modify absorption in additional blue, green and red spectral regions (Morel and Prieur, 1977; Bricaud et al., 1995; Simis et al., 2005; Kirk, 2011; IOCCG, 2014). Phytoplankton also contributes to scattering, and both absorption and scattering vary with cell size, pigment packaging, species composition and physiological state (Bricaud et al., 1995; Stramski et al., 2004; Kirk, 2011). CDOM is primarily an absorbing constituent, with strong absorption in the ultraviolet and blue spectral regions that decreases towards longer wavelengths (Bricaud et al., 1981; Kowalczyk et al., 2006; Coble, 2007). TSM contributes to both absorption and scattering, with mineral particles generally producing stronger scattering and backscattering signals, while organic detrital particles also contribute to absorption at shorter visible wavelengths, partly overlapping with CDOM absorption (Babin et al., 2003; Stramski et al., 2004; Kirk, 2011). Pure water itself absorbs strongly in the near-infrared and infrared regions (Morel and Prieur, 1977).

The angular distribution of scattering is described by the volume scattering function, $\beta(\theta, \lambda)$, from which total scattering and backscattering are derived (Mobley, 1994; Kirk,

2011). The spectral backscattering coefficient, $b_b(\lambda)$, represents scattering into the backward hemisphere:

$$b_b(\lambda) = 2\pi \int_{\frac{\pi}{2}}^{\pi} \beta(\theta, \lambda) \sin\theta d\theta \quad (3)$$

where $\beta(\theta, \lambda)$ is the volume scattering function, describing the angular distribution of scattered light at a given wavelength λ and angle θ . Backscattering is the scattering component most directly related to water-leaving radiance (Gordon et al., 1975; Morel and Prieur, 1977; Dekker et al., 1997; Lo Prejato et al., 2020). Increased absorption reduces the probability that photons leave the water column, whereas increased backscattering increases the fraction of light redirected towards the surface. The ratio between backscattering and absorption therefore controls much of the magnitude and spectral shape of the remotely measured signal (Gordon et al., 1975; Kirk, 1984; Lo Prejato et al., 2020).

AOPs depend on both the IOPs of the water and the ambient light field. These are not properties of the aquatic medium alone, but also depend on illumination geometry, sky conditions, surface roughness and the angular distribution of radiance within the water column (Preisendorfer, 1976; Mobley, 1994; Kirk, 2011). In water colour remote sensing, the most relevant AOPs include the remote sensing reflectance ($R_{rs}(\lambda)$), water-leaving reflectance ($R(\lambda)$) and the diffuse attenuation coefficient for downwelling irradiance ($K_d(\lambda)$) (Mobley, 1994; Kirk, 2011). $R_{rs}(\lambda)$ and $R(\lambda)$ describe the spectral signal measured by *in situ* radiometers and satellite sensors, whereas $K_d(\lambda)$ describes the vertical attenuation of downwelling light. $K_d(\lambda)$ is also used to characterise the underwater light field and to estimate the euphotic depth, commonly defined by the 1% surface light level relevant for photosynthesis (Kirk, 2011).

The distinction between IOPs and AOPs is important for interpreting satellite-derived water quality products. Satellite sensors measure radiance at the sensor level and after atmospheric correction the resulting water-leaving signal is used to retrieve water quality parameters. In optically complex coastal waters similar optical signals may arise from different combinations of absorption and scattering processes (Werther et al., 2025; Müller et al., 2026). This limits the use of universal algorithms and supports the need for *in situ* optical measurements, regional validation of retrieval methods and optical water type classification (Darecki and Stramski, 2004; Kowalczyk et al., 2006; Kratzer and Moore, 2018; Uudeberg et al., 2019; Soomets et al., 2022; Paper II; Paper III).

1.4 Aim and Objectives

The overall aim of this thesis is to assess how satellite remote sensing can be used to detect and interpret processes influencing coastal water quality in the eastern Baltic Sea, with emphasis on optically complex Estonian coastal waters. The thesis links water-column optical variability, regional retrieval performance and multi-sensor observations of coastal water quality responses to natural and anthropogenic forcing.

The specific objectives were:

- to determine how thermohaline structure and upwelling-driven water mass displacement alter the vertical distribution of IOPs and OSCs, and how these changes affect AOPs and the remotely sensed water-leaving signal (Paper I);
- to evaluate the applicability of Sentinel-3 OLCI data, standard processing chains and empirical algorithms for estimating reflectance, IOPs and water quality parameters in the Baltic Sea (Paper II);

- to assess whether and how optical water type classification improves the retrieval of CDOM absorption in boreal inland and coastal waters (Paper III);
- to quantify decadal variability in MERIS-derived TSM and CDOM near Estonian harbours and assess the influence of wind conditions, river discharge and vessel traffic on the observed TSM and CDOM variability (Paper IV);
- to develop and apply a Sentinel-1 SAR-based approach for mapping flood extent and frequency in boreal floodplains, including open-water flooding and flooding under vegetation (Paper V);
- to combine Sentinel-1 flood mapping with Sentinel-3 OLCI-based CDOM retrievals to evaluate flood-induced water quality variability in coastal waters influenced by riverine input.

2 Materials and Methods

2.1 Study Areas

2.1.1 Baltic Sea and Freshwater Areas

This research focuses mainly on optically complex waters in the eastern Baltic Sea region, including the Gulf of Finland, Pärnu Bay, Matsalu Bay, Moonsund Sea and Estonian harbour areas (Papers I–IV, Figure 2). Additional study areas from the Southern Baltic Sea (Paper II) and the Western Gotland Basin (Paper III), together with boreal lakes in Estonia and Finland (Paper III), were included to cover a broader range of optical conditions (Figure 2).

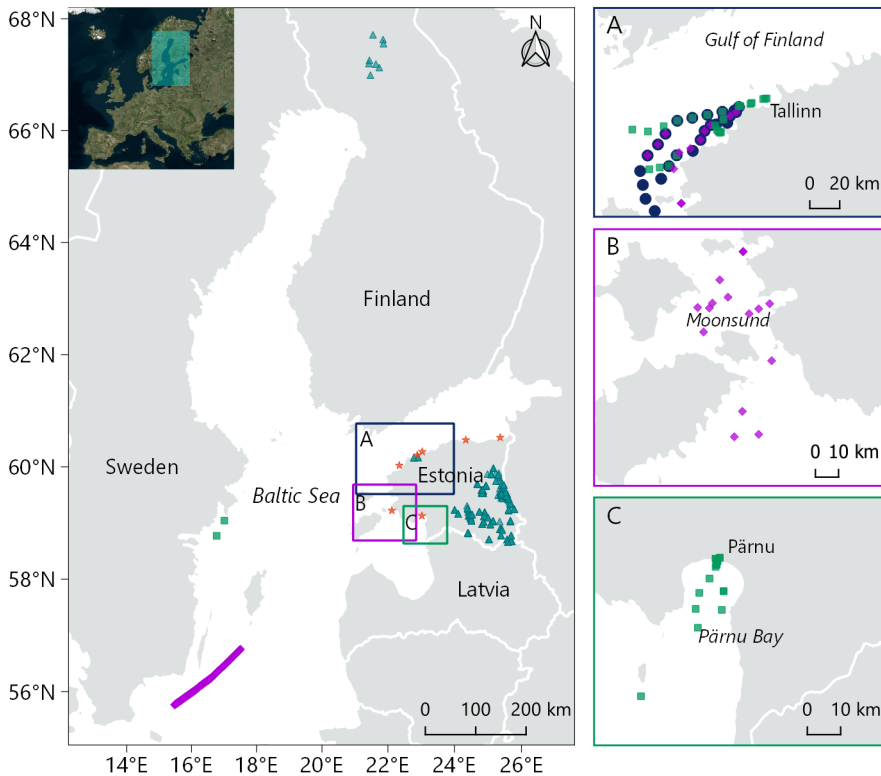


Figure 2. Study areas and in situ measurement locations used in Papers I–IV. The main panel shows the overall spatial coverage of the study in the Baltic Sea region and boreal lakes. Panels A–C provide detailed views of the Gulf of Finland, the Moonsund area and Pärnu Bay. Symbols indicate the datasets used in individual papers: blue circles denote Paper I stations, purple diamonds Paper II stations, blue-green triangles Estonian and Finnish lake sites from Paper III, green squares coastal and offshore sites from Paper III, and orange stars harbour areas analysed in Paper IV.

The Gulf of Finland is the easternmost sub-basin of the Baltic Sea, with a mean depth of approximately 37 m and a maximum depth of 123 m at Paldiski Deep (Leppäranta and Myrberg, 2009). The area is affected by seasonal stratification, wind-driven mixing,

upwelling and riverine inputs (Alenius et al., 1998; Leppäranta and Myrberg, 2009; Uiboupin and Laanemets, 2009). Pärnu Bay, Matsalu Bay and Moonsund Sea represent shallow and semi-enclosed coastal waters of western Estonia with strong riverine influence. Pärnu Bay is a well-mixed bay in the north-eastern Gulf of Riga, with a mean depth of approximately 4.7 m and a maximum depth of about 8 m. Wind-driven resuspension from sandy, clayey and muddy bottom sediments can produce rapidly changing TSM conditions (Kartau et al., 2011; Uusõue et al., 2022). Matsalu Bay is part of the Moonsund Sea system and forms a brackish estuarine basin influenced by the Kasari River, with an average depth of about 1.5 m and a maximum depth of 3.5 m (Vetemaa et al., 2006; Ivask et al., 2012). Moonsund Sea is connected to the Baltic Proper and the Gulf of Riga through several straits, and its physical and biogeochemical conditions vary strongly due to alternating water masses, restricted water exchange and sediment resuspension (Astok et al., 1999; Suursaar et al., 2009).

Additional Baltic Sea study areas included the Southern Baltic Sea and coastal waters near the Swedish coast in the Western Gotland Basin, representing more open and optically different conditions compared with the shallow Estonian coastal bays.

The freshwater study areas included 51 boreal lakes in Estonia and Finland, covering a broad gradient from transparent to CDOM-rich brown-water systems.

The harbour study areas included Tallinn, Kunda, Sillamäe, Virtsu and Pärnu, located along the Estonian coast. Tallinn and Virtsu are mainly passenger harbours, whereas Kunda, Sillamäe and Pärnu are mainly cargo harbours.

2.1.2 Floodplains in Estonia

Flood-related analyses were carried out in major floodplain and riverine systems in Estonia (Paper V, Figure 3). The Sentinel-1 flood mapping methodology was developed and tested in three floodplain areas: Matsalu, Soomaa and Alam-Pedja. Matsalu is a coastal floodplain at the Kasari River delta, bordering Matsalu Bay, with a region of interest (ROI) of 1068 km². Soomaa is an inland riverine floodplain in the Pärnu River basin, influenced by the Halliste, Navesti and Raudna rivers, with a ROI of 255 km². Alam-Pedja is an inland floodplain along the Emajõgi River in central Estonia, with a ROI of 546 km². These sites include protected floodplain grasslands, wetlands, bogs and forested floodplains. The thesis also includes flood-prone riverine areas connected to the Keila, Kasari and Pärnu rivers. These areas were used to link riverine flood dynamics with CDOM variability in the receiving coastal waters.

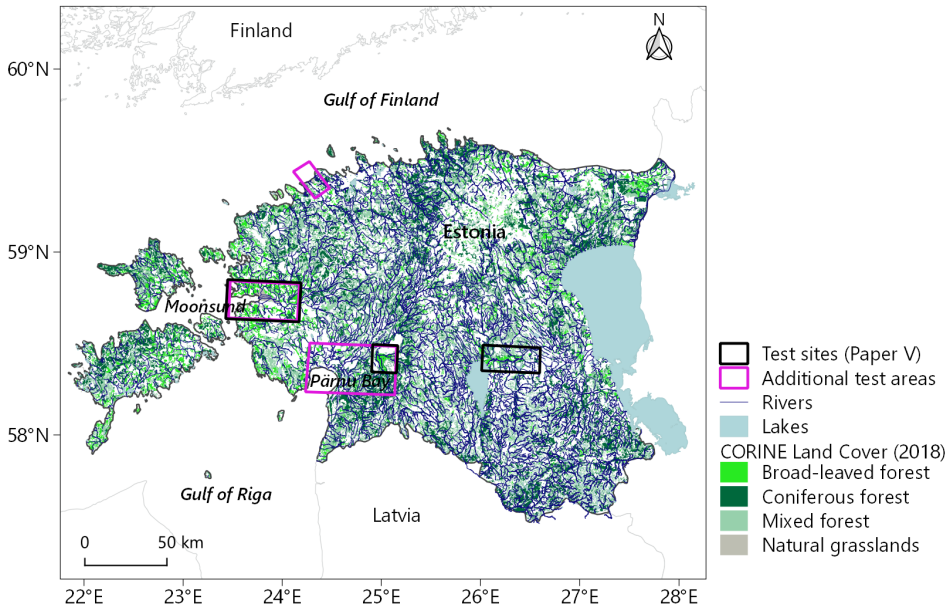


Figure 3. Study areas used in the flood-related analyses. The map shows the floodplain test sites analysed in Paper V and the additional test areas used to examine the relationship between Sentinel-1-based flood extent and coastal variability in coloured dissolved organic matter (CDOM). This variability was assessed from optical water type (OWT) based Sentinel-3 OLCI estimates of the CDOM absorption coefficient at 442 nm ($a_{\text{CDOM}(442)}$) in river-influenced coastal waters.

2.2 Data

An overview of the data types used in this study is presented in Table 1. The datasets include *in situ* optical measurements and water quality parameters (Papers I–III), and CTD temperature and salinity profiles (Paper I). Satellite datasets include optical satellite data (Papers I–V), thermal infrared satellite data (Paper I), and Sentinel-1 radar data (Paper V). Ancillary data include hydrological observations (Papers IV–V), meteorological data (Papers I, IV–V), vessel traffic statistics (Paper IV), drone-based validation data (Paper V), and spatial data layers (Paper V).

Table 1. Overview of the *in situ*, satellite and ancillary datasets used in Publications I–V. Data volume is reported according to data type and refers to measurements, profiles, satellite images, analysis cases, stations, spatial data layers or observations. IOPs: inherent optical properties; CTD profiles: conductivity, temperature and depth profiles; Chl-*a*: chlorophyll-*a*; TSM: total suspended matter; CDOM: coloured dissolved organic matter; Ferrybox: shipborne flow-through measurements of chlorophyll-*a* and phycocyanin fluorescence, and turbidity.

Data Type	Publication					Data volume
	I	II	III	IV	V	
<i>In situ data</i>						
Reflectance (RAMSES)	✓	✓	✓			836
IOPs (ac-s)	✓	✓				124
CTD profiles	✓					94
Chl- <i>a</i>	✓	✓	✓			716
TSM	✓	✓	✓			716
CDOM		✓	✓			432
Secchi depth	✓	✓	✓			542
Ferrybox		✓				2662
Satellite data						
Optical satellite data	✓	✓	✓	✓	✓	482
Thermal infrared satellite data	✓					11
Radar satellite data					✓	416
Ancillary data						
Meteorological data	✓			✓	✓	6
Hydrological data				✓	✓	7
Vessel traffic data				✓		5
Spatial data layers					✓	8
Drone observations					✓	44

2.2.1 *In Situ* Data

The *in situ* optical dataset included spectral reflectance measurements and IOP measurements. Spectral reflectance data were available for the analysis of vertical optical variability, Sentinel-3 OLCI product evaluation and optical water type (OWT) based retrieval development (Papers I–III). IOP data included spectral absorption and attenuation coefficients measured with an ac-s instrument, while scattering coefficients were derived from attenuation and absorption measurements (Papers I–II). In the vertical profile dataset, optical measurements were accompanied by CTD temperature and salinity profiles from the Gulf of Finland (Paper I).

The *in situ* water quality dataset included Chl-*a*, TSM, CDOM absorption and Secchi depth. Chl-*a* and TSM were included in the vertical optical dataset, the Sentinel-3 OLCI validation dataset and the OWT dataset (Papers I–III). CDOM absorption was included in the Sentinel-3 OLCI validation and OWT datasets (Papers II–III), while Secchi depth was included in all three *in situ* datasets (Papers I–III). Additional suspended matter fractions, SPIM (Suspended Particulate Inorganic Matter) and SPOM (Suspended Particulate Organic Matter), were included in the Sentinel-3 OLCI validation dataset (Paper II).

2.2.2 Remote Sensing Data

Satellite datasets included optical, thermal infrared and radar satellite data. Optical satellite data comprised Sentinel-3 OLCI, Sentinel-2 MSI and Envisat MERIS imagery.

Sentinel-3 OLCI full resolution (FR) Level-1 (L1) data with 300 m spatial resolution were used as the main optical satellite input and processed with the Case-2 Regional CoastColour (C2RCC) processor to derive atmospherically corrected reflectance and water quality-related outputs (Papers I–III). In Paper III, Sentinel-3 OLCI and Sentinel-2 MSI spectral response functions were also used to convolve *in situ* reflectance spectra into sensor-specific bands.

Sentinel-2 MSI L1 data with 10–60 m spatial resolution were used for optical-based flood mapping (Paper V). MERIS full resolution L1 data with 300 m spatial resolution were used for the long-term coastal water quality analysis and processed with the Case II Regional (C2R) processor (Paper IV).

Thermal infrared satellite data included Terra/Aqua MODIS Level-2 sea surface temperature (SST) products and Sentinel-3 SLSTR Level-2 SST products, both with 1 km spatial resolution (Paper I). Radar satellite data consisted of Sentinel-1 C-band SAR Ground Range Detected (GRD) products acquired in Interferometric Wide (IW) and Extended Wide (EW) swath modes (Paper V). The satellite datasets are summarised in Table 2.

Table 2. Satellite datasets used in Publications I–V. The datasets include optical, thermal infrared and radar satellite data from Sentinel-3 OLCI and SLSTR, Sentinel-2 MSI, Envisat MERIS, Terra/Aqua MODIS and Sentinel-1 SAR. L1: Level 1; L2: Level 2; GRD: Ground Range Detected; C2RCC: Case 2 Regional CoastColour processor; C2R: Case II Regional processor; MNDWI: modified normalized difference water index; IOPs: inherent optical properties; AOPs: apparent optical properties; OSCs: optically significant constituents; SST: sea surface temperature.

Sensor	Product level	Time Period	Spatial Resolution	Data Processing Method	Purpose of Use	Paper
OLCI	L1	2016, 2018, 2020	300 m	C2RCC	IOPs, AOPs, OSCs	I, II, III
MERIS	L1	2002–2011	300 m	C2R	OSCs	IV
MSI	L1	2017, 2019	Resampled to 10 m	MNDWI threshold	Flood mapping	V
MODIS	L2	2015–2016	1 km	Quality, Ground, and Cloud Masking	SST	I
SLSTR	L2	2020	1 km	Quality, Ground, and Cloud Masking	SST	I
SAR	L1 GRD	2017, 2019, 2020	IW: 5×20 m, EW: 20×40 m	Incidence angle dependent threshold	Flood mapping	V

2.3 Methodology

2.3.1 Measurements of Water Quality Parameters

Analysed water quality parameters included Chl-*a*, TSM, CDOM absorption and Secchi depth (Papers I–III). Chl-*a* concentrations were determined spectrophotometrically after pigment extraction, and TSM concentrations were measured gravimetrically from filtered water samples (Papers I–III). In Paper II, suspended matter was additionally separated into inorganic and organic fractions, SPIM and SPOM.

CDOM absorption was measured from filtered water samples using spectrophotometric analysis (Papers II–III). In Paper II, CDOM absorption spectra were measured over the wavelength range of 350–750 nm. The empirical CDOM algorithm analysis used $a_{\text{CDOM}}(412)$ as the reference variable, whereas the comparison with C2RCC-derived absorption products used $a_{\text{CDOM}}(443)$ (Paper II). In Paper III, the OWT-guided approach used a_{CDOM} at the wavelength 442 nm. Secchi depth was measured with a standard Secchi disk and used as a water transparency parameter (Papers I–III).

2.3.2 Measurements of Inherent Optical Properties

IOP measurements included spectral absorption and attenuation coefficients (Papers I–II). In Paper I, vertical profiles of absorption coefficient ($a(\lambda)$) and attenuation coefficient ($c(\lambda)$) were measured with a WETLabs ac-s instrument in the wavelength range 402–732 nm. The profiles were measured in the upper 25 m of the water column. The scattering coefficient ($b(\lambda)$) was derived from the measured $a(\lambda)$ and $c(\lambda)$:

$$b(\lambda) = c(\lambda) - a(\lambda). \quad (4)$$

The ac-s profiles were corrected for instrument drift, temperature, salinity and scattering effects. CTD profiles of temperature, salinity and depth were measured simultaneously and used to describe the thermohaline structure of the upper water column (Paper I). In Paper II, the *in situ* validation dataset included surface layer measurements of $a(\lambda)$ and $c(\lambda)$, while $b(\lambda)$ and backscattering coefficient ($b_b(\lambda)$) measurements were available for part of the dataset.

2.3.3 Measurements of Reflectance

Reflectance measurements were carried out with TriOS RAMSES hyperspectral radiometers using profiling, near-surface and above-water measurement setups (Papers I–III). The analysed spectral range was 350–900 nm.

In Paper I, the measurement system included one irradiance sensor measuring downwelling irradiance, $E_d(0^+, \lambda)$, and one radiance sensor measuring upwelling radiance, $L_u(0^-, \lambda)$, just beneath the water surface. Water-leaving radiance above the water surface was derived as:

$$L_w(0^+, \lambda) = T_L L_u(0^-, \lambda), \quad (5)$$

where T_L combines the effects of refraction of water and Fresnel reflectance at the air–water interface. Spectral irradiance reflectance was then calculated as:

$$R(\lambda) = \pi \frac{L_w(0^+, \lambda)}{E_d(0^+, \lambda)}. \quad (6)$$

In Paper II, boat-based measurements used $L_u(\lambda)$ and $E_d(\lambda)$, and reflectance was calculated as:

$$R(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)}. \quad (7)$$

Measurements from the research vessel Salme used $E_d(\lambda)$ and upwelling irradiance, $E_u(\lambda)$, measured just below the water surface, and irradiance reflectance was calculated as:

$$R(\lambda) = \frac{E_u(\lambda)}{E_d(\lambda)}. \quad (8)$$

Above-water triple-radiometer measurements were used in Papers II and III. These measurements included total radiance from the water surface, $L_t(\lambda)$, sky radiance, $L_{sky}(\lambda)$, and $E_d(\lambda)$. $L_w(\lambda)$ was obtained by correcting the measured total radiance for reflected sky radiance:

$$L_w(\lambda) = L_t(\lambda) - \rho L_{sky}(\lambda), \quad (9)$$

where ρ is the air-sea interface reflection coefficient. Remote sensing reflectance was then expressed as:

$$R_{rs}(\lambda) = \frac{L_w(\lambda)}{E_d(\lambda)}. \quad (10)$$

In Paper III, the corresponding dimensionless water-leaving reflectance was calculated as:

$$R(\lambda) = \pi R_{rs}(\lambda) = \pi \frac{L_t(\lambda) - \rho L_{sky}(\lambda)}{E_d(\lambda)}. \quad (11)$$

2.3.4 Simulated Apparent Optical Properties

Simulated AOPs were calculated from measured IOPs to represent the optical response of different water masses in the Gulf of Finland (Paper I). The simulations were performed for IOPs measured at the surface layer, 10 m depth and 20 m depth. Spectral irradiance reflectance, $R(\lambda)$, was simulated from absorption and backscattering according to Gordon et al. (1975) and Kirk (1984):

$$R(\lambda) = (-0.629\mu_0 + 0.975) \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}, \quad (12)$$

where $b_b(\lambda)$ is the backscattering coefficient, $a(\lambda)$ is the absorption coefficient, and μ_0 is the cosine of the refracted solar beam just beneath the surface. A value of $\mu_0=0.88$ was adopted from Alikas et al. (2015), representing conditions typical of Estonian inland and coastal waters in the period of June–August. The backscattering coefficient required for the simulations was approximated from the scattering coefficient as (Herlevi, 2002):

$$b_b(\lambda) = 0.015 * b(\lambda). \quad (13)$$

The spectral diffuse attenuation coefficient, $K_d(\lambda)$, was calculated from absorption and scattering using the radiative transfer model by Kirk (2011):

$$K_d(\lambda) = \mu_0^{-1} [a^2(\lambda) + (g_1 * \mu_0 - g_2) a(\lambda) * b(\lambda)]^{0.5}, \quad (14)$$

where $a(\lambda)$ is the absorption coefficient and $b(\lambda)$ is the scattering coefficient. The constants g_1 and g_2 account for the angular distribution of scattered light and the geometry of the underwater light field. In this study, $g_1=0.43$ and $g_2=0.19$ were adopted from Kirk (2010), and $\mu_0=0.88$ was adopted from Alikas et al. (2015).

The optical depth $z_{90}(\lambda)$, representing the depth from which 90% of the water-leaving signal originates, was calculated as (Gordon and McCluney, 1975):

$$z_{90}(\lambda) = \frac{1}{K_d(\lambda)}. \quad (15)$$

2.3.5 Analysis of Optical Properties in Thermohaline Conditions

The vertical variability of optical properties was analysed in relation to thermohaline structure in the Gulf of Finland (Paper I). Temperature and salinity profiles were used to classify the water column into three regimes: mixed conditions, intermediate conditions and stratified conditions with a distinct thermocline. The classification was based on the vertical structure of the upper 25 m water column.

For each regime, the vertical distribution of $a(\lambda)$, $c(\lambda)$, derived $b(\lambda)$, Chl- a and TSM was compared between the surface layer and deeper water layers. The ratio $b(\lambda)/a(\lambda)$ was used to assess the relative dominance of scattering and absorption under different thermohaline conditions.

Simulated AOPs were used to evaluate how the observed vertical IOP structure affected the optical response of different water masses. $R(\lambda)$, $K_d(\lambda)$ and $z_{90}(\lambda)$ were calculated for the surface layer, 10 m and 20 m depth, and compared between mixed, intermediate and stratified conditions (Paper I).

2.3.6 Optical Water Type Guided Approach for Estimating CDOM

The estimation of CDOM absorption at 442 nm, $a_{\text{CDOM}}(442)$, was based on an OWT-guided approach (Paper III). OWTs were assigned from the spectral shape of measured water-leaving reflectance, $R(\lambda)$, using similarity between individual spectra and predefined OWT reference spectra. The classification divided the dataset into five OWTs: Clear, Moderate, Turbid, Very Turbid and Brown. The same classification was applied to hyperspectral $R(\lambda)$ and to $R(\lambda)$ convolved to Sentinel-3 OLCI and Sentinel-2 MSI spectral bands. For $a_{\text{CDOM}}(442)$ estimation, 21 published empirical CDOM algorithms were tested separately for each OWT and spectral configuration (Paper III). Model selection was based on repeated k-fold cross-validation with 10 folds and 10 repeats. The algorithm ranking combined scaled error and bias metrics: root mean square error (RMSE), root mean square logarithmic error (RMSLE), mean absolute error (MAE), mean absolute percentage error (MAPE) and bias, together with the coefficient of determination (R^2) and p-value thresholds. Lower error and bias values, higher R^2 values and statistically significant p-values resulted in higher ranking scores. The scores were summed, and the highest-ranked CDOM algorithm was selected separately for each OWT and sensor-specific spectral configuration. The selected OWT-based CDOM algorithms were then applied to Sentinel-3 OLCI imagery to derive satellite-based $a_{\text{CDOM}}(442)$ products.

2.3.7 Sentinel-1 Flood Mapping Algorithms

The Sentinel-1 SAR flood mapping algorithm was developed for detecting open-water flooding (OWF) and flooding under vegetation (FUV) (Paper V). Sentinel-1 SAR data were pre-processed using calibration, noise filtering and terrain correction. OWF was mapped using incidence-angle-dependent backscatter thresholds for IW VH and EW HV data. FUV was mapped from EW HH data using a fixed backscatter threshold, as no clear incidence-angle dependence was detected for flooded forest areas. Here, VH, HV and HH denote vertical transmit–horizontal receive, horizontal transmit–vertical receive and horizontal transmit–horizontal receive polarization, respectively. The threshold conditions are given in Table 3.

Post-processing was used to reduce false detections and retain hydrologically plausible flood areas. Water lookalikes were removed using ancillary spatial layers, including inland water bodies, shoreline data, elevation information, forest cover and a building layer. OWF extent was estimated as the water-covered area outside the official shoreline within each ROI (Paper V).

Table 3. Threshold conditions used for Sentinel-1-based flood mapping (Paper V). The table shows the selected Sentinel-1 acquisition mode, polarization and backscatter threshold condition used to classify open-water flooding (conditions No. 1–2) and flooding under vegetation (condition No. 3). θ denotes the local incidence angle, and SD denotes the standard deviation adjustment applied in the threshold equation.

S1 Mode	Polarization	Threshold for Water Mapping	SD	No.
IW	VH	$Water < -0.30 \times \theta - 12.13 + 2 \times SD$	1.43	1
EW	HV	$Water < -0.23 \times \theta - 19.12 + 2 \times SD$	2.26	2
EW	HH	$Flooded\ forest > -3.15 - SD$	1.06	3

Sentinel-2 MSI data were used as an optical reference dataset for assessing OWF mapping accuracy. The modified normalized difference water index was calculated as:

$$MNDWI = \frac{B3 - B11}{B3 + B11}, \quad (16)$$

where B3 is the MSI green band and B11 is the shortwave infrared band. Band 11 was resampled to 10 m, and water areas were extracted using the condition $MNDWI > 0.6$. OWF accuracy was assessed using overall accuracy and the kappa hat coefficient. FUV was assessed using drone photographs and field observation points (Paper V).

3 Results and Discussion

3.1 Understanding Baltic Sea Coastal Waters as a Complex Optical Environment

3.1.1 Horizontal Variability of Optical Water Parameters

The horizontal variability of optical water parameters was analysed across several spatial scales: surface-layer variability in the Gulf of Finland (Paper I), contrasting Baltic Sea water conditions used for Sentinel-3 OLCI validation (Paper II), and long-term coastal gradients along the Estonian coastline derived from MERIS time series in harbour-adjacent areas (Paper IV). These datasets show that the horizontal optical structure of the Baltic Sea coastal zone is not controlled by a single water quality parameter. Chl- a , TSM and CDOM vary partly independently, and their combined effect determines absorption, scattering and reflectance in optically complex coastal waters.

In the Gulf of Finland, surface-layer optical variability was moderate compared with the vertical contrasts discussed in Section 3.1.2, but the measured ranges show that the near-surface water was not optically uniform (Paper I). The surface-layer IOPs varied substantially: the beam attenuation coefficient $c(440)$ ranged from 0.94 to 7.56 m^{-1} , the scattering coefficient $b(440)$ from 0.42 to 6.86 m^{-1} , and the absorption coefficient $a(440)$ from 0.45 to 0.89 m^{-1} (Figure 3 in Paper I). Attenuation was therefore mainly controlled by scattering rather than absorption. Surface Chl- a ranged from 0.4 to 20.6 mg/m^3 , while TSM varied from 0.1 to 6.7 mg/L (Table 1 in Paper I). The corresponding $R(\lambda)$ spectra had the highest reflectance in the green region, around 550–580 nm, and lower reflectance in the blue and red regions, with a local minimum near 670 nm linked to Chl- a absorption (Figure 4 in Paper I). This spectral structure is consistent with Baltic Sea studies showing that CDOM suppresses blue reflectance, while particles and phytoplankton affect the green, red and near-infrared parts of the spectrum (Darecki and Stramski, 2004; Kowalczyk et al., 2006; Kratzer and Moore, 2018).

The Sentinel-3 OLCI validation dataset showed that optical conditions differed substantially between the analysed Baltic Sea water bodies (Paper II). The dataset covered contrasting coastal and open-water conditions, including Matsalu Bay, Moonsund Sea (Hiiumaa Strait) and the Southern Baltic Sea. The absorption coefficient varied by approximately one order of magnitude across the studied waters (Figure 2 in Paper II). In the clearest sites, absorption was only about 45–65% higher than typical central Baltic Sea values, whereas in Matsalu Bay it was almost one order of magnitude higher. This reflects the strong influence of CDOM-rich inflow from surrounding wetlands and shows that even within the Baltic Sea, the optical baseline can differ substantially between coastal systems (Paper II).

This interpretation is also supported by Ligi (2017), who showed that absorption values in Estonian coastal waters differed strongly even within a relatively limited coastal region. In that study, absorption coefficients measured along the Estonian coast varied substantially between Kõiguste, Kihnu, Vormsi, Matsalu and Haapsalu, and the highest Estonian coastal values were about ten times higher than values measured in clearer Swedish coastal waters. Ligi (2017) also showed that Estonian coastal absorption values may overlap with those measured in Lake Peipsi, indicating that parts of the Baltic Sea coastal zone can optically resemble highly absorbing inland and estuarine waters more than open marine waters. This supports the need for regional and water-type-sensitive

interpretation in Baltic Sea coastal remote sensing, rather than assuming a uniform optical response across coastal waters.

The long-term MERIS analysis showed that horizontal optical variability along the Estonian coast was also evident in the five harbour-adjacent study areas analysed in Paper IV. Annual mean TSM concentrations varied by almost one order of magnitude, from 1.93 ± 0.38 mg/L near Tallinn Harbour to 14.94 ± 3.50 mg/L near Pärnu Harbour. Lower values were observed near Kunda and Sillamäe, 3.40 ± 0.81 and 3.96 ± 1.35 mg/L, respectively, whereas Virtsu showed higher inter-annual variability, with a mean annual TSM of 6.97 ± 1.97 mg/L (Table 3 in Paper IV). This spatial contrast indicates that MERIS-derived TSM concentrations were influenced by local coastal conditions, particularly water depth and exposure to wind- and wave-driven resuspension.

The comparison with wind data showed that the influence of wind forcing depended on the temporal scale of analysis. Annual mean wind speed did not explain annual mean TSM variability, whereas correlations between monthly mean wind speed and monthly mean TSM concentrations were found in several harbour-adjacent areas. The relationship was most consistent near Kunda and Sillamäe, where monthly wind speed coincided with TSM variability in most of the analysed years. In Pärnu Bay, the decrease in TSM during 2006–2007 was linked to a shift in dominant wind direction from south-westerly to westerly winds, which reduced resuspension in the shallow and semi-enclosed bay. In contrast, no consistent relationship between wind speed and TSM was found in Virtsu, suggesting that suspended matter variability in the Moonsund area was shaped by more complex hydrodynamic conditions than wind speed alone. These results are consistent with previous studies showing that wind-driven resuspension and local bathymetry strongly affect suspended matter distribution in shallow Baltic Sea coastal waters (Kratzer and Tett, 2009; Raudsepp et al., 2011; Kyrliuk and Kratzer, 2019).

CDOM showed a different spatial pattern from TSM. The lowest annual mean CDOM was observed near Tallinn Harbour in the Gulf of Finland, 0.12 ± 0.03 m⁻¹, whereas the highest values occurred near Pärnu Harbour where the annual mean CDOM reached 1.57 ± 0.34 m⁻¹. CDOM values in Virtsu, Kunda and Sillamäe were lower than in Pärnu but higher than in Tallinn, with annual mean values of 0.41 ± 0.13 , 0.28 ± 0.15 and 0.26 ± 0.08 m⁻¹, respectively (Table 4 in Paper IV). This difference between TSM and CDOM patterns indicates that suspended matter and dissolved organic matter absorption were controlled by partly different processes. TSM can increase due to resuspension in shallow, wind-exposed areas, while CDOM is more directly linked to riverine and catchment-derived dissolved organic matter. This is consistent with earlier Baltic Sea studies showing that terrestrial dissolved organic matter shapes coastal CDOM gradients. For example, Vaičiūtė et al. (2015) found that Nemunas River discharge influenced CDOM variability in the Curonian Lagoon, while Sipelgas et al. (2004) showed CDOM gradients along the Estonian coastline. In Paper IV, the same process was most evident near Pärnu Harbour, where annual mean CDOM showed the clearest positive relationship with Pärnu River discharge. No comparable relationship was found at the other harbour sites located near river mouths, suggesting that the association between annual mean river discharge and CDOM variability was not explained by discharge magnitude alone, but also by the hydrodynamic connection between the river mouth and the analysed harbour-adjacent area.

3.1.2 Vertical Variability of Optical Water Parameters

The vertical profiles of IOPs and OSCs in the Gulf of Finland showed that differences between the surface layer and 20 m depth depended on the thermohaline structure of the water column, being smallest under mixed conditions and most pronounced under stratified conditions (Paper I; Figure 4). In summer, the Gulf of Finland is commonly characterised by an upper mixed layer, a seasonal thermocline at approximately 10–20 m depth and a colder intermediate layer, while wind-driven upwelling and downwelling can modify the position and strength of these layers (Alenius et al., 1998; Liblik and Lips, 2011; Kikas and Lips, 2016). This physical setting provides the basis for interpreting how the vertical redistribution of OSCs is expressed in the measured IOP profiles.

The vertical distribution of Chl-*a* and TSM differed most clearly between mixed and stratified profiles (Figure 4; Table 3 in Paper I). Between the surface and 20 m, Chl-*a* decreased by 33.3% under mixed conditions and by 96.1% under stratified conditions, while TSM decreased by 29.4% and 73.3%, respectively. Similar vertical structuring of phytoplankton biomass has been reported in the Gulf of Finland, where sub-surface Chl-*a* maxima occurred in the lower part of the seasonal thermocline at depths of 14.5–35 m, with layer thicknesses of 1.5–9 m and Chl-*a* concentrations up to 7.6 mg/m³ (Lips et al., 2010). Lips et al. (2011) also showed that sub-surface biomass maxima may form below the strongest vertical density gradient, linking phytoplankton vertical distribution to stratification and physical forcing.

The IOP profiles followed the vertical redistribution of OSCs, especially through changes in scattering (Figure 4; Table 2 in Paper I). In mixed profiles, *c*(440) decreased by only 16.4% between the surface and 20 m, whereas under stratified conditions the decrease reached 69.1%. The corresponding decrease in *b*(440) was 21.5% under mixed conditions and 85.7% under stratified conditions. Absorption varied less strongly, with *a*(440) decreasing by 5.9% and 43.9%, respectively. Thus, the vertical attenuation gradient was mainly associated with the decline in particle-related scattering below the thermocline. Since vertical CDOM data were not available in Paper I, the absorption component cannot be directly separated into CDOM and particulate absorption.

The ratio *b*(440)/*a*(440) (from about 2.1 in the surface layer to 0.4–0.5 at 20 m depth) summarised the shift in the relative contribution of scattering and absorption in the Gulf of Finland profiles. In the upper mixed layer, *b*(440)/*a*(440) > 1, indicating scattering-dominated attenuation. Below the thermocline, *b*(440)/*a*(440) < 1, indicating absorption-dominated attenuation (Figure 4). In stratified profiles, the correlation between the median temperature profile and *b*(440)/*a*(440) was $R^2=0.99$, showing that the optical transition followed the thermohaline structure rather than a fixed depth level. This result is comparable with Berthon and Zibordi (2010), who showed that the scattering-to-absorption ratio in the Baltic Sea (Bothnian Bay and Baltic Proper) can vary strongly between water masses: values higher than 1.5 occurred in the upper 0–15 m layer of the Baltic Proper, whereas values below 0.5 were observed in the northern Bothnian Bay, where CDOM absorption was high and not accompanied by a corresponding increase in particle scattering. In the Gulf of Finland profiles (Paper I), the decrease in *b*(440)/*a*(440) with depth was instead linked to the sharp reduction of scattering below the thermocline.

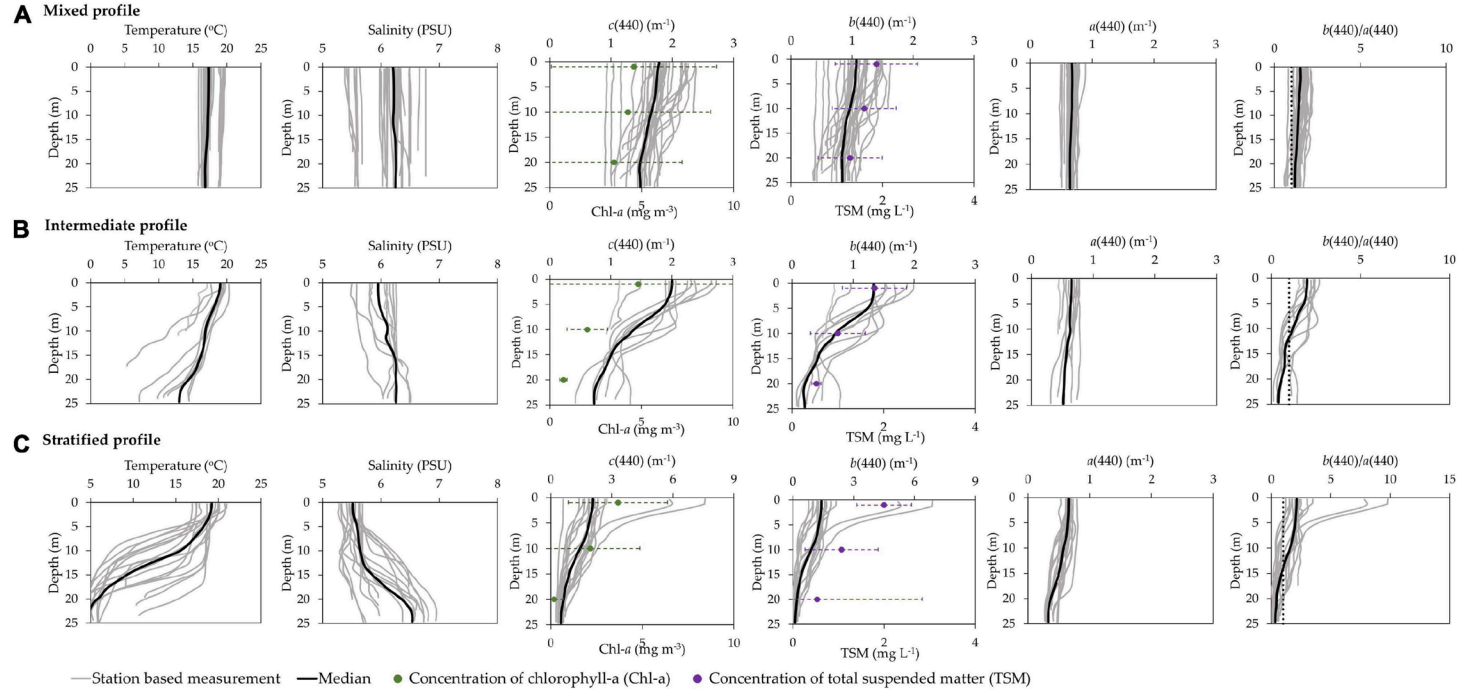


Figure 4. Vertical profiles of temperature, salinity, attenuation coefficient ($c(440)$), scattering coefficient ($b(440)$), absorption coefficient ($a(440)$) and $b(440)/a(440)$ at the wavelength of 440 nm during different hydrodynamic situations: (A) mixed water column down to a 25 m depth (the vertical temperature gradient was consistently $<0.1^\circ\text{C m}^{-1}$), (B) intermediate situation with steady vertical decrease in temperature (the vertical temperature gradient was steadily $\geq 0.1^\circ\text{C m}^{-1}$), (C) stratified profile (there was a layer with a vertical temperature gradient $\geq 0.1^\circ\text{C m}^{-1}$ under the layer where the gradients were steadily $<0.1^\circ\text{C m}^{-1}$). The dotted line on the $b(440)/a(440)$ graph represents the boundary from which either the absorption $b(440)/a(440) < 1$ or scattering $b(440)/a(440) > 1$ dominates. In addition, the median concentrations of chlorophyll-a (Chl-a) and total suspended matter (TSM) are given with the interquartile range. Reproduced from Paper I.

3.2 Remote Sensing Retrieval of Optical Water Quality Parameters

3.2.1 Limitations of Standard Satellite Retrievals in Baltic Sea Waters

The evaluation of Sentinel-3 OLCI showed a clear difference between the performance of atmospheric correction and the retrieval of IOPs and water quality parameters in Baltic Sea waters (Paper II). C2RCC-derived water-leaving reflectance spectra were realistic in shape and magnitude under non-bloom conditions (Figures 3–5 in Paper II). Band-wise correlations between C2RCC-derived water-leaving reflectance and *in situ* reflectance were highest in the green, red and near-infrared bands. For boat-based measurements, correlations reached $R=0.82$ at 560 nm, $R=0.77$ at 490 and 620 nm, and $R=0.68$ at 665–681 nm (Table 4 in Paper II). These results show that C2RCC atmospheric correction retained useful spectral information in several OLCI bands, although the low water-leaving signal constrained the blue spectral region.

The main limitation appeared in the subsequent retrieval of IOPs. In C2RCC, the IOP inversion is performed by neural networks (NNs) trained on radiative-transfer simulations (Müller et al., 2026). In Paper II, none of the C2RCC-derived IOPs showed statistically significant correlations with corresponding *in situ* measurements. Figure 5 compares C2RCC-derived absorption and scattering products with measured optical properties. The weak agreement indicates that the NN-based in-water inversion did not resolve the Baltic Sea IOP structure reliably, even where the water-leaving reflectance was realistic. This is consistent with the non-unique nature of the inverse problem, where different combinations of absorption and scattering may produce similar spectral signals (Müller et al., 2026).

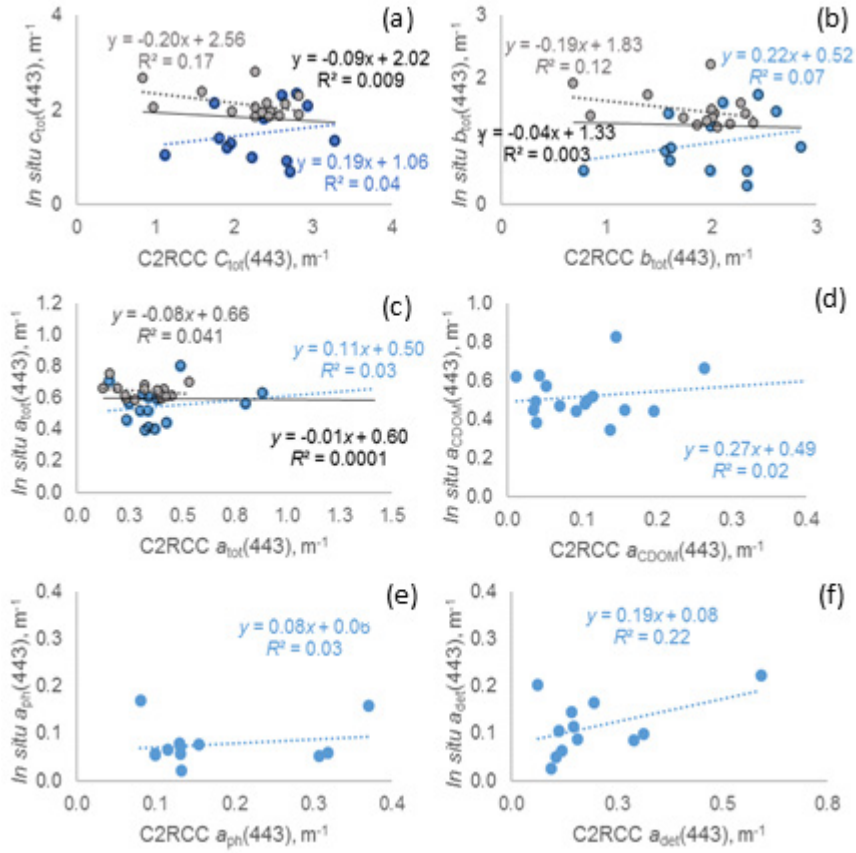


Figure 5. Comparison of inherent optical properties (IOPs) derived with the Case 2 Regional CoastColour (C2RCC) processor and corresponding in situ measurements in Baltic Sea waters. Panels show C2RCC-derived values plotted against in situ values for (a) total attenuation coefficient ($c_{\text{tot}}(443)$), (b) total scattering coefficient ($b_{\text{tot}}(443)$), (c) total absorption coefficient ($a_{\text{tot}}(443)$), (d) coloured dissolved organic matter (CDOM) absorption coefficient ($a_{\text{CDOM}}(443)$), (e) phytoplankton absorption coefficient ($a_{\text{ph}}(443)$), and (f) detrital absorption coefficient ($a_{\text{det}}(443)$). Grey dots indicate measurements from the research vessel (R/V) Salme, blue dots indicate boat-based measurements, and the black regression line represents the combined R/V Salme and boat dataset. Modified from Paper II.

The limited IOP retrieval was also reflected in the derived water quality products. In C2RCC, constituent concentrations are derived from retrieved IOPs using empirical bio-geo-optical models (Müller et al., 2026). C2RCC-derived Chl-*a* and TSM products performed only slightly better than the IOPs from which they were calculated, but the explained variance remained low. For direct *in situ* comparisons, R^2 remained low, reaching 0.25 for Chl-*a* and 0.11 for TSM (Figure 8 in Paper II). The Ferrybox comparison gave higher R^2 values, up to 0.56 for Chl-*a*, but the scatter remained large. C2RCC Chl-*a* ranged from 0 to 11 mg/m^3 when Ferrybox Chl-*a* was around 2.5 mg/m^3 . The same product dependence was reported by Ansper-Toomsalu et al. (2024). For Sentinel-3 OLCI,

C2RCC-derived total absorption explained more variation than individual absorption components, but the relationship remained moderate ($R^2=0.33$). The C2RCC-derived CDOM absorption product had the highest R^2 among the tested $a_{\text{CDOM}}(443)$ algorithms, but the relationship was weak ($R^2=0.10$). For Sentinel-2 MSI, C2RCC-derived TSM showed stronger agreement with *in situ* TSM ($R^2=0.74$). For Sentinel-3 OLCI, TSM retrieval was reliable mainly at lower concentrations and overestimated higher values (Ansper-Toomsalu et al., 2024).

The weak performance of the standard products is consistent with the optical conditions described in Section 3.1. Baltic Sea waters have high and spatially variable CDOM absorption, while particle composition varies between shallow coastal areas and bloom-dominated waters. Dense cyanobacterial blooms add another limitation because they strongly affect the red and near-infrared part of the spectrum. In Paper II, C2RCC atmospheric correction produced unrealistic water-leaving reflectance spectra in dense cyanobacterial bloom conditions, where the corrected spectra lost the expected bloom-related signal above 700 nm (Figure 6 in Paper II). Cyanobacterial accumulations are also difficult to validate with point-based *in situ* data, because Chl-*a* may vary by orders of magnitude within one OLCI pixel under bloom conditions (Kutser, 2004; Reinart and Kutser, 2006; Simis et al., 2017).

Empirical algorithms applied to C2RCC-derived water-leaving reflectance performed better than the standard C2RCC output products for several parameters (Paper II). For Chl-*a*, the best-performing algorithms used green, red and near-infrared bands rather than standard blue-green band ratios (Figure 9 in Paper II). This agrees with Ligi et al. (2017), who showed that the standard blue-green Chl-*a* algorithm performed very poorly for Baltic Sea reflectance data ($R^2=0.0054$), whereas red and near-infrared band-ratio algorithms showed stronger relationships, including R^2 values around 0.4–0.56 for field reflectance data and above 0.9 for modelled spectra. Soomets et al. (2022) further showed that their best tested Sentinel-3 OLCI band-ratio algorithm used 665, 709 and 754 nm bands and outperformed the Sentinel-3 OLCI C2RCC Chl-*a* product ($R^2=0.67$ and 0.55, respectively). These results confirm the relevance of red and near-infrared bands for Chl-*a* retrieval in CDOM-rich Baltic Sea waters.

The parameter-specific results showed that retrieval performance depends on both the target parameter and the optical composition of the water masses (Paper II). TSM retrieval was affected by differences in particle composition. R/V Salme measurements were linked mainly to organic material during cyanobacterial conditions, whereas boat measurements in shallow coastal waters were more influenced by resuspended inorganic particles. CDOM retrieval was constrained by the available validation range. Only one sampling station had a relatively high CDOM value compared with most of the sampled values, $a_{\text{CDOM}}(412)=3.2 \text{ m}^{-1}$, which strongly influenced the regression. This value is not high for Baltic Sea coastal waters. For instance, Ligi et al. (2017) reported measured $a_{\text{CDOM}}(412)$ values from 0.28 to 13.46 m^{-1} , while Kutser et al. (2009) estimated $a_{\text{CDOM}}(420)$ values above 30 m^{-1} in Matsalu Bay and 5–15 m^{-1} in the river plume flowing into the Muhu Strait.

3.2.2 Optical Water Type Guided Retrieval of $a_{\text{CDOM}}(442)$

Following the limitations of standard retrievals shown in Section 3.2.1, Paper III used an OWT classification to select empirical $a_{\text{CDOM}}(442)$ models according to the optical structure of the water. The classification followed the scheme introduced by Uudeberg et al. (2019) and was based on key features of measured $R(\lambda)$ spectra, including the

wavelength of the reflectance maximum, spectral slope and reflectance amplitude. In Paper III, the OWT-guided approach was applied to several optical water quality parameters, whereas this thesis focuses on the $a_{\text{CDOM}}(442)$ retrieval component.

The classification separated boreal inland and coastal waters into five OWTs with distinct bio-optical conditions (Figures 3–4 in Paper III): 1) Clear OWT had reflectance maxima in the green spectral region, between approximately 540 and 580 nm, and represented waters with high transparency and low OSC concentrations; 2) Moderate OWT had a similar green-region maximum but higher OSC concentrations, with no single constituent dominating the optical signal; 3) Turbid OWT had the highest reflectance values and was primarily associated with elevated TSM; 4) Very Turbid OWT had a reflectance maximum in the red region, approximately 685–715 nm, and represented Chl-*a* dominated bloom conditions; 5) Brown OWT had low $R(\lambda)$ values and a maximum shifted towards the red part of the spectrum, reflecting CDOM-dominated dark waters.

For each OWT, 21 published empirical algorithms were evaluated for estimating $a_{\text{CDOM}}(442)$ using hyperspectral (RAMSES), OLCI, and MSI reflectance bands. Model performance differed more between OWTs than between spectral configurations (Table 4 in Paper III). Key results are as follows:

- Clear OWT: The best model for RAMSES was the log–log regression based on the Kallio et al. (2008) 560/660 nm reflectance ratio, while the Menken et al. (2006) 665/560 nm ratio performed best for both OLCI and MSI. This was the only OWT where the selected models explained 74% of the variance in measured $a_{\text{CDOM}}(442)$ across all three spectral configurations.
- Moderate OWT: The best hyperspectral model was based on the Ficek et al. (2011) 570/655 nm reflectance ratio, whereas the Menken et al. (2006) 665/560 nm ratio was selected for both OLCI and MSI configurations. The R^2 values were lower than in Clear OWT, reaching 0.42 for RAMSES, 0.33 for OLCI and 0.35 for MSI. This indicates that $a_{\text{CDOM}}(442)$ retrieval was less stable when CDOM absorption occurred together with increased OSC concentrations, but without one clearly dominant constituent.
- Turbid OWT: Similar to Moderate OWT, the Ficek et al. (2011) 570/655 nm ratio for RAMSES, and the Menken et al. (2006) 665/560 nm ratio for OLCI and MSI gave the best performance. The R^2 values were 0.31 for RAMSES, 0.45 for OLCI and 0.44 for MSI. Compared with Clear OWT, the lower performance reflects the stronger influence of TSM on the reflectance signal, which can reduce the specificity of red-to-green ratios for CDOM retrieval.
- Very Turbid OWT: The best model was the Ammenberg et al. (2002) red-to-green reflectance ratio for all spectral configurations. The selected linear regression model used 664/550 nm for RAMSES and 665/560 nm for OLCI and MSI, with R^2 values of 0.42, 0.38 and 0.39, respectively. The performance was limited by the Chl-*a* dominated optical signal, as this OWT is associated with bloom conditions and a pronounced reflectance peak at red spectral region.
- Brown OWT: The best models were log-transformed multiple linear regressions. The Brezonik et al. (2005) model using blue and near-infrared reflectance data performed best for RAMSES and OLCI, whereas the Griffin et al. (2011) model using 665 nm and the 560/490 nm ratio performed best for MSI. The corresponding R^2 values were 0.38 for RAMSES and 0.41 for both OLCI and MSI.

Across all OWTs, the OWT-guided $a_{\text{CDOM}}(442)$ retrieval showed similar performance for hyperspectral and satellite spectral configurations (Figure 6). The correlations between measured and predicted $a_{\text{CDOM}}(442)$ were 0.88 for RAMSES and 0.87 for both

OLCI and MSI. However, the highest $a_{\text{CDOM}}(442)$ values in Brown OWT were underestimated, indicating that very high CDOM absorption remained difficult to retrieve even after optical pre-classification.

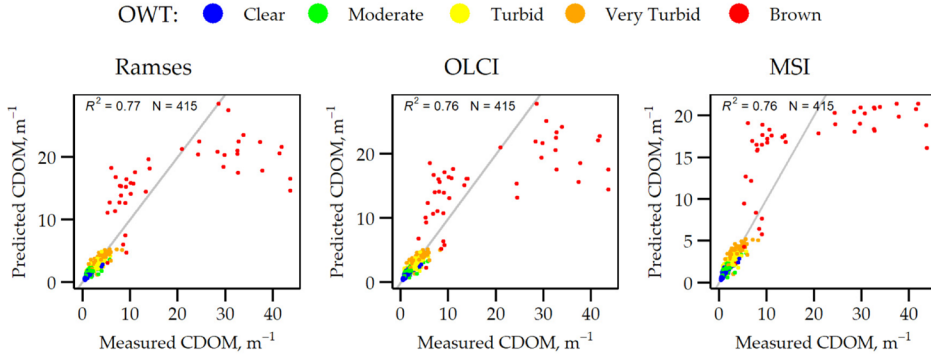


Figure 6. Optical water type (OWT) guided retrieval of the coloured dissolved organic matter (CDOM) absorption coefficient at 442 nm ($a_{\text{CDOM}}(442)$) from hyperspectral and sensor-specific reflectance configurations. Measured $a_{\text{CDOM}}(442)$ values are compared with values predicted from hyperspectral TriOS RAMSES reflectance and from in situ reflectance spectra convolved to Sentinel-3 OLCI and Sentinel-2 MSI spectral bands. Colours indicate the five OWTs: Clear, Moderate, Turbid, Very Turbid and Brown. The line shows a 1:1 relationship. The figure shows good overall agreement, but limited performance for high CDOM Brown OWT waters. Reproduced from Paper III.

The underestimation in Brown OWT occurred mainly at the highest $a_{\text{CDOM}}(442)$ values. In Paper III, Brown OWT represented the high-CDOM, low-reflectance end of the combined dataset of inland and coastal waters, with a reflectance maximum shifted towards longer wavelengths and a median $a_{\text{CDOM}}(442)$ of 13.6 m^{-1} . Figure 4 in Paper III shows that this class had a substantially higher $a_{\text{CDOM}}(442)$ range and lower Secchi depth than the other OWTs. These conditions were driven mainly by very CDOM-rich inland waters, although similar optical conditions may occur locally in strongly river-influenced coastal embayments. Baltic Sea coastal waters usually cover lower a_{CDOM} ranges than the upper end of Brown OWT, although elevated values occur in river-influenced coastal systems, such as Matsalu Bay, Pärnu Bay, the Gulf of Riga, the Gulf of Gdansk and the Öre Estuary (Kutser et al., 2009; Ligi et al., 2017; Kratzer and Moore, 2018). The Brown OWT bias should be interpreted as a high-CDOM retrieval limit rather than as the general performance of the OWT-guided approach in eastern Baltic coastal waters.

3.3 Remote Sensing of Coastal Water Quality Dynamics

3.3.1 Upwelling-Induced Changes in Optical Parameters

Upwelling modifies not only the thermohaline structure of the water column, but also the optical signal of the surface water measured by remote sensors (Paper I). This effect was quantified by simulating AOPs from measured IOPs at the surface layer, 10 m and 20 m depth, representing how $R(\lambda)$, $K_d(\lambda)$ and $z_{90}(\lambda)$ would change if water masses from below the thermocline were transported into the surface layer during upwelling. The simulated response was then compared with independent RAMSES $R(\lambda)$ measurements

collected during an upwelling event and tested with Sentinel-3 OLCI reflectance data together with SLSTR SST fields. Such changes are particularly relevant in the Gulf of Finland, where coastal upwelling can affect large areas and form filaments extending tens of kilometres offshore or even across the gulf (Zhurbas et al., 2008; Uiboupin et al., 2012).

The simulated $R(\lambda)$ spectra showed that water masses from below the thermocline had a lower and smoother optical signal than the surface layer (Figure 4 in Paper I). Between the surface and 20 m depth, reflectance in the photosynthetically active radiation region ($R(\text{PAR})$) decreased by 68.8% under intermediate and by 61.5% under stratified conditions (Table 4 in Paper I). The reduction in $R(\lambda)$ was most evident in the green spectral region, where the surface-water spectra had a clear maximum at 550–580 nm, whereas spectra representing water from deeper layers were lower and smoother. This pattern follows the lower Chl- a and TSM concentrations below the thermocline and is consistent with Baltic Sea studies showing that cold upwelled water can initially coincide with low Chl- a regions during the active phase of upwelling, before nutrient-driven biological responses develop later (Uiboupin et al., 2012; Dabuleviciene et al., 2018, 2020).

The response of $K_d(\lambda)$ was smaller than the change in $R(\lambda)$, but it altered the optical depth represented by remote sensing. From the surface to 20 m depth, $K_d(\text{PAR})$ decreased by 28.1% under intermediate and by 37.5% under stratified conditions, while $K_d(490)$ decreased by 38.8% and 51.6%, respectively (Table 4 in Paper I). The $z_{90}(\lambda)$ simulations showed that the water layer contributing to the remotely sensed signal was deepest in the green spectral region, where $z_{90}(\lambda)$ could increase from about 2.3 m to 4.3 m when water originating from deeper layers was represented at the surface (Figure 5 in Paper I). This agrees with Simis et al. (2017), who showed that the depth contributing to water-leaving radiance in Baltic Sea waters increases under low-biomass conditions, especially near 560 nm.

The simulated optical response was supported by independent RAMSES $R(\lambda)$ measurements collected during an upwelling event (Figure 7). The upwelled water had SST of 4.8 °C, Secchi depth of 12.2 m and Chl- a of approximately 0.5 mg/m³, whereas nearby non-upwelled coastal waters had SST of about 15 °C, Secchi depth of 3.3–3.7 m and Chl- a of 17.5–20.6 mg/m³. The measured spectra separated typical coastal water, with a clear 550–580 nm maximum, from upwelled water with a lower and smoother $R(\lambda)$ shape. The spectral contrast reflects the replacement of productive, particle-rich surface water by optically clearer water from below the thermocline during upwelling.

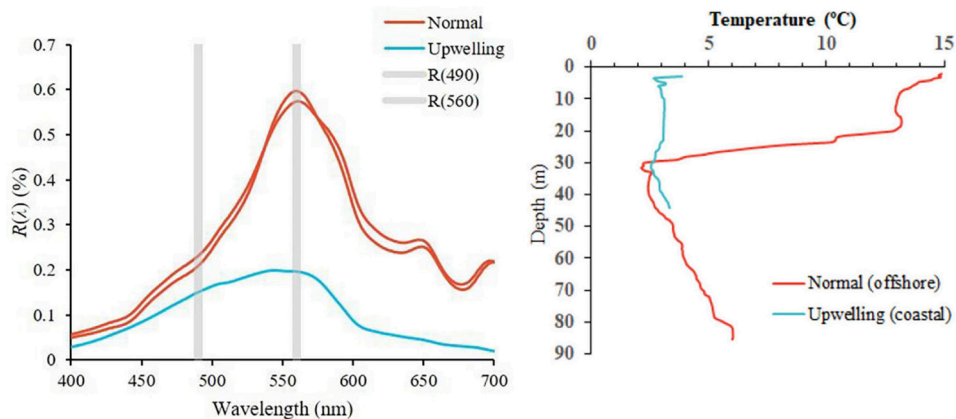


Figure 7. The spectral irradiance reflectance ($R(\lambda)$) of in situ measurements during upwelling and normal situations (left panel). The corresponding measured temperature profiles indicate strong coastal upwelling with surface temperature below 5°C (right panel). Reproduced from Paper I.

The same upwelling event was captured in the OWT-based analysis in Paper III. The Gulf of Finland station measured during this event had the highest Secchi depth in the dataset, 12.2 m, together with low OSC concentrations, and was assigned to Clear OWT. The reduced accuracy of the OWT-guided Secchi depth model at these high transparency values indicates that upwelling can temporarily shift coastal waters into an optical range where some retrieval models are less well constrained.

The spectral difference between upwelled and non-upwelled water was quantified using the ratio $R(490)/R(560)$. Based on RAMSES spectra, $R(490)/R(560) \geq 0.77$ was defined as the threshold for separating upwelled water from typical coastal surface water, and the same condition was then applied to Sentinel-3 OLCI data (Paper I). The area identified from the reflectance ratio corresponded well with low SST areas in SLSTR imagery (Figure 7 in Paper I). The ratio provides an optical indicator of upwelled water and can be useful when SST data are not simultaneously available or when higher spatial detail from optical imagery is needed.

3.3.2 Harbour-Related Effects on TSM and CDOM

CDOM did not show a direct relation to harbour-related activity in Paper IV. The highest CDOM values occurred near Pärnu Harbour, where annual mean CDOM was positively, but not significantly, related to the mean annual discharge of the Pärnu River ($R=0.59$, $p=0.075$; Table 6 in Paper IV).

The effect of harbour-related activity was most evident in TSM through vessel-induced resuspension (Paper IV). Annual vessel visits were significantly related to mean annual TSM in Tallinn Harbour, where vessel traffic was highest ($R=0.66$, $p=0.035$; Figure 9 in Paper IV). An increase in vessel visits from approximately 4300 to 12 300 corresponded to an increase in mean annual TSM from 1.3 to 2.5 mg/L. No significant relationship was found in Pärnu and Kunda, where annual vessel visits remained below 1000 (Figure 9 in Paper IV). Vessel-related resuspension was therefore detectable in MERIS-based annual TSM statistics only under sufficiently intensive traffic conditions. Similar effects of vessel activity on suspended sediments have been reported in port and lagoon environments. Briciu-Burghina et al. (2014) linked turbidity events in Dublin Port to vessel activity, while

Rapaglia et al. (2015) showed that ship wakes caused sediment remobilisation in the Venice Lagoon.

The detectability of harbour-related TSM changes depends on the local natural background. Raag et al. (2014) showed that monthly mean TSM near Estonian commercial harbours ranged from 0.75–2.60 mg/L near Tallinn to 10.04–24.23 mg/L near Pärnu. In Pakri Bay, Raag et al. (2014) assessed dredging-induced turbidity by comparing MERIS-derived TSM during the dredging period with monthly background TSM conditions. The impact threshold was set at 2.26 mg/L above background TSM, accounting for natural variability and retrieval uncertainty. Harbour-related TSM increases should therefore be evaluated against local background variability, particularly in shallow coastal waters where wind-driven resuspension and seasonal changes can produce turbidity patterns comparable to those caused by harbour activities.

3.3.3 Flood-Induced Variability in Coastal CDOM

Paper V developed the Sentinel-1 SAR workflow used for mapping OWF and FUV. OWF was mapped from IW VH and EW HV data, which provided the strongest separation between dry land and open water. FUV was mapped from EW HH data, selected from the backscatter contrast between flooded and unflooded forest areas. The OWF thresholds were incidence-angle dependent, whereas FUV was mapped with a fixed HH threshold, as flooded-forest backscatter showed no consistent incidence-angle dependence in the analysed dataset (Table 3).

OWF mapping reached overall accuracies of 93.6–97.8%, with kappa hat coefficient values of 0.62–0.94, depending on site and acquisition mode (Table 6 in Paper V). This validated OWF methodology is also used in the Estonian Environment Agency's national operational open-water extent mapping service (Estonian Environment Agency, n.d.). FUV remained less constrained than OWF, as water below vegetation could not be directly validated with optical satellite imagery. Drone photographs and field observations confirmed that EW HH detected inundated vegetated areas, but FUV accuracy could not be quantified in the same way as OWF (Paper V).

The Sentinel-1 flood maps showed that gauge water level did not represent floodplain inundation equally well across different floodplain settings. In inland floodplains, OWF extent was strongly related to gauge water level, with $R^2=0.94$ for Alam-Pedja and $R^2=0.62$ for Soomaa. In the Matsalu coastal river delta floodplain, the relationship with the Kasari hydrological station was weaker, with $R^2=0.34$ for IW VH and $R^2=0.38$ for EW HV (Figure 7 in Paper V). The weaker relationship in Matsalu reflects the influence of coastal water-level conditions in addition to river water level.

The Sentinel-1 methodology developed in Paper V was applied to four selected flood events: one in the Pärnu river system, one in the Keila river system and two in the Kasari river system. Mapped flood extent was compared with coastal $a_{\text{CDOM}}(442)$ derived from Sentinel-3 OLCI using the OWT-based retrieval developed in Paper III. Coastal $a_{\text{CDOM}}(442)$ was extracted from pixels located at least 500 m from the shoreline and in water deeper than 2 m to reduce land adjacency and shallow-water effects. Flood mapping areas followed the actual floodplain location in each river system, rather than a fixed distance from the river mouth. The timing of the $a_{\text{CDOM}}(442)$ increase in the receiving coastal waters was then compared with the mapped inundation period (Figure 8).

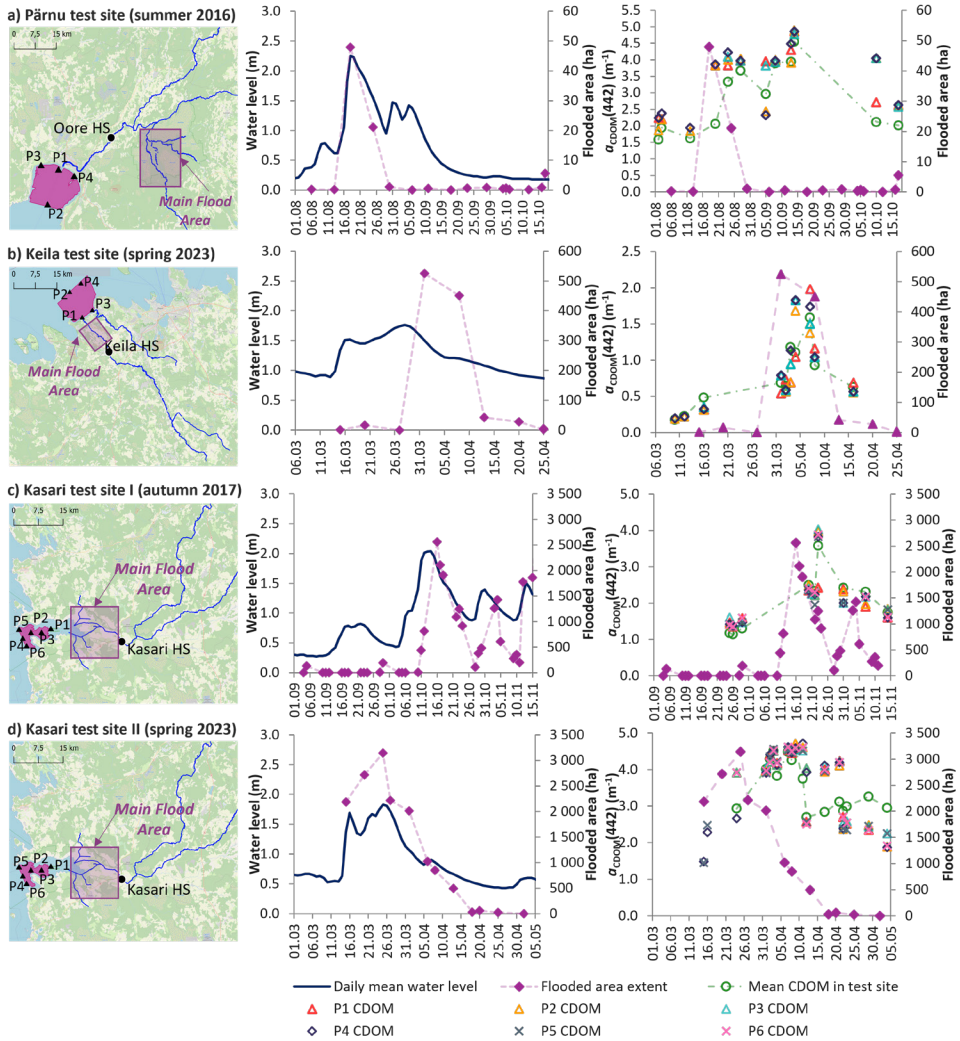


Figure 8. Integration of Sentinel-1 flood mapping with optical water type (OWT) based Sentinel-3 OLCI retrieval of the coloured dissolved organic matter (CDOM) absorption coefficient at 442 nm ($a_{CDOM}(442)$) to assess flood-related CDOM variability in river-influenced coastal waters. Four flood events are shown: a) Pärnu test site, summer 2016; b) Keila test site, spring 2023; c) Kasari test site I, autumn 2017; and d) Kasari test site II, spring 2023. For each event, the left panel shows the riverine flood mapping area and the coastal points used for extracting OLCI-derived $a_{CDOM}(442)$ estimates. The middle panel shows hydrological station water level together with Sentinel-1 mapped flood extent, and the right panel shows coastal $a_{CDOM}(442)$ estimates at individual points and as the site mean. HS denotes hydrological station.

The temporal correspondence between Sentinel-1 derived flood extent and hydrological station water level depended on the station location relative to the mapped floodplain area (Figure 8). At the Pärnu test site, daily mean water level and mapped flood extent showed close agreement, with nearly coincident peaks. In the Kasari and

Keila test sites, the mapped floodplain areas were located downstream from the hydrological stations, and flood extent increased after the rise in water level. This indicates downstream propagation of high-water conditions across the floodplain and river corridor.

Mapped flood peaks were followed by higher $a_{\text{CDOM}}(442)$ in the receiving coastal waters. Coastal $a_{\text{CDOM}}(442)$ increased approximately 1.6–2.7 times after the flood period. The increase was evident in both point-based estimates and the mean $a_{\text{CDOM}}(442)$ of the river-influenced bay area. For the analysed events, the highest $a_{\text{CDOM}}(442)$ values occurred on average about seven days after the flood peak. Figure 9 illustrates the spatial pattern in the Pärnu case, where elevated OLCI-derived $a_{\text{CDOM}}(442)$ values occurred in the river-influenced inner bay after the August 2016 flood event. These results complement Paper IV by linking the previously observed Pärnu River influence on harbour-area CDOM to short-term flood-related $a_{\text{CDOM}}(442)$ changes.

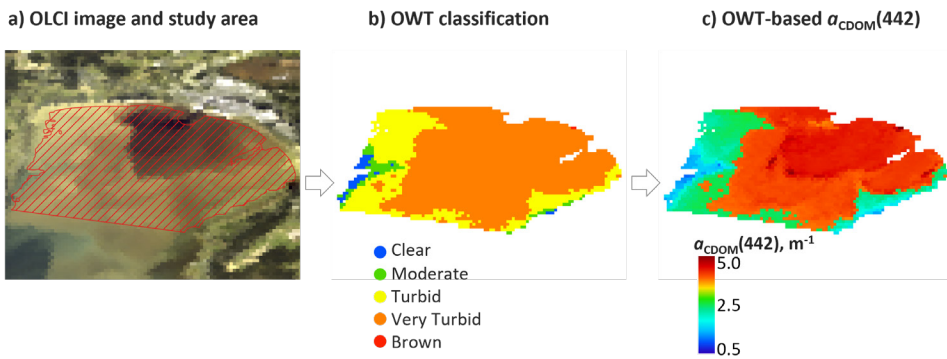


Figure 9. Example of optical water type (OWT) based retrieval of the coloured dissolved organic matter (CDOM) absorption coefficient at 442 nm ($a_{\text{CDOM}}(442)$) in Pärnu Bay after the August 2016 flood event. The workflow is shown for a Sentinel-3 OLCI image acquired on 28 August 2016: a) OLCI image with the Pärnu Bay coastal analysis area, b) pixel-wise OWT classification, and c) OWT-based $a_{\text{CDOM}}(442)$ distribution. Elevated $a_{\text{CDOM}}(442)$ values in the inner bay indicate CDOM-rich water associated with riverine and flood-related input.

4 Conclusions

The main aim of this thesis was to assess how satellite remote sensing can be used to detect and interpret processes influencing coastal water quality in the eastern Baltic Sea, with emphasis on optically complex Estonian coastal waters. The results show that reliable satellite-based water quality assessment in this region requires process-based interpretation of optical variability, regionally evaluated retrieval methods and multi-sensor analysis of the drivers affecting coastal waters. The main conclusions are as follows:

- **Thermohaline structure modifies the optical water column mainly through the vertical redistribution of OSCs.** In the Gulf of Finland, stratification separated particle-rich surface waters from optically different deeper layers. This was expressed most clearly in particle-related scattering, with $b(440)$ decreasing by 85.7% between the surface and 20 m depth under stratified conditions.
- **Upwelling altered the optical signal of the surface layer and could be identified from reflectance data.** Simulations showed that when deeper water reached the surface, reflectance in the photosynthetically active spectral range decreased by up to 68.8%. At the same time, the optically clearer upwelled water increased the depth represented by the water-leaving signal, particularly in the green part of the spectrum. The ratio $R(490)/R(560) \geq 0.77$ provided an optical indicator of upwelled water, complementing SST-based detection where SST data are unavailable or too coarse.
- **The standard Case 2 Regional CoastColour processor (C2RCC) workflow for Sentinel-3 OLCI was limited mainly at the retrieval stage from water-leaving reflectance to IOPs and water quality parameters.** The atmospherically corrected water-leaving reflectance retained useful spectral information, with correlations up to $R=0.82$ at 560 nm, but the C2RCC-derived IOPs and standard Chl-*a* and TSM products showed weak agreement with *in situ* data. This indicates that, in Baltic Sea coastal waters, atmospherically corrected OLCI reflectance can support further empirical retrievals, whereas the standard C2RCC product outputs require regional evaluation before use.
- **Regionally adapted empirical algorithms improved water quality retrievals when the optical conditions of the water were accounted for.** Chl-*a* retrieval benefited from green, red and NIR bands rather than standard blue-green ratios, which are limited by CDOM absorption in Baltic Sea waters. For $a_{CDOM}(442)$, the OWT approach separated the dataset into five optical water types and enabled algorithms to be selected according to the reflectance characteristics of each water type. The resulting $a_{CDOM}(442)$ estimates agreed well with *in situ* measurements across hyperspectral, OLCI and MSI configurations ($R \geq 0.87$), while very high CDOM absorption in Brown OWT remained difficult to retrieve reliably.
- **Long-term MERIS observations showed that vessel-related resuspension was detectable in satellite-derived TSM only under high traffic intensity and must be evaluated against local background variability.** The relationship between vessel traffic and mean annual TSM was evident in Tallinn Harbour, where annual vessel traffic exceeded 6000 visits, but not in harbours with fewer than 1000 annual vessel visits. In shallow coastal waters, wind-driven resuspension and seasonal variability can generate turbidity patterns similar to those associated with harbour activity. This

highlights the need for site-specific background information when assessing harbour-related impacts on suspended matter dynamics.

- **The developed Sentinel-1 SAR-based flood mapping method enabled both open-water flooding and flooding under vegetation to be detected, with open-water flood mapping accuracies of 93.6–97.8% and kappa hat coefficient values of 0.62–0.94.** The method was developed for Estonian floodplains. The Sentinel-1 results complemented hydrological station data by showing where, how extensively and how persistently floodwater occurred across the floodplain. The open-water flood mapping approach is also used in the Estonian Environment Agency's operational open-water extent service.
- **Combining Sentinel-1 flood maps with OWT-based Sentinel-3 OLCI $a_{\text{CDOM}}(442)$ retrieval showed a delayed coastal CDOM response to floodplain inundation.** At the Pärnu, Keila and Kasari test sites, coastal $a_{\text{CDOM}}(442)$ increased approximately 1.6–2.7 times after flood events, with the maximum response occurring on average about seven days after the mapped flood peak. For the analysed events, multi-sensor analysis linked upstream flood dynamics with short-term CDOM variability in the receiving coastal waters. The observed delay was event- and site-specific.

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Abstract

Processes Influencing Coastal Water Quality in the Eastern Baltic Sea as Observed from Remote Sensing Data

Coastal water quality in the Baltic Sea is shaped by physical forcing, biogeochemical processes and human activities that modify the concentration, composition and vertical distribution of optically significant constituents (OSCs), such as coloured dissolved organic matter (CDOM), total suspended matter (TSM) and phytoplankton. In the eastern Baltic Sea, these constituents are affected by riverine inputs, flood-driven export, sediment resuspension, seasonal stratification and upwelling. These processes modify absorption and scattering in the water column and, therefore, the light signal measured by ocean colour satellite sensors. Its interpretation is difficult because CDOM, suspended particles and phytoplankton can vary partly independently while producing overlapping effects in the visible spectrum.

The main aim of this dissertation was to assess how satellite remote sensing can be used to detect and interpret processes influencing coastal water quality in the eastern Baltic Sea, with emphasis on optically complex Estonian coastal waters. The work combined *in situ* reflectance measurements, inherent optical properties (IOPs) and water quality measurements with optical, thermal infrared and radar satellite data. Sentinel-3 OLCI and Envisat MERIS were used as the main optical data sources for water quality analyses, MODIS and SLSTR for sea surface temperature (SST), Sentinel-1 SAR for flood mapping, and Sentinel-2 MSI as an optical reference dataset for validating Sentinel-1 derived open-water flood (OWF) extent. The analysis linked three aspects of coastal water quality remote sensing: the optical variability of the water column, the performance of satellite-based retrieval methods, and the use of multi-sensor observations to analyse coastal responses to natural and anthropogenic forcing.

Optical measurements showed that thermohaline structure affected the vertical distribution of OSCs in the Gulf of Finland, which was expressed in the IOP profiles mainly through changes in particle-related scattering. Under stratified conditions, the scattering coefficient at 440 nm ($b(440)$) decreased by 85.7% between the surface and 20 m depth, indicating a strong reduction in particle-related scattering below the thermocline. Simulations based on measured IOPs showed that optically clearer subsurface water reaching the surface during upwelling may reduce reflectance in the photosynthetically active spectral range by up to 68.8%. At the same time, the optically detectable layer became deeper, especially in the green spectral region, where the optical depth from which 90% of the water-leaving signal originates (z_{90}) increased from 2.3 to 4.3 m. The measured upwelling case confirmed the lower and smoother reflectance signal of upwelled water, and the ratio $R(490)/R(560) \geq 0.77$ provided an optical indicator that complemented SST-based upwelling detection.

The evaluation of Sentinel-3 OLCI data showed that atmospheric correction, IOP retrieval and the derivation of water quality products introduced different uncertainties in Baltic Sea waters. The atmospherically corrected water-leaving reflectance retained useful spectral information, especially in the green, red and near-infrared regions, whereas C2RCC-derived IOPs and standard Chl-*a* and TSM products showed weak agreement with *in situ* measurements. Empirical algorithms applied to the water-leaving reflectance gave more reliable estimates than the standard C2RCC product outputs,

although performance differed between parameters, band combinations and validation datasets.

Optical water type (OWT) classification improved CDOM retrieval by allowing empirical algorithms to be selected according to reflectance shape and bio-optical conditions. The dataset was separated into five OWTs, from clear waters with low OSC concentrations to CDOM-rich brown waters. The results showed that $a_{\text{CDOM}}(442)$ retrieval could not be described by one universal empirical relationship across boreal inland and coastal waters. OWT-based estimates agreed well with measurements across hyperspectral, OLCI and MSI spectral configurations, with $R \geq 0.87$. The main limitation occurred in Brown OWT, where very high $a_{\text{CDOM}}(442)$ values, mainly associated with optically extreme CDOM-rich lakes, remained difficult to retrieve reliably.

Long-term MERIS time series were used to assess inter-annual variability in TSM and CDOM near Estonian harbours in relation to vessel traffic, wind conditions and river discharge. Vessel-related sediment resuspension was detectable in satellite-derived TSM only under sufficiently intensive traffic conditions. In Tallinn Harbour, where traffic exceeded 6000 vessel visits per year, mean annual TSM increased with traffic intensity. No comparable relationship was found in harbours where annual vessel traffic remained below 1000 visits. Wind conditions were related to monthly TSM variability in several harbour-adjacent areas, but annual mean wind speed did not explain inter-annual TSM variability. Mean annual CDOM showed the clearest positive relationship with mean annual discharge of the Pärnu River near Pärnu Harbour, whereas no corresponding pattern was found at the other harbour sites located near river mouths.

A Sentinel-1 SAR-based method was developed and applied to map flood extent and frequency in Estonian boreal floodplains, including both open-water flooding (OWF) and flooding under vegetation (FUV). OWF was mapped from IW VH and EW HV data using local incidence angle-dependent backscatter thresholds, while FUV was mapped from EW HH data using a fixed backscatter threshold. Compared with point-based hydrological station data, the Sentinel-1 analysis provided spatially explicit information on where and how persistently floodwater occurred across the floodplain. The Sentinel-1 flood maps were then combined with Sentinel-3 OLCI $a_{\text{CDOM}}(442)$ retrievals based on OWT-specific algorithms to evaluate flood-induced CDOM variability in river-influenced coastal waters. At the Pärnu, Keila and Kasari test sites, coastal $a_{\text{CDOM}}(442)$ increased approximately 1.6 to 2.7 times after flood events, with the maximum response occurring on average about seven days after the mapped flood peak. This delay was consistent across the analysed events and indicates a site-specific lag between floodplain inundation and the CDOM response in the receiving coastal waters.

The analyses show that satellite remote sensing can be used to detect and interpret process-driven changes in optical properties and water quality parameters in Estonian coastal waters of the eastern Baltic Sea. Such interpretation requires consideration of: (1) how the water-leaving optical signal is formed, (2) when and which regionally adapted or site-specific algorithms should be applied, and (3) which processes affect water quality and, consequently, the optical properties of the water. The combination of *in situ* optical measurements, regionally adapted remote sensing algorithms, optical water type based CDOM retrieval, and multi-sensor satellite observations enabled the observed optical variability to be linked to water-mass displacement during upwelling, vessel traffic-induced sediment resuspension, and riverine and flood-related inputs.

Lühikokkuvõte

Kaugseire andmetest hinnatud rannikuvee kvaliteeti mõjutavad protsessid Läänemere idaosas

Läänemere rannikuvee kvaliteet kujuneb looduslike protsesside ja inimtegevuse koosmõjul. Rannikuvee muutlikkus nii ajas kui ruumis on põhjustatud mitmetest protsessidest. Jõgedega kanduvad merre orgaaniline aine ja heljum. Suurvee ajal võib rannikumerre jõuda tavapärasest rohkem jõeäärsetelt aladelt pärinevat orgaanilist ainet. Põhjasetteid tõstavad veesambasse tuule tekitatud lainetus ja hoovused, aga ka laevaliiklus. Rannikuvee optilisi omadusi mõjutavad lisaks veesamba kihistumine ja süvaveeerge ehk *upwelling*. Kõik need protsessid muudavad vees leiduvate optiliselt aktiivsete ainete sisaldust ja jaotust ning seeläbi ka seda, kuidas päikesekiirgus vees neeldub ja hajub.

Satelliitkaugseire võimaldab neid muutusi hinnata kaudselt. Osa vees hajunud päikesekiirgusest väljub veest tagasi atmosfääri. See veest väljuv kiirgus kannab endas teavet vee optiliste omaduste kohta. Satelliidisensor registreerib kogu sensorini jõudva kiirguse, millest veest väljuv signaal moodustab vaid väikese osa. Pärast atmosfääri mõju eemaldamist saab hinnata vee peegeldumisspektrit. Peegeldumisspektri tugevus ja kuju sõltuvad sellest, kuidas vesi ja selles sisalduvad optiliselt aktiivsed ained kiirgust neelavad ja hajutavad. Läänemeres kujundavad kaugseire peegeldumisspektrit eelkõige vees sisalduvad värvunud lahustunud orgaaniline aine ehk CDOM, heljum ja fütoplankton ning nende sisaldus ja jaotus vees võivad kiiresti ning üksteisest osaliselt sõltumatult muutuda. Selline muutlikkus on üks põhjus, miks ookeanivete jaoks välja töötatud standardsed veekvaliteedi parameetrite satelliidiproduktid optiliselt keerukates ranniku- ja sisevetes piisavalt usaldusväärselt ei toimi. Satelliidiandmete tõlgendamisel tuleb seega arvestada nii veest väljuva optilise signaali kujunemise, kasutatavate kaugseirealgoritmide sobivuse (piirangutega) kui ka vee optilisi omadusi mõjutavate protsessidega.

Doktoritöö eesmärk oli uurida satelliitkaugseire võimalusi Läänemere idaosas rannikuvee optiliste omaduste ja veekvaliteedi muutuste hindamiseks ning neid muutusi kujundavate protsesside analüüsimiseks. Töös kasutati nii optiliste parameetrite kohtmõõtmiste (*in situ*) andmeid kui ka satelliidiandmetest tuletatud näitajaid. Rannikuvee optiliste parameetrite hindamiseks kasutati Sentinel-3 OLCI ja Envisat MERIS andmeid. Merepinna temperatuuri (SST) hinnati Terra/Aqua MODIS ja Sentinel-3 SLSTR mõõtmiste põhjal. Üleujutuste kaardistamiseks kasutati Sentinel-1 SAR radarandmeid ning avatud vee üleujutuse kaardistuse valideerimiseks Sentinel-2 MSI optilisi andmeid.

Töö tulemusena selgus, et veesamba termohaliinne struktuur mõjutab vee esmaseid optilisi parameetreid optiliselt aktiivsete ainete vertikaalse jaotuse kaudu. Soome lahes avaldus see eelkõige vees sisalduvate osakestega seotud valguse hajumises. Kihistunud veesambas vähenes hajumiskoeffitsient lainepikkusel 440 nm ($b(440)$) veepinna ja 20 m sügavuse vahel 85,7%. Koos sellega muutus ka valguse nõrgenemise iseloom: ülemises segunenud veekihi domineeris hajumine, termokliinist allpool aga neeldumine. Süvaveeerge korral võib selline sügavamast veekihist pärit optiliselt selgem veemass jõuda pinnakihti ning oluliselt muuta veest väljuvat optilist signaali. Mõõdetud esmaste optiliste parameetrite põhjal tehtud simulatsioonid näitasid, et vee peegeldustegur fotosünteesiliselt aktiivses spektripiirkonnas (400–700 nm) võib sellises olukorras väheneda kuni 68,8%. Samuti muutub vee peegeldumisspektri kuju nähtava valguse

piirkonnas laugemaks. Optiliselt selgema vee tõttu suureneb ka satelliidisensorile nähtava pinnakihi paksus. Rohelises spektripiirkonnas võib 90% veest väljuvast optilisest signalist pärineda umbes 4 m paksusest pinnakihist, samas kui tüüpilises Soome lahe rannikuvees pärineb see ligikaudu 2 m paksusest kihist. Pinnale kerkinud veemassi oli võimalik eristada ka vee peegeldustegurite suhte $R(490)/R(560) \geq 0,77$ alusel. Vastav tingimus annab merepinna temperatuuri kõrval täiendava võimaluse süvavee kerke mõjuala tuvastamiseks optiliste satelliitandmete põhjal.

Satelliidiandmetest tuletatud vee optiliste omaduste ja veekvaliteedi parameetrite usaldusväärsus sõltub nii atmosfäärikorreksioonist kui ka sellele järgnevast andmetöötlusest. Sentinel-3 OLCI andmete puhul hinnati vastavaid etappe eraldi C2RCC (*Case 2 Regional CoastColour*) töötlusahela abil. Atmosfäärikorreksiooni järel saadud vee peegeldumisspektrid olid mitteõitsengu tingimustes üldiselt realistlikud nii spektri kuju kui peegeldusteguri väärtuste poolest. Kooskõla *in situ* mõõtmistega oli parem rohelises, punases ja lähiinfrapunases spektripiirkonnas, samas kui suuremad erinevused ilmnesid spektri sinises osas. Tiheda tsüanobakterite õitsengu korral ei andnud atmosfäärikorreksioon siiski usaldusväärset peegeldumisspektrit. C2RCC töötlusahela järgmises etapis kasutatakse saadud vee peegeldumisspektrit närvivõrgul põhineva bio-optilise mudeli sisendina. Mudeli abil hinnatakse vee esmaseid optilisi parameetreid. Läänemere tingimustes ei leitud C2RCC-ga tuletatud esmaste optiliste parameetrite ja *in situ* mõõtmiste vahel statistiliselt olulist seost. Seetõttu ei olnud piisavalt usaldusväärsed ka nende põhjal arvutatud klorofüll a , heljumi ja CDOM-i hinnangud.

Kuna atmosfäärikorreksiooni järel saadud vee peegeldumisspektrid olid mitteõitsengu tingimustes siiski kasutatavad, hinnati nende põhjal ka empiiriliste algoritmide sobivust veekvaliteedi parameetrite hindamiseks. Mitmed testitud spektraalsete kanalite suhtel põhinevad empiirilised algoritmid andsid veekvaliteedi parameetrite hindamisel paremaid tulemusi kui C2RCC standardne närvivõrgupõhine lähenemine. Empiiriliste algoritmidega oli võimalik hinnata klorofüll a , heljumit, CDOM-i ja Secchi ketta sügavust, kuigi tulemuste täpsus erines parameetrite vahel. Algoritmide sobivus sõltus hinnatavast parameetrist, vee bio-optilistest omadustest ja kasutatud spektraalkanalitest. Kõige paremini toimusid algoritmid, mis kasutasid rohelise, punase ja lähiinfrapunase spektripiirkonna kanaleid. Näiteks klorofüll a hindamisel andsid need Läänemere rannikuvee tingimustes paremaid tulemusi kui standardsed sinise ja rohelise spektripiirkonna peegeldustegurite suhted.

Lisaks rakendati doktoritöös CDOM-i hindamisel optiliste veetüüpide ehk OWT-de põhiste lähenemist, mis võimaldas arvestada vee bio-optiliste erinevustega. Selle asemel, et rakendada kogu andmestikule ühte algoritmi, jaotati veed peegeldumisspektri omaduste põhjal viide bio-optiliselt erinevasse veetüüpi ning iga veetüübi jaoks kasutati testitud algoritmide seast sobivaimat CDOM-i hindamise algoritmi. OWT-põhised $a_{\text{CDOM}}(442)$ hinnangud olid *in situ* mõõtmistega heas kooskõlas nii hüperspektraalsete andmete, kui ka OLCI ja MSI spektraalkanalite korral, kus $R \geq 0,87$. Meetodi peamine piirang avaldus väga suure CDOM-i neeldumisega vete korral, kui $a_{\text{CDOM}}(442)$ väärtusi üle 20 m^{-1} ei olnud enam võimalik usaldusväärselt hinnata. Selliseid tingimusi esineb eelkõige väga CDOM-rikastes sisevetes. Enamiku Läänemere rannikuvee puhul ei ole see piirang määrav.

Töös hinnati ka pikaajaliste Envisat MERIS aegridade põhjal heljumi ja CDOM-i muutlikkust Eesti sadamate lähialadel. Analüüsis arvestati laevaliiklust, tuuleolusid ja jõgede äravoolu. Laevaliiklusega seotud setete resuspensiooni mõju oli satelliidiandmetest hinnatud heljumi kontsentratsioonides tuvastatav ainult intensiivse

laevaliiklusega Tallinna sadama piirkonnas (>6000 laevakülastust aastas). Aastakeskmine heljumi kontsentratsioon vee pinnakihi suurenemise seal koos laevaliikluse intensiivsusega. Alla 1000 laevakülastusega sadamates vastavat seost ei leitud. Tuuleolud olid seotud heljumi kuuphise muutlikkusega mitmes sadamapiirkonnas, kuid aastakeskmine tuulekiirus ei selgitanud heljumi aastate vahelist muutlikkust. Pärnu sadama piirkonnas seostus Pärnu jõe suurenemine äravooli kõrgema aastakeskmise CDOM-i kontsentratsiooniga, kuigi seos ei olnud statistiliselt oluline. Teistes jõesuudmete lähedal asuvates sadamates oli CDOM-i seos jõe äravooluga nõrk.

Eraldi käsitleti doktoritöös jõgedega seotud üleujutussündmusi. Üleujutuste ulatuse ja esinemissageduse hindamiseks töötati välja Sentinel-1 SAR andmetel põhinev meetod, mida rakendati Eesti boreaalsetel lammialadel. Meetod võimaldas kaardistada nii avatud vee üleujutust, kui ka taimestiku all esinevat vett. Avatud vee kaardistamisel kasutati sisendina Sentinel-1 IW VH ja EW HV polarisatsiooniga andmeid. Radari tagasihajunud signaali võrreldi lokaalsest langemisnurgast sõltuva läviväärtusega. Taimestiku all esinevat üleujutust kaardistati EW HH andmete põhjal, kasutades fikseeritud tagasihajumise läviväärtust. Avatud vee üleujutuse kaardistuse üldine täpsus oli 93,6–97,8% ning kapp koefitsient jäi vahemikku 0,62–0,94. Võrreldes hüdromeetriaajaamade mõõtmisandmetega võimaldas Sentinel-1 hinnata üleujutuse ruumilist ulatust ja püsivust kogu lammialal.

Üleujutustega seotud lühiajaliste muutuste hindamiseks rannikuvee CDOM-is seoti Sentinel-1 SAR andmetest kaardistatud üleujutuse ulatus OWT-põhiste Sentinel-3 OLCI $a_{CDOM}(442)$ hinnangutega. Pärnu, Keila ja Kasari jõesüsteemides analüüsiti nelja valitud üleujutussündmust ning kaardistusala määratleti igas jõesüsteemis eraldi vastavalt kohaliku üleujutusala paiknemisele. Analüüsitud sündmuste järel suurenes rannikuvee $a_{CDOM}(442)$ ligikaudu 1,6–2,7 korda. Suurim CDOM-i kontsentratsiooni kasv rannikuvees järgnes kaardistatud üleujutuse tipule keskmiselt umbes seitsme päevase viiteajaga.

Käesolev töö näitas, et satelliitkaugseire abil saab Läänemere idaosas (sh Eesti rannikumeres) hinnata vee optilisi omadusi ja veekvaliteedi parameetreid ning seostada neid rannikuvee kvaliteeti mõjutavate protsessidega. Kaugseireandmete usaldusväärsaks rakendamiseks tuleb arvestada: (1) kuidas kujuneb veest väljuv optiline signaal (vee peegeldumisspekter), (2) millal ja kuidas kasutada piirkondlikult kohandatud ehk asukohapõhiseid algoritme ning (3) millised protsessid mõjutavad vee kvaliteeti ja selle kaudu ka vee optilisi omadusi. *In situ* optiliste mõõtmiste kasutamine, piirkondlikult kohandatud kaugseire algoritmide rakendamine, optiliste veetüüpide põhise värvunud lahustunud orgaanilise aine hindamine ja mitme sensori satelliidiandmete ühendamine võimaldasid eristada süvaveekerke, laevaliiklusega seotud setete resuspensiooni ning jõgede ja üleujutuste mõju rannikuvee optilistele parameetritele.

Appendix 1

Publication I

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Impact of Thermohaline Conditions on Vertical Variability of Optical Properties in the Gulf of Finland (Baltic Sea): Implications for Water Quality Remote Sensing

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Vertical variability of inherent optical properties (IOPs) affect the water quality retrievals from remote sensing data. Here, we studied the vertical variability of IOPs and simulated apparent optical properties (AOPs) in the Gulf of Finland (Baltic Sea) under three characteristic (non)stratification conditions. In the case of mixed water column, the vertical variability of optically significant constituents (OSC) and IOPs was relatively small. While in case of stratified water column the IOPs of surface layer were three times higher compared to the IOPs below the thermocline and the IOPs were strongly correlated with the physical parameters (temperature, salinity). Measurements of IOPs in stratified water column showed that the ratio of scattering ($b(440)$) to absorption ($a(440)$) changed under the thermocline ($b(440)/a(440) < 1$) i.e., absorption became the dominant component of attenuation under thermocline while the opposite is true for the upper layer. Simulated (from IOPs) spectral irradiance reflectance ($R(\lambda)$) and spectral diffuse attenuation coefficient ($K_d(\lambda)$) from deeper layers (below thermocline) have significantly smaller magnitude and smoother shape. This becomes relevant during upwelling events—a common process in the coastal Baltic Sea. We quantified the effect of upwelling on surface water properties using simulated AOPs. The simulated AOPs (from IOPs measurements) showed a decrease of the signal up to 68.8% and an increase of optical depth ($z_{90}(\lambda)$) from 2.3 to 4.3 m in the green part of the spectrum in case upwelled water mass reaches the surface. In the coastal waters a vertical decrease of $K_d(\lambda)$ in the PAR region (400–700 nm) by 6.8% (surface to 20 m depth) was observed, while vertical decrease of chlorophyll-*a* (Chl-*a*) and total suspended matter (TSM) was 31.7 and 42.1%, respectively. The ratio $R(490)/R(560) \geq 0.77$ indicates also the upwelled water mass. The study showed that upwelling is a process that, in addition to biological activity, horizontal transport of OSC, and temperature changes, alters the optical signal of surface water measured by a remote sensor. Knowledge about the vertical variability of IOPs and AOPs relation to upwelling can help the parametrization of remote sensing algorithms for retrieving water quality estimates in the coastal regions.

Keywords: upwelling, inherent optical properties, apparent optical properties, reflectance, diffuse attenuation coefficient, Gulf of Finland

INTRODUCTION

The remote sensing of ocean colour is a valuable tool for synoptic regional- and global-scale water-quality data estimation [e.g., the concentration of chlorophyll-*a* (Chl-*a*) and total suspended matter (TSM)]. Continuous monitoring of the optical quality of water bodies helps to understand different natural processes better, as well as to detect environmental threats such as eutrophication and harmful algal blooms (Ritchie et al., 2003; Glasgow et al., 2004). However, the interpretation of data from passive optical remote sensing is sometimes complicated, not only because of the disturbing influence of the atmospheric effects but also because of some specific characteristics of the object under investigation—the upper layer of the ocean. This is particularly true in the case of marginal seas and inland waters. These waters are optically complex and commonly known as Case 2 waters (Morel and Prieur, 1977), being a function of at least three optically significant constituents (OSC) [phytoplankton pigments, coloured dissolved organic matter (CDOM), and total suspended matter], which may vary independently of one another.

In the Baltic Sea, the composition and concentrations of OSC are highly variable over short spatial scales. Hence, standard remote sensing algorithms developed for Case 2 waters often fail in this area (e.g., Attila et al., 2013, 2018; Toming et al., 2017). In open and coastal waters of the Baltic Sea, CDOM is the dominant optical component (Kirk, 1984; Kowalczyk et al., 2006; Kratzer and Tett, 2009; Kratzer and Moore, 2018). For instance, according to Kratzer and Moore (2018), the CDOM absorption values range between 0.6 and 1.2 m^{-1} (Gulf of Finland), 1.5 and 13.0 m^{-1} (Gulf of Riga), and 0.2 and 0.3 m^{-1} (Bornholm Sea). In the coastal areas, there are also significant loads of TSM, which increase with proximity to the coast (Kratzer and Tett, 2009). Additionally, Kyrliuk and Kratzer (2019) showed that the Gulf of Gdańsk and Gulf of Riga, which are shallow coastal basins of the Baltic Sea, have a large variability of TSM concentrations, compared to the other basins. The mean values ($\pm$ standard deviation) over a 3-year period (summer) were $2.80 \pm 3.90 \text{ g m}^{-3}$ and $1.56 \pm 2.00 \text{ g m}^{-3}$, respectively. In addition to spatial variability OSC also show great seasonal variation in the Baltic Sea. The phytoplankton distribution is strongly influenced by the temperature of surface water and the availability of specific nutrients (nitrate, phosphate). Diatoms and dinoflagellates dominate the spring bloom occurring after ice melt and cyanobacteria dominate during summer and early autumn (Wasmund, 1994; Gasinaite et al., 2005; Kownacka et al., 2018; Hjerne et al., 2019). In this case, the optical properties of these phytoplankton groups are so different that some studies have indicated that seasonal remote sensing algorithms are needed (Ligi et al., 2017; Simis et al., 2017). According to the review by Kratzer and Moore (2018) the Chl-*a* variability in the Baltic Sea ranges from 0.3 to 130 mg m^{-3} (in the Gulf of Finland from 1.2 to 130 mg m^{-3}). From the high-resolution Hyperion imagery, Reinart and Kutser (2006) showed that the chlorophyll concentration may rise up to $\sim 300 \text{ mg m}^{-3}$ during cyanobacteria bloom in the Gulf of Finland. Kutser (2004)

showed concentrations up to 1,000 mg m^{-3} in case of thick cyanobacterial accumulations.

In addition, the coastal zones of the Baltic Sea are often affected by upwellings induced by alongshore winds. This causes the mixing of clear water masses from deeper layers and turbid surface layer water (Gidhagen, 1987; Myrberg and Andrejev, 2003; Lehmann et al., 2012; Omstedt et al., 2014). Numerous studies of this phenomenon in the Baltic Sea have been carried out using remote sensing methods (Kahru et al., 1995; Lehmann et al., 2012; Omstedt et al., 2014), model simulations (Myrberg and Andrejev, 2003; Zhurbas et al., 2008; Laanemets et al., 2009; Väli et al., 2011) and field observations (Haapala and Alenius, 1994; Vahtera et al., 2005; Suursaar and Aps, 2007; Kuvaldina et al., 2010; Kikas and Lips, 2016). The narrow, elongated Gulf of Finland, an easternmost sub-basin of the Baltic Sea, is a well-known region of upwellings during the summer and autumn months when the water masses are relatively strongly stratified (Zhurbas et al., 2008; Gurova et al., 2013; Kikas and Lips, 2016). In this gulf, upwelling along one coast is usually accompanied by downwelling along the opposite coast (e.g., Zhurbas et al., 2008; Lips et al., 2009). Upwelling near the northern coast of the Gulf of Finland is induced by south-westerly winds and along the southern coast by north-easterly winds. Even though upwelling in the southern nearshore is less frequent (about 25% of the time) and not as persistent as near the northern coast (about 30% of the time) (Myrberg and Andrejev, 2003), intensive upwellings also occur near the southern coast of the gulf (Lips et al., 2009; Uiboupin and Laanemets, 2009). The changing wind patterns have apparently increased their frequency in the recent past (Soomere et al., 2015). In addition to changes in the temperature and salinity fields, upwelling events also affect the transport and distribution of sediments and dissolved substances in the marine environment (Nowacki et al., 2009; Dabuleviciene et al., 2018), thus affecting the inherent optical properties (IOPs) of the surface water. Moreover, upwelling plays a crucial role in boosting biological productivity as nutrient-rich water is advected upward into the photic layer, where the process of photosynthesis is promoted (Vahtera et al., 2005; Laanemets et al., 2009; Lips et al., 2009; Uiboupin et al., 2012). Usually the chlorophyll concentrations increase several days after the start of upwelling event. In the early phase (“active phase”) of the upwelling the advected water has low temperature and low OSC concentrations which will increase if the upwelled water remains in the euphotic zone.

Variation of IOPs is an indicator of changes in the concentrations and types of OSC in water. In particular, the light absorption coefficient ($a(\lambda)$) and backscattering coefficient ($b_b(\lambda)$) are important for optical modelling, since the reflectance can be derived from a function of the ratio of these coefficients. Additionally, these parameters play a key role in governing light propagation in the water column (Gordon, 1988; Morel and Gentili, 1993). Therefore, it is important to understand horizontal and vertical variations of the IOPs in different water masses in order to obtain reasonable estimates of water quality parameters from remote sensing imagery for the optically complex water bodies.

The objectives of the current study are: (1) to improve the knowledge about the vertical variability of IOPs in the coastal zone of Gulf of Finland (Baltic Sea); (2) to characterise the effect of different hydrodynamic conditions on vertical variability of IOPs; (3) and to quantify the impact of upwelling events on the signal measured by the optical remote sensor (using simulated reflectance).

MATERIALS AND METHODS

The Study Area

The Gulf of Finland is a eutrophied elongated basin in the north-eastern part of the Baltic Sea (**Figure 1**). It is relatively shallow, with a mean depth of 37 m and a maximum depth of 123 m (Paldiski Deep). The total water volume is about 1098 km³ (Leppäranta and Myrberg, 2009). Topographically, the Gulf is a direct continuation of the Baltic Proper and becomes shallower toward its eastern end. The surface area (29,948 km²) is small compared with the catchment area (423,000 km²) (HELCOM, 2015). The water column in deeper areas is also vertically stratified. A seasonal thermocline usually forms at the beginning of May and starts to erode by the end of August. The thermocline is usually situated at a depth of 10–20 m in such a way that a three-layer vertical structure can be distinguished: the upper mixed layer, the cold intermediate layer, and the near-bottom layer (Alenius et al., 1998; Liblik and Lips, 2011). During the winter, the water column is mixed down to the depth of the permanent halocline at 60–80 m (Haapala and Alenius, 1994; Alenius et al., 1998). The Gulf is strongly influenced by river runoff (114 km³/year), primarily from the Neva, and this influence is apparent not only in the low salinity but also in the optical properties of these waters (Alenius et al., 2003; Vazyulya et al., 2014; Ylöstalo et al., 2016; Sipilgas et al., 2018). The algal growth season is generally from early May to late August (Jaanus et al., 2011). Therefore, factors causing increased light attenuation (e.g.,

organic and inorganic matter) vary both spatially and temporally in the study area.

In situ Data

The *in situ* measurements for this study were conducted during seven field campaigns (**Table 1**). The IOPs measurements were performed during the two summers of 2015 (on July 20, July 30–31, August 12, August 25) and 2016 (on July 26–27 and August 3–4), and reflectance measurements to compare the results obtained from previous campaigns were performed during one campaign in the summer of 2018. Additionally, water samples from three different depths (surface layer (0–m), 10 m depth, and 20 m depth) were collected with a rosette sampler, and Secchi depth measurements were performed with a standard white disc with a 30 cm diameter. **Figure 1** shows the locations of *in situ* measurement stations.

Laboratory Measurements

The concentration of TSM (mg L⁻¹) was measured using a standard gravimetric technique. Mixed water sample 0.750 L was filtered through pre-combusted and pre-weighted Millipore membrane filters (pore size 0.45 μm, diameter 47 mm). The filters were rinsed with 40 ml distilled water in order to wash out salt residuals. The filters were then dried to a constant weight at the temperature of 105°C. The increase of filter weight indicates the TSM concentration (Strickland and Parsons, 1972; Mueller et al., 2003). A single value of TSM was determined from each water sample.

Chl-*a* concentration (mg m⁻³) was determined by filtering the water sample through Whatman GF/F glass microfiber filter (pore size 0.7 μm, diameter 47 mm), extracting the pigments with 96% ethanol and measuring spectrophotometrically (Thermo Helios γ) absorption at wavelengths of 665 and 750 nm. The values of Chl-*a* were calculated according to the method of Lorenzen (1967).

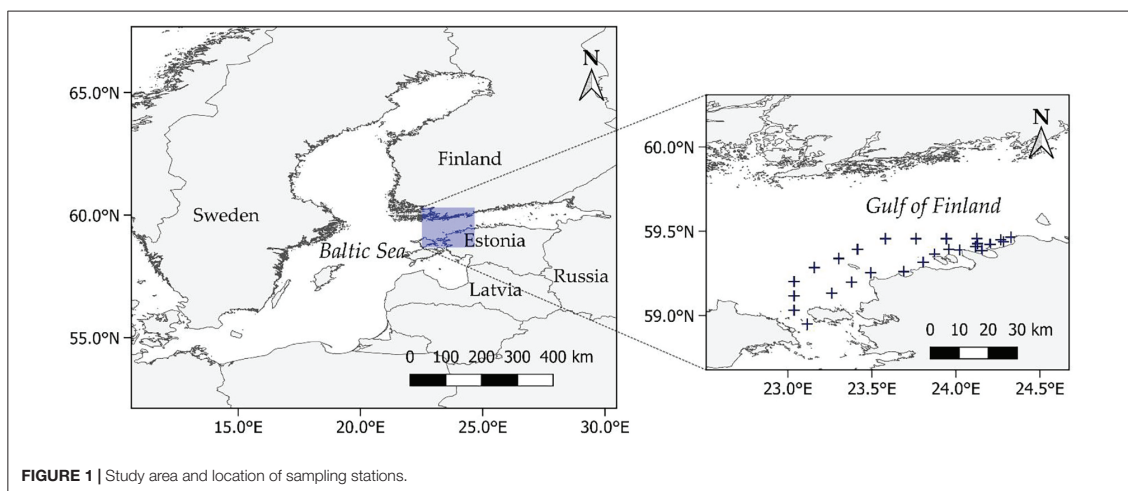


FIGURE 1 | Study area and location of sampling stations.

TABLE 1 | A summary of *in situ* measurements per study area campaign.

Date	No ^a	ac-s	CTD	TR ^b	Secchi Depth (m)	TSM (mg L ⁻¹)			Chl- <i>a</i> (mg m ⁻³)		
						0- m	10 m	20 m	0- m	10 m	20 m
20.07.15	10	+	+	-	3.0–4.0	1.6–3.7	0.3–2.3	0.5–1.9	4.6–15.1	6.9–11.2	4.0–8.7
30–31.07.15	20	+	+	-	3.5–5.5	0.1–3.6	0.1–2.5	0.7–1.7	2.0–4.6	2.2–4.7	1.1–5.1
12.08.15	11	+	+	-	2.5–3.5	1.1–3.3	0.3–2.0	0.0–1.2	5.1–8.6	1.2–3.2	0.5–0.9
25.08.15	7	+	+	-	3.5–5.5	1.5–3.3	–	–	1.8–6.0	–	–
26–27.07.16	22	+	+	-	2.0–5.5	0.8–4.5	0.3–2.8	0.3–2.9	0.4–5.4	0.6–4.6	0.0–3.0
3–4.08.16	21	+	+	-	1.5–4.0	0.9–6.7	1.1–6.1	0.4–3.6	1.7–6.3	1.5–5.8	0.1–4.3
04–05.07.18	3	-	+	+	3.3–12.2	1.7–3.7	0.9–1.9	0.4–0.5	0.5–20.6	0.1–9.0	0.1–1.8

^aNumber of measurement stations. ^bReflectance measurements with TriOS RAMSES radiometers.

Inherent Optical Properties

Inherent optical properties data were collected using a WETLabs spectral absorption and attenuation meter ac-s (Sea-Bird Scientific, 2020). The profiles of attenuation ($c(\lambda)$) and absorption ($a(\lambda)$) coefficient were measured in the wavelength range from 402 to 732 nm. Simultaneously CTD (conductivity, temperature, depth) (Sea-Bird) profilers were used to record the temperature, salinity and depth. The water column profiles were measured to a depth of 25 m.

Three analysis steps are necessary to obtain accurate $a(\lambda)$ and $c(\lambda)$ from ac-s measurements: (1) pure water calibration of the ac-s data, (2) temperature and salinity corrections, and (3) scattering corrections (Papadopoulou et al., 2015).

In the current study, pure water calibration of ac-s drift corrections was applied based on the most recent instrument pure water calibration spectra. All ac-s measured values correspond to the total absorption and attenuation coefficients minus water.

Measured CTD data was used to apply temperature and salinity corrections for the ac-s data using Compass post-processing software provided by WetLabs. Processing started by merging ac-s raw data with CTD data, as a function of time and by interpolating the $c(\lambda)$ and $a(\lambda)$ values to concurrent wavelengths.

The proportional scattering method (Equation 1) was applied for scattering correction. According to the ac-s protocol document (WETLabs, 2011), the application of the proportional scattering method requires the assumption of negligible absorption in a reference wavelength (λ_{ref}) and the wavelength independence of volume scattering function (VSF). The Baltic Sea waters are CDOM rich Case II waters (Kirk, 1984; Kowalczuk et al., 2006; Kratzer and Tett, 2009; Kratzer and Moore, 2018), therefore the corresponding wavelength of negligible absorption and independent of VSF was chosen 720 nm.

$$a_{proportional}(\lambda)$$
$$= a_{mts}(\lambda) - \left(a_{mts}(\lambda_{ref}) \frac{b_{mts}(\lambda)}{b_{mts}(\lambda_{ref})} \right) \tag{1}$$

where, $a_{mts}(\lambda)$ is the absorption coefficient corrected for temperature, salinity and instrument drift, and $b_{mts}(\lambda)$ is obtained from $c_{mts}(\lambda)-a_{mts}(\lambda)$, where $c_{mts}(\lambda)$ is the

attenuation coefficient corrected for temperature, salinity and instrument drift.

Finally, the scattering coefficient ($b(\lambda)$) was calculated from post-processed $a(\lambda)$ and $c(\lambda)$ measurements as follows

$$b(\lambda) = c(\lambda) - a(\lambda). \tag{2}$$

Measured Apparent Optical Properties

Spectral irradiance reflectance ($R(\lambda)$) was calculated from measurements with TriOS RAMSES hyperspectral radiometers. The measurement system contained one TriOS RAMSES irradiance sensor measuring above-water downwelling irradiance ($E_d(\lambda)$) and one TriOS RAMSES radiance sensor measuring upwelling radiance ($L_u(\lambda)$) just beneath the water surface. The measured spectral range was from 350 to 900 nm. All measured spectra were linearly interpolated to a 1 nm step. First, the water-leaving radiance ($L_w(\lambda)$) above the sea surface was derived from $L_u(0^-, \lambda)$ by propagating the latter across the water-air interface using (Austin, 1974; Mueller, 2003),

$$L_w(0^+, \lambda) = \frac{1 - \rho}{n^2} L_u(0^-, \lambda) = T_L * L_u(0^-, \lambda), \tag{3}$$

where the n is the index of refraction of water, ρ is the Fresnel reflectance at the air-sea surface, and T_L combines these factors for simplifications. The index of refraction of air is taken to be 1. T_L takes a typical value of 0.543. Then, the $R(\lambda)$ was calculated as

$$R(\lambda) = \pi \frac{L_w(0^+, \lambda)}{E_d(0^+, \lambda)}. \tag{4}$$

The mean $R(\lambda)$ was calculated to represent the measurement station. $R(\lambda)$ values are presented in percentages in this study.

Simulated Apparent Optical Properties

The $R(\lambda)$ and spectral diffuse attenuation coefficient ($K_d(\lambda)$) were simulated for water mass at three different depths using the measured IOPs: surface layer, 10 and 20 m. $R(\lambda)$ was calculated according to the method by Gordon et al. (1975) and Kirk (1984):

$$R(\lambda) = (-0.629\mu_0 + 0.975) \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \tag{5}$$

where $b_b(\lambda)$ is the backscattering coefficient, $a(\lambda)$ is the absorption coefficient, and μ_0 is the cosine of the refracted solar

beam just beneath the surface. The $\mu_0 = 0.88$ was adopted from Alikas et al. (2015), which should represent Estonian coastal waters and lakes in the period of June–August. In simulations, the value of μ_0 was taken as constant. The backscattering coefficient was calculated as $b_b(\lambda) = 0.015 * b(\lambda)$ (Herlevi, 2002). The values of $a(\lambda)$ and $b(\lambda)$ were taken from measurements at depths: 0 m (surface water) 10 and 20 m and the $R(\lambda)$ value was simulated from IOPs measured at corresponding depths.

The radiative transfer model presented by Kirk (2010) was applied to calculate $K_d(\lambda)$ as a function of IOPs and respective light conditions. The method estimates $K_d(\lambda)$ from $a(\lambda)$ and $b(\lambda)$ over the depth where downward irradiance is reduced to 1% of that penetrating the surface:

$$K_d(\lambda) = \mu_0^{-1} [a^2(\lambda) + (g_1 * \mu_0 - g_2)a(\lambda) * b(\lambda)]^{0.5} \quad (6)$$

where the cosine of the refracted solar beam just beneath the surface $\mu_0 = 0.88$ (Alikas et al., 2015) and the constants $g_1 = 0.43$ and $g_2 = 0.19$ were adopted from Kirk (2010).

As seen from Equations 5 and 6, apparent optical properties (AOPs) depend on IOPs and light conditions above the water surface. In this study, the light conditions are taken as constants. Therefore, simulations present how the IOPs of different water masses affect variability of the AOPs.

The spectra of optical depth ($z_{90}(\lambda)$) were simulated according to Equation 7 (Gordon and McCluney, 1975). This shows the surface layer depth from which 90% of radiation received by the satellite sensors originates:

$$z_{90}(\lambda) = \frac{1}{K_d(\lambda)}. \quad (7)$$

Satellite Dataset

Terra/Aqua Moderate Resolution Imaging Spectroradiometer (MODIS) sea surface temperature (SST) maps were used to describe the temporal and spatial variability of SST around the study site in the period 2015–2016. Standard Level-2 SST products were downloaded from NASA's OceanColor Web (NASA's OceanColor Web, 2020) and processed in Sentinel Application Platform (SNAP), where specific classification and quality flags were applied over the study area. The flags applied were ATMFAIL, LAND, CLDICE, NAVWARN, MAXAERITER, ATMWARN, SEAICE, NAVFAIL, FILTER, SSTWARN, and SSTFAIL (NASA's OceanColor Web, 2020).

In addition, Sentinel-3 data were used to test whether optical sensor data could be used to distinguish upwelling water masses. Data were taken from June 14, 2020 and June 21, 2020, at a time of intensive upwelling in the study area (Estonian Weather Service, 2020). The choice of dates was determined by the presence of upwelling and a cloud-free image.

The Sentinel-3 Sea and Land Surface Temperature Radiometer (SLSTR) SST Level-2 product (WST) was used to show the SST fields. The products were downloaded from the ESTHub Satellite Data Portal (ESTHub Services, 2020), which is the Estonian Land Board's national mirror site for Copernicus satellite data. Quality, ground, and cloud masks were applied in SNAP.

The Sentinel-3 Ocean and Land Colour Instrument (OLCI) full resolution (FR) Level-1 data was used for the analysis

of $R(\lambda)$ data. Level-1 images were processed with the Case-2 Regional CoastColour (C2RCC) atmospheric correction processor v1.15 in the ESTHub Processing Platform (ESTHub Services, 2020). In parametrisation of C2RCC algorithm the average temperature and salinity values of corresponding period and study area were used.

RESULTS

Distribution of Temperature and Salinity

Figure 2 illustrates the variability of the SST retrieved from MODIS imagery. These SST maps show that the temperature fields can be quite variable in the narrow gulf. The satellite imageries reveal that in the second half of August 2015, an upwelling occurred on the north-western coast of Estonia (in the southern Gulf of Finland), in which the temperature differences between the cold upwelled water originating from the deeper layers and the surrounding water reached to about 9°C. Between July 25 and August 3 on 2016, the SST map also shows a weak upwelling region along the Finnish coast which is accompanied by downwelling event along the southern coast.

Temperature and salinity profiles measured at filed campaigns are shown in Figure 3. There were no significant differences in the horizontal distribution of the temperature at the surface layer during different observation days. However, the vertical distribution of temperature and salinity varied considerably between the observation days. On July 20, 2015 and July 30–31, 2015 measurement cruises, the upper 25 m water column was well-mixed and the temperature and salinity profiles were almost homogeneous. Local weather data (Estonian Weather Service, 2020) revealed that before the measurement campaigns, western winds were dominant. As a result, a downwelling event occurred which caused the water column to mix up to a 25 m depth. The SST from MODIS data also show that the temperature was higher on July 20, 2015 (Figure 2) along the north-western coast of Estonia, indicating the downwelling event.

In general, the analysis of thermohaline structure (temperature–salinity curves) revealed three different situations in terms of vertical stratification: (1) well mixed profiles down to 25 m, (2) intermediate situation (steady decrease in temperature or increase in salinity with depth), and (3) stratified profiles with distinct thermocline (clear distinction between the upper mixed layer, thermocline and the layer under the thermocline) (Figure 3). In case of the mixed profile, the vertical temperature gradient was consistently $<0.1^\circ\text{C m}^{-1}$. In the intermediate situation, the vertical temperature gradient was steadily $\geq 0.1^\circ\text{C m}^{-1}$. In the case of stratified profiles, there was a layer with a vertical temperature gradient $\geq 0.1^\circ\text{C m}^{-1}$ under the layer where the gradients were steadily $<0.1^\circ\text{C m}^{-1}$. The water column profile types form the basis for the further analysis of the IOPs and AOPs.

Distribution of Inherent Optical Properties

The vertical variability of IOPs was analysed in case of three different (non)stratification conditions. At the surface layer,

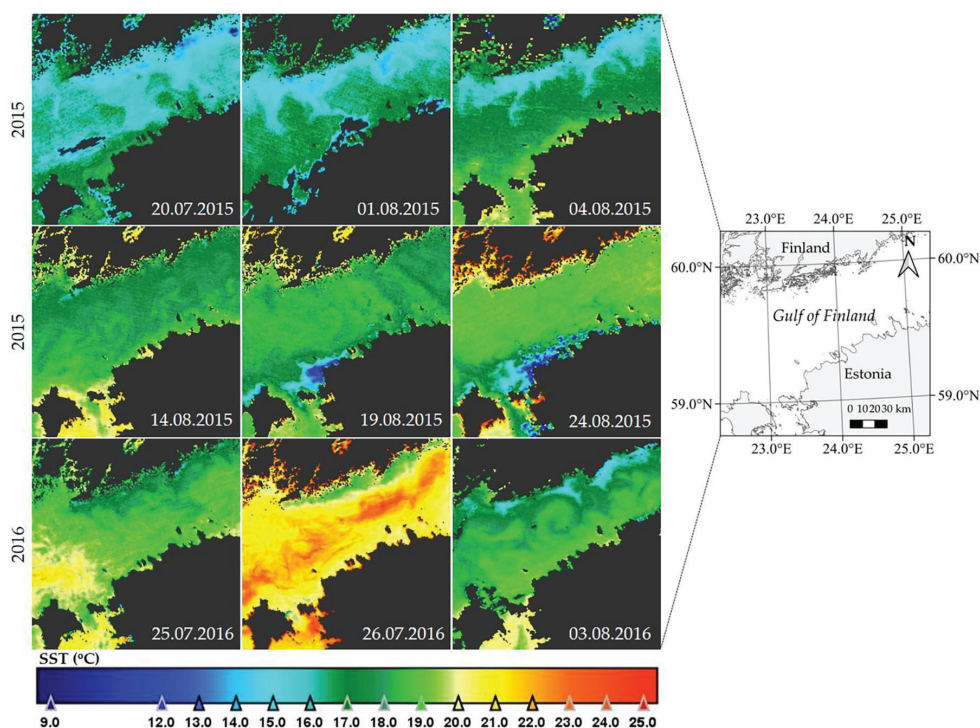


FIGURE 2 | Sea Surface Temperature (SST) maps from MODIS data for the 2015 and 2016 monitoring period. Coastal upwelling regions with lower surface temperature can be observed.

the measured attenuation coefficient at 440 nm ($c(440)$) varied between 0.94 and 7.56 m^{-1} . The scattering coefficient at 440 nm ($b(440)$) varied between 0.42 and 6.86 m^{-1} . The distribution of the absorption coefficient showed less variability, being 0.45 and 0.89 m^{-1} at 440 nm ($a(440)$).

The median values of IOPs measured at the surface layer, 10 and 20 m depth in three different hydrodynamic situations are shown in **Table 2**. The corresponding OSC (Chl-*a* and TSM) are given in **Table 3**. The vertical distribution of IOPs coincides with the changes in thermohaline structure (**Figure 3** and **Table 2**). The density boundary at the thermocline prevents mixing of the upper and lower water masses. As a result, the vertical transport of OSC between the water layers is impeded.

In the case of stratified water column (**Figure 3C**), the vertical profiles of temperature, $c(440)$ and $b(440)$ were similar, and all three parameters decreased rapidly at the thermocline. For instance, the median values of $c(440)$ and $b(440)$ decreased by 1.43 ($2.07\text{--}0.64 \text{ m}^{-1}$) units and 1.20 ($1.40\text{--}0.20 \text{ m}^{-1}$) units, respectively, over the measured water column (0–25 m). Additionally, the ratio of $b(440)$ to $a(440)$ changed under the thermocline ($b(440)/a(440) < 1$), which demonstrates that absorption became the dominant component of attenuation. The correlation (r^2) between median profiles of temperature and

the $b(440)/a(440)$ was 0.99. Although there were no significant changes in the vertical distribution of $a(440)$, there was a slight shift of about 0.29 units for $a(440)$. Below the thermocline, there were no significant changes in the IOPs down to a 25 m depth.

In the case of the intermediate situation (**Figure 3B**) where stratification was not so obvious, but the temperature was decreasing with depth, a similar pattern occurred as in case of the strongly stratified situation. The $b(440)$ decreased smoothly with depth so that $a(440)$ became dominant at a certain depth, the r^2 between median profiles of temperature and the $b(440)/a(440)$ was 0.86. The medians of $c(440)$ and $b(440)$ decreased from the surface layer to 25 m depth by 1.20 ($2\text{--}0.80 \text{ m}^{-1}$) units and 1.13 ($1.34\text{--}0.21 \text{ m}^{-1}$) units, respectively. A decrease of concentrations of OSC was also observed (**Table 3**). The measured profiles confirm that the change in distribution of IOPs profiles reveals the change in relative concentrations of the OSC (note changes in Chl-*a* and TSM concentrations).

In the mixed water column (**Figure 3A**), there is no density boundary and the vertical variability of IOPs was very small (<0.30 units in case of $c(440)$ and $b(440)$ and 0.04 units for $a(440)$). Therefore, the ratio of $b(440)/a(440)$ remained almost the same through the entire water column. The r^2 between median profiles of temperature and the $b(440)/a(440)$ was 0.89.

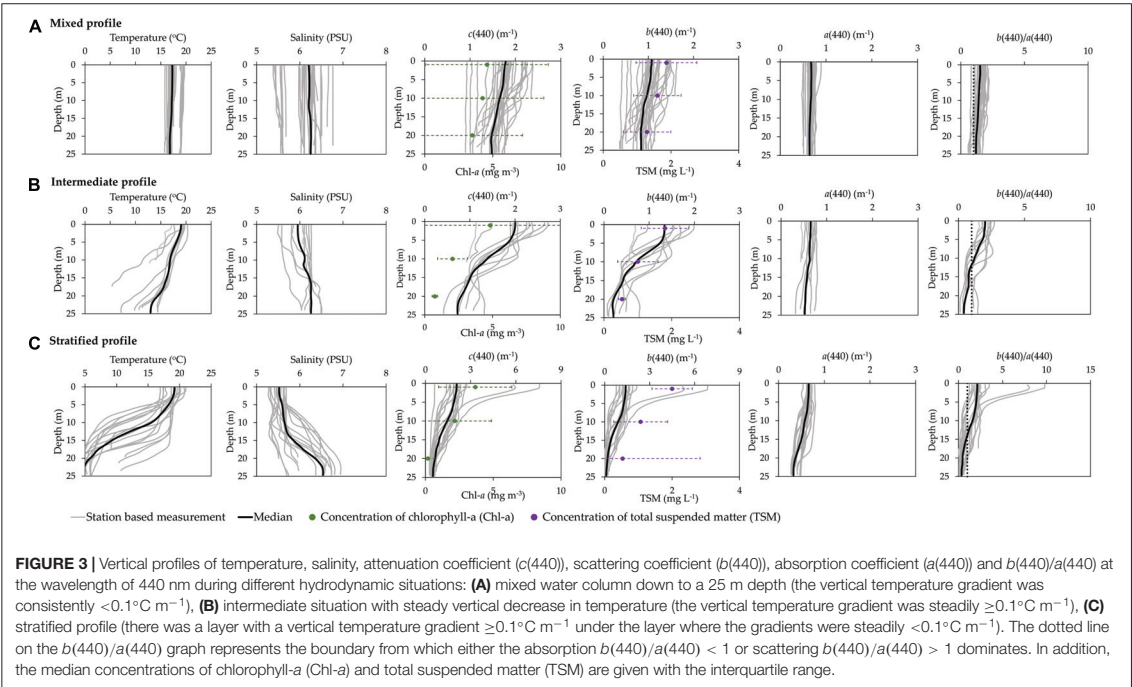


FIGURE 3 | Vertical profiles of temperature, salinity, attenuation coefficient ($c(440)$), scattering coefficient ($b(440)$), absorption coefficient ($a(440)$) and $b(440)/a(440)$ at the wavelength of 440 nm during different hydrodynamic situations: **(A)** mixed water column down to a 25 m depth (the vertical temperature gradient was consistently $<0.1^{\circ}C\ m^{-1}$), **(B)** intermediate situation with steady vertical decrease in temperature (the vertical temperature gradient was steadily $\geq 0.1^{\circ}C\ m^{-1}$), **(C)** stratified profile (there was a layer with a vertical temperature gradient $\geq 0.1^{\circ}C\ m^{-1}$ under the layer where the gradients were steadily $<0.1^{\circ}C\ m^{-1}$). The dotted line on the $b(440)/a(440)$ graph represents the boundary from which either the absorption $b(440)/a(440) < 1$ or scattering $b(440)/a(440) > 1$ dominates. In addition, the median concentrations of chlorophyll-a (Chl-a) and total suspended matter (TSM) are given with the interquartile range.

Profile	0- m			10 m			20 m		
	$c(440)$ (m^{-1})	$a(440)$ (m^{-1})	$b(440)$ (m^{-1})	$c(440)$ (m^{-1})	$a(440)$ (m^{-1})	$b(440)$ (m^{-1})	$c(440)$ (m^{-1})	$a(440)$ (m^{-1})	$b(440)$ (m^{-1})
Mixed	1.77 (0.31)	0.68 (0.14)	1.07 (0.27)	1.66 (0.27)	0.67 (0.11)	0.97 (0.28)	1.48 (0.45)	0.64 (0.08)	0.84 (0.43)
Intermediate	2.00 (0.72)	0.65 (0.20)	1.34 (0.49)	1.38 (0.76)	0.63 (0.13)	0.71 (0.76)	0.80 (0.49)	0.53 (0.21)	0.21 (0.46)
Stratified	2.07 (0.56)	0.66 (0.06)	1.40 (0.53)	1.44 (0.91)	0.57 (0.14)	0.89 (0.79)	0.64 (0.24)	0.37 (0.15)	0.20 (0.20)

Values are medians, with the interquartile range given in parentheses.

TABLE 3 | *In situ* measured optically significant constituents (OSC), such as the concentration of total suspended matter (TSM) and chlorophyll-a (Chl-a) for different hydrodynamic situations at different depths.

Profile	0- m		10 m		20 m	
	TSM ($mg\ L^{-1}$)	Chl-a ($mg\ m^{-3}$)	TSM ($mg\ L^{-1}$)	Chl-a ($mg\ m^{-3}$)	TSM ($mg\ L^{-1}$)	Chl-a ($mg\ m^{-3}$)
Mixed	1.9 (0.9)	4.6 (4.5)	1.6 (0.7)	4.3 (4.5)	1.3 (0.7)	3.5 (3.7)
Intermediate	1.8 (0.7)	4.8 (5.8)	1.0 (0.6)	2.0 (1.1)	0.5 (0.1)	0.7 (0.2)
Stratified	2.0 (0.6)	3.7 (2.7)	1.1 (0.8)	2.2 (2.7)	0.5 (2.3)	0.2 (0.5)

Values are medians, with the interquartile range given in parentheses.

In addition, the vertical variability of OSC was small (Table 3 and Figure 3).

Vertical profiles of measured IOPs (Figure 3) in study area show that: (1) in the upper mixed layer scattering contributed most to attenuation, i.e., scattering

dominated over the absorption; (2) the vertical distribution of the scattering coefficient coincides with the vertical distribution of the attenuation coefficient; (3) and below the density layer, absorption becomes the dominant factor in the attenuation, i.e., the ratio of $b(440)/a(440)$

becomes lower than one in the south-western coast of Gulf of Finland.

Distribution of Simulated Apparent Optical Properties

The following analysis is based on the division of water masses by stratification of the water column. $R(\lambda)$ and $K_d(\lambda)$ were simulated from IOPs measured at different depths. By simulating the AOPs from IOPs for different water masses enabled to evaluate the changes in optical parameters that might occur when a water mass rises from deeper layers to the surface layer as a result of an upwelling event.

Variability of simulated $R(\lambda)$ in the PAR region (400–700 nm) is shown in **Figure 4A**. $R(\lambda)$ at 400 nm ranged from 0.31 to 3.94 units, at 550 nm from 0.92 to 12.98 units and at 700 nm from 0.31 to 5.52 units for the surface layer. $R(\lambda)$ simulated from IOPs measured at 20 m depth were 0.01–1.01, 0.28–3.99, and 0.09–1.79 units depending on water mass stratification. The spectral shape of simulated $R(\lambda)$ showed highest reflection in the green part of the spectrum, in particular, at 550–580 nm and lower reflection in blue and red part of the spectrum which is typical spectral shape for Case II water type. A minimum of 670 nm was also observed, which corresponds to the absorption of Chl-*a*. The spectra that represent water mass at a 20 m depth are considerably smoother at the longer wavelengths due to the lower particles concentrations at this depth.

The $K_d(\lambda)$ calculated from the $a(\lambda)$ and $b(\lambda)$ measurements at three depths are shown in **Figure 4B**. The spectral dependence of $K_d(\lambda)$ curves at different depths is quite similar. However, the numerical value of $K_d(\lambda)$ varied greatly and the variation was largest at shorter wavelengths (400–550 nm). It is known that, in this spectral region, Chl-*a* and CDOM have the main influence on the optical parameters. For instance, the greatest decrease in $K_d(\text{PAR})$ in one station was 40.8%, which resulted in

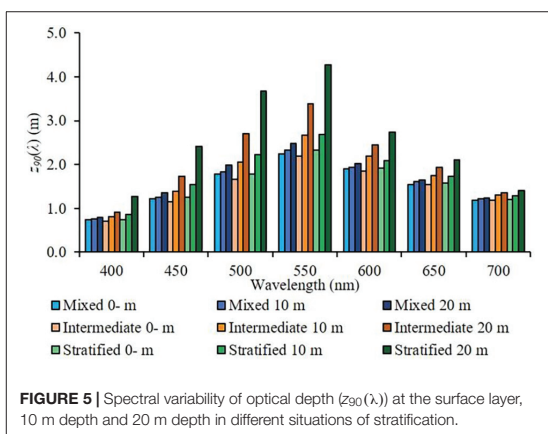


FIGURE 5 | Spectral variability of optical depth ($z_{90}(\lambda)$) at the surface layer, 10 m depth and 20 m depth in different situations of stratification.

corresponding changes in Chl-*a* (80.1%) and TSM (61.4%). The smallest vertical decrease of $K_d(\text{PAR})$ (6.8%) occurred when Chl-*a* and TSM decreased from the surface layer to 20 m by 31.7 and 42.1%, respectively.

Evaluation of the differences in $z_{90}(\lambda)$ revealed that the thickness of the water layer, which would be detected by optical remote sensing instruments depends on the wavelength and water mass (**Figure 5**). It was found that the informative layer is largest in the wavelength range of 550–600 nm, where the median value of $z_{90}(\lambda)$ was 2.1 m. The lowest $z_{90}(\lambda)$ values were in the 400, 450, and 700 nm spectral region, where the median $z_{90}(\lambda)$ values were 0.7, 1.2 and 1.2 m, respectively. However, simulations indicate that in the case of intensive coastal upwelling when water mass from deeper layers reaches the surface the $z_{90}(\lambda)$ might exceed 4 m (550 nm), and values in the 400, 450, and 700 nm spectral region might be up to 1.3, 2.4, and 1.4 m, respectively.

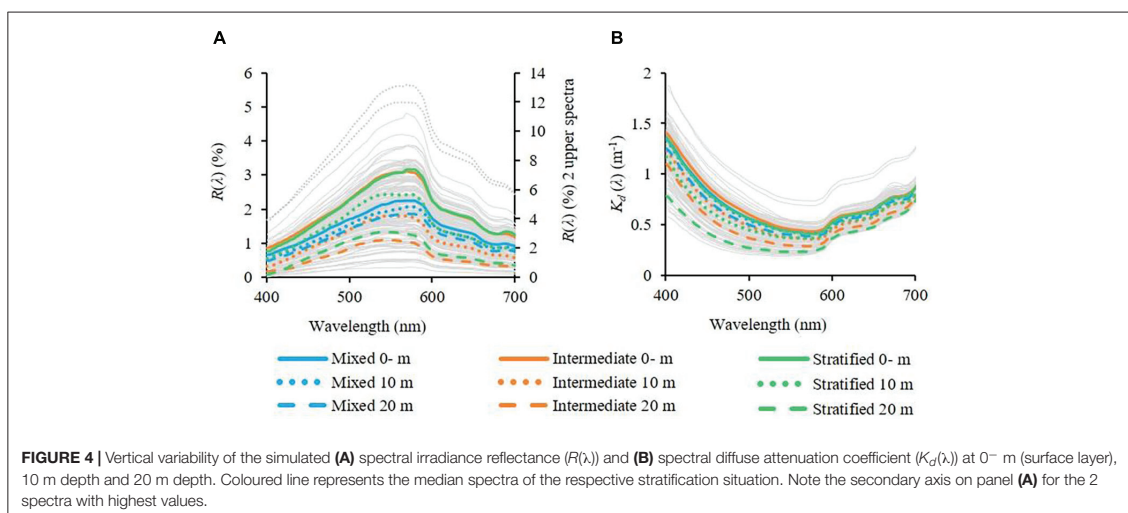


FIGURE 4 | Vertical variability of the simulated (A) spectral irradiance reflectance ($R(\lambda)$) and (B) spectral diffuse attenuation coefficient ($K_d(\lambda)$) at 0-m (surface layer), 10 m depth and 20 m depth. Coloured line represents the median spectra of the respective stratification situation. Note the secondary axis on panel (A) for the 2 spectra with highest values.

Detection of Upwelling Zone From Apparent Optical Properties

In section 3.3 we demonstrated the changes in $R(\lambda)$ and $K_d(\lambda)$ values that might occur when a water mass rises from deeper layers to the surface layer as a result of an upwelling event. Simulation indicated that $K_d(\text{PAR})$ decreases up to 37.5% and $R(\text{PAR})$ 61.5% in the subsurface layer (Table 4). The simulated results of $R(\lambda)$ for different water masses were compared with measurements of $R(\lambda)$ (with TriOS RAMSES radiometers) from an independent dataset collected during the upwelling event on July 4–5, 2018 (Figure 6). The strong upwelling event occurred in the region of the study area (south-western part of the Gulf of Finland). The SST dropped to 4.8°C, whereas the Secchi depth was extremely high for summer time (in the context of the Baltic Sea), with a value of 12.2 m (Figure 6). The Chl-*a* values measured in the upwelling zone were around 0.5 mg m⁻³, which, given that the measurements were taken at the beginning of July, are rather low. On the contrary, outside the upwelling zone (two stations that were only 25–30 km from the upwelling station), the water temperature was about 15°C, the Secchi depth was 3.3–3.7 m, the concentration of Chl-*a* was 17.5–20.6 mg m⁻³ and TSM concentration was 3.5–3.7 mg L⁻¹. Two different types of water mass were distinguishable from the *in situ* $R(\lambda)$ spectra measured with Ramses instrument (Figure 6): (1) typical coastal water, which is strongly reflected in the green part of the spectrum (550–580 nm), and (2) upwelled water with considerably smoother $R(\lambda)$ spectra.

Due to the difference in $R(\lambda)$ spectra between the two water mass, a simple band ratio condition was tested to detect the upwelled water mass. The $R(490)/R(560)$ value was calculated from the upwelling *in situ* $R(\lambda)$ spectra (shown in Figure 6). Condition for the separation of upwelling zones ($R(490)/R(560) \geq 0.77$) was set ≥ 0.77 relying on *in situ* Ramses data collected on July 4–5, 2018. The characteristic spectra for upwelling and non-upwelling situations are shown in Figure 6.

We also tested the ratio condition to satellite data. Two cloud-free Sentinel-3 OLCI images acquired during intense upwelling events (July 14 and July 21, 2020) in the Gulf of Finland were chosen for testing. Figure 7 shows the combined result of the

SST and band ratio condition, where the latter is marked with a black hatched area on the SST map. The SST maps (Figure 7) show large upwelling areas along the southern coast of the Gulf of Finland, where the temperatures remained below 10°C. The figure shows how the horizontal distribution of the upwelling zone based on SST coincides quite well with the area indicated on the basis of the $R(\lambda)$ spectra from OLCI. Thus, the band ratio approach may be useful in order to assess whether upwelling is occurring if the SST data is not available.

DISCUSSION

The general aim of current study was to give an overview of the variation of optical parameters and the relationship of these parameters with thermohaline structure based on measurements made on the south-western coast of the Gulf of Finland. In the analysis of the IOPs distribution, the main focus was on a wavelength of 440 nm, because values close to this wavelength are used in Case-2 Regional processors to derive IOPs from remote sensing data, which are then used as a proxy for concentrations of OSC (Brockmann et al., 2016). The measurements of IOPs showed that in the upper mixed layer, the light attenuation process is mainly dominated by scattering. Sipelgas et al. (2004) also showed that the light scattering dominated over the absorption in the south-western coastal sea of the Gulf of Finland. However, they also demonstrated that in the Moonsund, which is near to our study area, where the optical properties of water are mainly influenced by the river inflow, the light absorption was found to be dominant. This discrepancy between the two studies indicates that the distribution of IOPs can change quite rapidly within a small spatial area.

The variation of OSC was moderate compared to other studies carried out in different region over the Baltic Sea. Chl-*a* varied between 0.36 and 15.06 mg m⁻³ and TSM between 0.80 and 4.40 mg L⁻¹. Therefore, also, the IOPs in the surface layer did not vary much. Different studies (Woźniak et al., 2011; Sipelgas and Raudsepp, 2015; Soja-Woźniak et al., 2017; Kratzer and Moore, 2018) have showed that intensive blooms (surface scums), resuspension, and anthropogenic impact (e.g., dredging),

TABLE 4 | Differences (%) between the concentration of optically significant constituents (OSC) such as the concentration of total suspended matter (TSM) and chlorophyll-*a* (Chl-*a*), and the spectral diffuse attenuation coefficient ($K_d(\lambda)$) and the spectral irradiance reflectance ($R(\lambda)$) at different wavelengths by respective depths and hydrodynamic situations.

Parameter	0– m and 10 m Difference (%)			0– m and 20 m Difference (%)		
	Mixed	Intermediate	Stratified	Mixed	Intermediate	Stratified
TSM	21.6	37.9	40.0	29.4	73.3	73.3
Chl- <i>a</i>	8.0	57.5	48.6	33.3	88.9	96.1
$K_d(\text{PAR})$	2.7	14.1	13.2	8.5	28.1	37.5
$K_d(490)$	3.4	19.2	20.4	10.9	38.8	51.6
$K_d(673)$	2.8	8.9	7.4	5.4	18.9	23.5
$R(\text{PAR})$	9.4	44.5	25.0	17.6	68.8	61.5
$R(565)$	9.6	42.4	21.8	17.1	65.9	58.1
$R(673)$	12.1	48.6	31.2	20.7	72.8	67.3

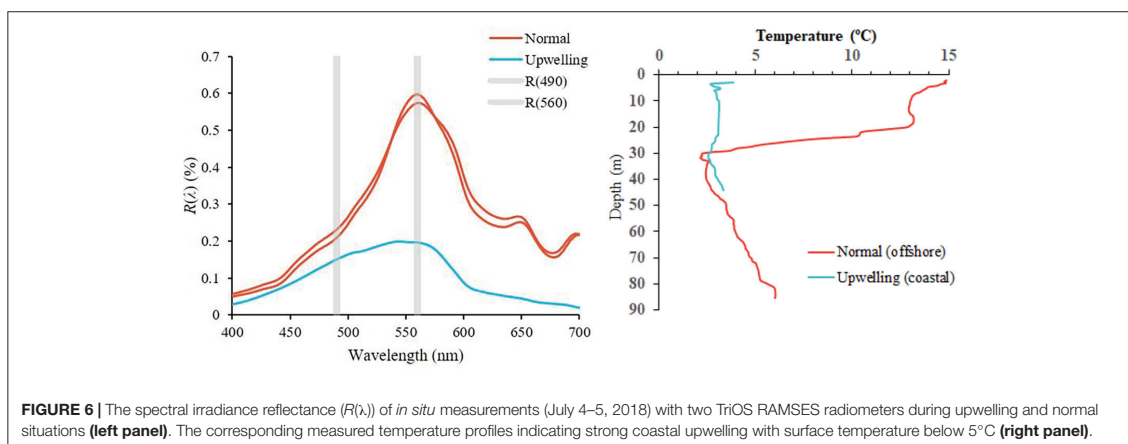


FIGURE 6 | The spectral irradiance reflectance ($R(\lambda)$) of *in situ* measurements (July 4–5, 2018) with two TriOS RAMSES radiometers during upwelling and normal situations (**left panel**). The corresponding measured temperature profiles indicating strong coastal upwelling with surface temperature below 5°C (**right panel**).

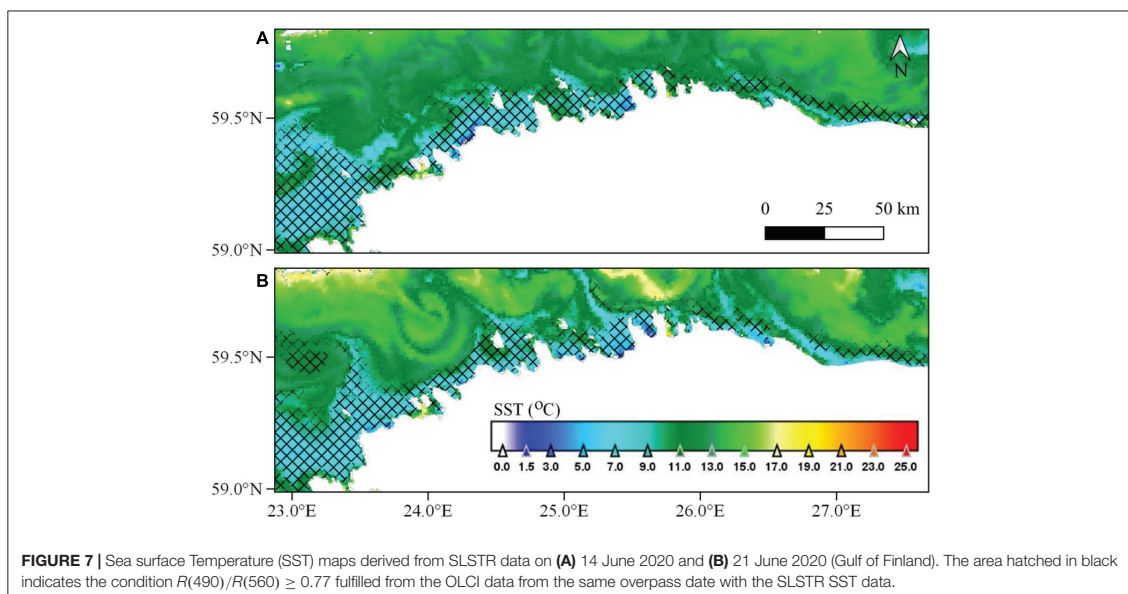


FIGURE 7 | Sea surface Temperature (SST) maps derived from SLSTR data on (A) 14 June 2020 and (B) 21 June 2020 (Gulf of Finland). The area hatched in black indicates the condition $R(490)/R(560) \geq 0.77$ fulfilled from the OLCI data from the same overpass date with the SLSTR SST data.

would significantly change the distribution of OSC and IOPs in much larger scale.

However, depending on the vertical distribution of OSC in different thermohaline conditions, a significant variation in the ratio of $b(440)$ to $a(440)$ was observed. In the mixed water column, the ratio was more stable than in the situation when stratification occurred. With an increase of depth, the $a(440)$ in the stratified water column became dominant in $c(440)$. Berthon and Zibordi (2010) obtained similar vertical distributions of IOPs in the Baltic Proper, where the surface (upper mixed) layer was dominated by scattering, whereas the intensity of scattering decreased with an increasing depth and in the deeper layers absorption became more dominant. Berthon and Zibordi (2010) also showed that the optical properties of the Baltic Sea vary considerably, depending on the regional characteristics. On

contrary to the Baltic Proper (closest to our study area), it was found that in the northern part of the Baltic Sea (Bothnian Bay), absorption was dominant within the upper 25 m water column. The reason for this was high absorption by CDOM resulting from the presence of humic matter brought by the numerous rivers. They found that in the Bothnian Bay, the contribution of CDOM to absorption was up to 35% higher than in the Baltic Proper. Unfortunately, CDOM concentrations were not measured in the present study, which makes it difficult to assess directly the contribution of CDOM to beam attenuation. However, previous studies (Sipelgas et al., 2004; Ylöstalo et al., 2016; HELCOM, 2018; Kratzer and Moore, 2018) have shown that Baltic Proper and western Gulf of Finland (our study area) have also high absorption of CDOM at 440 nm (up to 4.1 m^{-1}), but not as high as in the Bothnian Bay (up to 8.8 m^{-1}).

One of the reasons why the vertical distributions of optical parameters were compared was to evaluate the influence of upwelling event on the optical properties of surface water. During the development stage of an upwelling, more productive and turbid surface waters are pushed away from the shore. The water mass that rises from deeper layers of the stratified water column differs from the original water mass in terms of temperature, nutrients and OSC, which, as a result, changes the optical properties of the surface layer. For instance, Uiboupin et al. (2012) showed that in the case of an upwelling event, the area influenced by upwelled water might cover up to 40% of the total area of the Gulf of Finland in the Baltic Sea. Moreover, filaments of upwelled water may spread much farther, reaching several tens of kilometres out into the sea and in some case, cross the entire Gulf of Finland (Zhurbas et al., 2008). Several studies have demonstrated that in the case of an intensive upwelling front, the low Chl-*a* regions coincide with the cold upwelled water area and concentrations may drop down by an order of magnitude (Uiboupin et al., 2012; Dabuleviciene et al., 2018, 2020). The latter proves that the upwelling is an important process that, in addition to temperature changes, alters the optical signal of surface water measured by a remote sensor. Therefore, it is important to quantify the influence of upwelling water on remote sensing signal.

We quantified the change in magnitude and spectral shape of remote sensing signal in upwelling conditions by simulating the AOPs ($K_d(\lambda)$ and $R(\lambda)$). Delpeche-Ellmann et al. (2018) showed that the cooler water most likely originates from intermediate water masses at depths between 15 and 30 m. In our study, AOPs ($K_d(\lambda)$ and $R(\lambda)$) were calculated from the measured $a(\lambda)$ and $b(\lambda)$ and simulated to represent water masses at three different depths: surface layer, 10 and 20 m. It is considered that AOPs simulated from IOPs measured below the density barrier represent water masses in an upwelling condition. For instance, Lips et al. (2009) showed that during an intensive upwelling event in the central Gulf of Finland, the cold intermediate layer water was mixed with the water from the upper mixed layer, with a share of 85 and 15%, respectively. Calculations of AOPs showed that water below thermocline has substantially lower values of $R(\text{PAR})$, the decrease could be between 61.5 and 68.8%. The variation in the shapes of $R(\lambda)$ spectra was also observed under different stratification conditions. The spectra of the deeper water layers under the thermocline had significantly less spectral dependency, $R(\lambda)$ spectra were no longer representing typical coastal water, which is strongly reflected in the green part of the spectrum. Our results represent the theoretical simulations of AOPs in upwelling conditions, however in natural environment during the upwelling, waters from different layers are both advected and mixed.

Another important aspect is the significant differences in the spectral values of $z_{90}(\lambda)$ under upwelling condition. Our analyses indicate that the thickness of the water layer measured by the remote sensor may increase compared to the typical coastal water condition from 2.3 to 4.3 m in the green region of the spectrum. Simis et al. (2017) demonstrated that 90% of water-leaving radiance at 560 nm exceeded 5 m if the biomass (Chl-*a*) was less than 5 mg m⁻³. Otherwise, the mean values of

$z_{90}(\lambda)$ were 1.0, 3.0–3.5, and 1.5 m, in the blue, green and red spectral region, respectively. The latter are also comparable to the results obtained in the present study. Furthermore, both studies show that the most informative spectral region for the Baltic Sea waters is located near 550–560 nm. The above analysis about variability of the $z_{90}(\lambda)$ for different water masses highlights the need for an additional optical classification of waters prone to the upwelling phenomenon.

The obtained simulation results of $R(\lambda)$ for different water masses were confirmed by measurements of $R(\lambda)$ from an independent dataset of TriOS RAMSES radiometers collected during the upwelling event. Two different types of water masses were distinguishable (Figure 6): (1) typical coastal water which is strongly reflected at 550–580 nm and (2) upwelled water with considerably smoother $R(\lambda)$ spectra. Such a difference in the shape of $R(\lambda)$ spectra may have an effect on the use of algorithms to derive OSC concentrations found as a result of the classification of optical water types, where reflectance spectrum features are associated with a specific bio-optical condition. Such classification approaches are widely used in the remote sensing of water bodies (Vantrepotte et al., 2012; Shen et al., 2015; Jackson et al., 2017; Spyarakos et al., 2018; Uudeberg et al., 2019, 2020). Based on the difference in the $R(\lambda)$ spectrum shapes in the current study, it is suggested that the ratios between $R(490)$ and $R(560)$ values can be used as an indicator for the detection of upwelled water (in this work $R(490)/R(560) \geq 0.77$). The applicability of the proposed band ratio approach was tested for discerning upwelling events in satellite imagery. Comparison of satellite SST and reflectance band ratio derived from OLCI image showed good agreement, low SST values (below 10°C) coincided with the upwelling area indicated by the band ratio algorithm (Figure 7). Implementation of ratio condition to optical remote sensing imagery allows separating the upwelling region also from missions Sentinel-2 or Landsat which are not primarily designed for SST estimation.

The SST based approach has been widely used for monitoring upwelling events. However, the band ratio method proposed in this work offers an alternative way to estimate the pixels belonging to the upwelled water region from optical satellite images. In addition, the acquisition of optical and temperature sensors is not always simultaneous, which prevents the use of this data in synergy. For instance, Sentinel-2 satellites do not include thermal infrared sensors like Sentinel-3 and Terra/Aqua. Besides, the spatial resolution of optical sensors is often significantly higher than of the thermal infrared sensors, thus providing more detailed added value.

Previous studies have shown how biological (phytoplankton, primary production), chemical (phosphate, nitrate), and physical (temperature, salinity) patterns change at different stages of upwelling (Vahtera et al., 2005; Lips et al., 2009; Uiboupin et al., 2012), but there is no detailed information on how the optical properties of water change during upwelling in the Gulf of Finland. As there was no time series of such data in the present work, it is planned for the future to perform additional measurements and analyse how the optical properties of water change over time (before, during and after upwelling) in the Gulf of Finland region. The current study revealed the consequences of

upwelling in optical properties in the Gulf of Finland. However, the conclusions cannot be automatically expanded to the other basins of the Baltic Sea as the vertical distribution of IOPs differ between basins of the Baltic Sea (Berthon and Zibordi, 2010; Soja-Woźniak et al., 2017; Kratzer and Moore, 2018). However, upwelling is a frequent process also in other basins of the Baltic Sea (Lehmann et al., 2012; Dabuleviciene et al., 2018, 2020; Bednorz et al., 2021), therefore future research is needed to quantify the effect of upwelling on the remote sensing signal/retrievals in the other basins of the Baltic Sea.

CONCLUSION

On the basis of IOPs, OSC (Chl-*a* and TSM) and vertical profiles of temperature and salinity, the optical parameters of the south-western part of the Gulf of Finland (Baltic Sea) have been investigated. The analysis of the thermohaline structure revealed three different situations in terms of vertical stratification: (1) mixed water column down to 25 m depth, (2) intermediate situation (steady decrease in temperature or increase in salinity with depth), and (3) stratified profiles with a distinct thermocline. The comparison of the vertical profiles of temperature and IOPs showed similar patterns in vertical variability. In the situation of a mixed water column, the optical parameters did not change significantly through the entire water column. In the stratified water column, the concentrations of OSC changed considerably and the vertical variability of attenuation and scattering was significantly higher compared to the mixed layer [i.e., the difference of $c(440)$ between surface and 20 m depth was 69.1 and 16.4%, respectively]. The analysis of IOPs in the case of stratified water column showed that the ratio of scattering $b(440)$ to absorption $a(440)$ changed under the thermocline ($b(440)/a(440) < 1$) i.e., absorption became the dominant component of attenuation under thermocline while the opposite is true for upper layer. The results showed that the stratification of the water column is related to the variability of the optical parameters through the distribution of OSC.

The values of $R(\lambda)$ and $K_d(\lambda)$ were calculated from IOPs measured at three different depths: surface layer, 10 and 20 m. The performed simulation allow to assume how surface $R(\lambda)$ values would change if upwelling events occur. The results showed that in the upwelling region, the signal measured by the remote sensor may decrease up to 68.8% as a result of deep water uptake. Additionally, the $R(\lambda)$ spectra would be considerably smoother, as the strong reflection in the green part of the spectrum (550–580 nm) is diminished. Moreover, the $z_{90}(\lambda)$ —the thickness of the water layer measured by the remote

sensor—of upwelled water may increase from 2 to 4 m in the green part of the reflectance spectra compared to the typical coastal water of the Baltic Sea. The study also showed that the small vertical decrease of $K_d(\text{PAR})$ by 6.8% (from surface to 20m depth) corresponds to much larger Chl-*a* and TSM decreased by 31.7 and 42.1%, respectively. It is suggested that the AOPs and IOPs can be used as an indicator for the detection of upwelled water mass from remote sensing data: 1) $R(490)/R(560) \geq 0.77$; 2) $b(440)/a(440) < 1$. The application of ratio condition $R(490)/R(560) \geq 0.77$ to the optical imagery allows determining the upwelled water mass in more detail (spatially) than with the SST approach and is in synergy with derived ocean colour retrievals. Allowing estimation of upwelling zone independently for SST data. All these aspects show that upwelling is an important process that, in addition to temperature changes, alters the optical signal of surface water measured by a remote sensor. Knowledge of IOPs and AOPs relation to upwelling can help the parametrisation of remote sensing algorithms for retrieving water quality estimates in the coastal regions.

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

AA, RU, and LS: conceptualisation, methodology, software, formal analysis, data curation, visualisation, and writing—original draft preparation. AA, LS, RU, and KU: investigation and writing—review and editing.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Appendix 2

Publication II

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Article

Mapping Water Quality Parameters with Sentinel-3 Ocean and Land Colour Instrument Imagery in the Baltic Sea

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Abstract: The launch of Ocean and Land Colour Instrument (OLCI) on board Sentinel-3A in 2016 is the beginning of a new era in long time, continuous, high frequency water quality monitoring of coastal waters. Therefore, there is a strong need to validate the OLCI products to be sure that the technical capabilities provided will be used in the best possible way in water quality monitoring and research. The Baltic Sea is an optically complex waterbody where many ocean colour products, performing well in other waterbodies, fail. We tested the performance of standard Case-2 Regional/Coast Colour (C2RCC) processing chain in retrieving water reflectance, inherent optical properties (IOPs), and water quality parameters such as chlorophyll *a*, total suspended matter (TSM) and coloured dissolved organic matter (CDOM) in the Baltic Sea. The reflectance spectra produced by the C2RCC are realistic in both shape and magnitude. However, the IOPs, and consequently the water quality parameters estimated by the C2RCC, did not have correlation with in situ data. On the other hand, some tested empirical remote sensing algorithms performed well in retrieving chlorophyll *a*, TSM, CDOM and Secchi depth from the reflectance produced by the C2RCC. This suggests that the atmospheric correction part of the processor performs relatively well while IOP retrieval part of the neural network needs extensive training with actual IOP data before it can produce reasonable estimates for the Baltic Sea.

Keywords: OLCI; Sentinel-3; Baltic Sea; C2RCC

1. Introduction

The launch of Ocean and Land Colour Instrument (OLCI) on board ESA Sentinel-3A satellite in February 2016 and the planned near future launch of identical sensor on Sentinel-3B opened a new era in coastal water remote sensing. Previous ocean colour sensors (Sea-Viewing Wide Field-of-View Sensor (SeaWiFS); Moderate Resolution Imaging Spectroradiometer (MODIS); and Medium Resolution Imaging Spectrometer (MERIS)) were one-off scientific missions not designed for water quality monitoring. Sentinel satellites, launched in the Copernicus program, are designed to provide continuous long-term data flow to allow monitoring of environmental parameters with high accuracy enabling not only operational monitoring but also studies on environmental change. OLCI is a follow up of MERIS mission (2002–2012) with improved capabilities. Its spectral configuration is specifically

designed for optically complex coastal and inland waters, i.e., it has spectral bands in red and near-infrared (NIR) part of spectrum where most of the useful spectral information, needed to retrieve different water quality parameters, is situated [1–8].

The Baltic Sea is an extraordinarily complex study object for ocean colour remote sensing. High amount of coloured dissolved organic matter (CDOM) received from boreal forest in the catchment area makes the water dark. This means that the water leaving signal is very low requiring highly sensitive remote sensing devices and very accurate atmospheric correction (typically more than 95% of the signal measured by satellites originates from atmosphere not water). In addition, sun elevation is low during most of the year. Low salinity (down to 0 Practical Salinity Unit (psu) in some parts) and high latitudes are the cause why large portion of the Baltic Sea is covered by ice in winter. There are two distinct phytoplankton seasons in the Baltic Sea [9]. Diatoms dominate the spring bloom that occurs after ice melt and cyanobacteria dominate during summer and early autumn. Optical properties of these two assemblages are so different that seasonal remote sensing algorithms may be needed [10,11]. There are also indications that the seasonality is changing [12,13].

The optical complexity of the Baltic Sea is probably one of the reasons why Copernicus Marine Environment Monitoring Services (CMEMS) have not managed to develop ocean colour products that perform reasonably well. For example, the correlation between CMEMS chlorophyll *a* product and in situ data is $r^2 = 0.20$ [14] while for some wavelengths of the reflectance products r^2 is around 0.5. The neural network used to retrieve chlorophyll *a* and reflectance products first estimates inherent optical water properties (IOPs) such as the total absorption coefficient, the absorption coefficients of pigments, detritus and CDOM, and the particulate backscattering, which are then used to calculate derived products (such as the chlorophyll *a*, total suspended matter, Secchi depth, etc.). These products are provided at the global scale and for some regional seas, but not for the Baltic Sea. Therefore, it is not possible to validate the CMEMS IOP products and there is need to find other methods to retrieve water quality parameters in the Baltic Sea.

Estimation of the phytoplankton biomass (usually expressed as chlorophyll *a* concentration) is especially complicated in the Baltic Sea during cyanobacterial season when blooms may cover area of more than 200,000 km² [15]. Cyanobacteria, unlike most phytoplankton, can regulate their buoyancy and in calm conditions (wind below 2 m s^{−1}) choose the depth optimal for their growth. Vertical distribution of the biomass has significant impact on the measured reflectance [16] and consequently our ability to estimate cyanobacterial biomass. Moreover, cyanobacteria that have lost their buoyancy control form surface scum that may be several centimetres thick. It is not possible to estimate the biomass within the scum as the thickness cannot be estimated and the amount of still alive cells (chlorophyll *a*) may be significantly lower on the surface of the scum (due to photodegradation) than inside of it. Obviously, it is not possible to estimate phytoplankton biomass below the opaque scum. It has been shown that the cyanobacterial blooms are extremely heterogeneous and chlorophyll *a* may vary by three orders of magnitude within one OLCI pixel [4]. This causes problems in algorithm development and validation. First of all, the in situ sample collected with typical point measurement does not represent the same situation satellites are detecting. In addition, the reflectance measured by satellite does not represent the actual situation. For example, pixel that is partially covered with surface scum (high NIR reflectance, similar to terrestrial plants) and partially with relatively clear water below (negligible reflectance in NIR) is often detected as subsurface bloom (peak between 700–710 nm) [4].

Despite the above-mentioned complexity, studies demonstrate reasonable performance of remote sensing, at least at regional scales and/or in open parts of the Baltic Sea. Different remote sensing products (chlorophyll *a*, CDOM, suspended matter, diffuse attenuation coefficient, etc.) have been developed or adopted for the Baltic Sea [3,4,6,8,11,17–28]. Many of the recent studies rely on MERIS data and the results can probably be implemented on Sentinel-3 OLCI data as well. The aim of this study was to test the performance of Sentinel-3A OLCI in coastal waters of the Baltic Sea by evaluating the results of atmospheric correction, ocean colour products produced by the standard processor

(C2RCC) and selected empirical algorithms that have shown promising results in the Baltic Sea when applied on other sensors or modelled data.

2. Materials and Methods

2.1. Study Sites and in Situ Data

In order to compile as many data sources as possible in testing the performance of Sentinel-3 OLCI, we used in situ data from three different sources:

- Field campaigns dedicated for Sentinel-2 and Sentinel-3 validation where bio-optical measurements were carried out from a boat with comprehensive set of optical instrumentation followed by water sample analysis in laboratory (circles on Figure 1).
- Bio-physical sampling campaigns on R/V Salme included both fixed station sampling with limited number of optical measurements (reflectance, IOPs), accompanied with water sampling, and ferrybox measurements between the stations (triangles and lines on Figure 1).
- Reflectance measurements collected for satellite data calibration and validation with Rfex systems [29] on ships of opportunity under the frame of the BONUS FerryScope project (www.ferryscope.org), along with in situ data collected with ferrybox systems (markers in the Southern part of the Baltic Sea).

Three dedicated field campaigns (16 measurements, on 24 May, 14 September, and 12 October 2016) were carried out from a boat. Water samples for the analysis of chlorophyll *a* (in mg m^{-3}), total suspended matter (TSM, in mg L^{-1}), inorganic fraction of suspended matter (SPIM, in mg L^{-1}), the organic fraction of suspended matter (SPOM, in mg L^{-1}) and a_{CDOM} (in m^{-1}) were collected from surface layer (top 0.5 m). Besides the water sampling, in situ data collection included reflectance measurements (described in Section 2.2), spectral absorption, attenuation, scattering and backscattering measurements (WetLabs AC-S, ECO-vsf3, ECO-bb3, Philomath, OR, USA), volume scattering at three angles and three wavelengths (WetLabs ECO-vsf3, Philomath, OR, USA), CTD (SeaBird, Philomath, OR, USA) data collection and fluorometric measurements of chlorophyll *a*, phycocyanin and CDOM (Trios, microFLU, Oldenburg, Germany).

Two ship cruises were conducted using the vessel R/V Salme (17 measurements, on 26 July and 3 August) in 2016. Reflectance measurements (described in Section 2.2) were carried out in fixed stations together with water sampling from surface layer (top 0.5 m) for the analysis of chlorophyll *a* (in mg m^{-3}) and total suspended matter (TSM, in mg L^{-1}). In addition, spectral absorption and attenuation in the wavelength range from 402 nm to 732 nm were measured at each station using AC-S instrument (WetLabs, Philomath, OR, USA).

A ferrybox system (by GO-Systemelektronik BlueBox-System) installed on board the R/V Salme collected data at 2 m depth between the fixed sampling stations (822 measurements on 26 July; 1088 measurements on 3 August 2016). During the cruises, water was pumped continuously through measuring system equipped with fluorometers for chlorophyll *a* (in mg m^{-3}), phycocyanin (ppb), and turbidity (NTU, ECO Fluorometers, WetLabs, Philomath, OR, USA). Measurements, together with GPS signal, were logged by BlueBox-system at 60 s frequency, giving a spatial resolution of about 250 m.

A time series of shipborne remote sensing reflectance (described in Section 2.2), chlorophyll *a* and turbidity (385 measurements, on 10 May 2016) were collected from the Southern Baltic Sea. This is a subset of data collected in the frame of the FerryScope project [30]. The mean time difference between Sentinel-3 OLCI and in situ data was approximately one day.

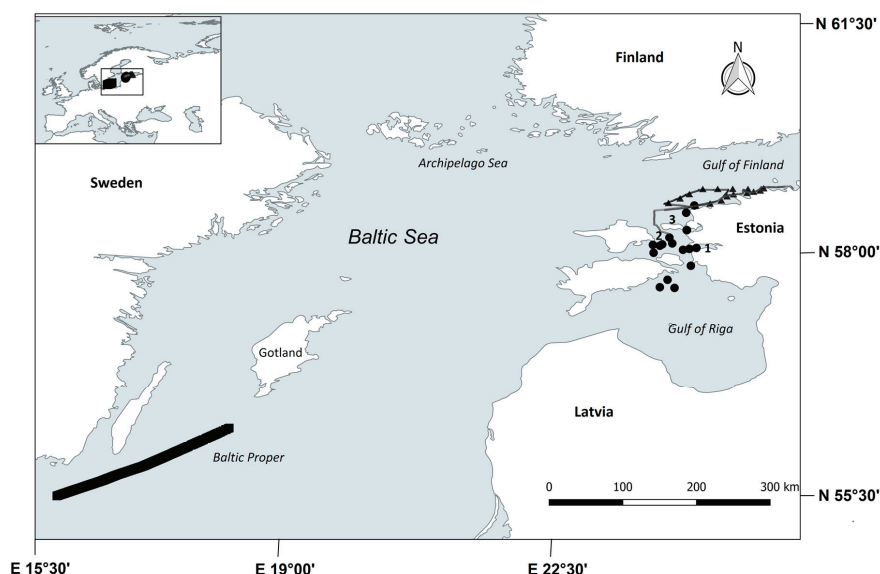


Figure 1. Locations of the sampling points: Squares, FerryScope; circles, boat measurements; triangles, research vessel R/V Salme; rout behind the triangles, R/V Salme ferrybox; 1, Matsalu Bay; 2, Hiuu Strait; and 3, Nordgrund.

Concentration of chlorophyll *a* was determined by filtering the water samples through Whatman GF/F glass microfibre filters (pore size 0.7 μm , diameter 47 mm, Whatman International Ltd., Mainstone, UK), extracting the pigments with ethanol (96%) and spectrophotometrically measuring absorption at wavelengths of 665 nm and 750 nm [31]. The values of chlorophyll *a* were calculated with the Lorenzen formula [32].

The concentration of TSM, was measured gravimetrically after filtration of the same amount of water through pre-weighed and pre-combusted (103–105 $^{\circ}\text{C}$ for 1 h) GF/F filters. The increase of filter weight indicates TSM concentration in the water sample. The inorganic fraction of suspended matter (SPIM) was measured after combustion at 550 $^{\circ}\text{C}$ for 30 min. The organic fraction of suspended matter (SPOM) was determined by subtraction of SPIM from TSM (ESS, 1993).

a_{CDOM} was measured with a spectrometer (Hitachi U-3010 UV/VIS, at the range of 350–750 nm) in water filtered through a Millipore 0.2 μm filter. Measurements were carried out in a 5 cm cuvette against distilled water and corrected for residual scattering according to [33]. $a_{\text{CDOM}}(412)$ was used for measuring CDOM concentration in the algorithm analyses. Different algorithms use different wavelengths for CDOM, but as Kowalczyk et al. [19] has shown, the slope of the CDOM in the Baltic Sea is relatively stable throughout the year so using a different wavelength as reference should not change the performance of the algorithm [11].

Secchi depth was measured from a boat and R/V Salme with a 30 cm diameter Secchi disk.

2.2. Reflectance Measurements

Reflectance measurements used in this study were collected in three different ways: the in situ measurements from a boat were carried out with radiance (L_u) and irradiance (E_d) sensor, the measurements from R/V Salme were performed with an irradiance (E_d) sensor and the measurements from ships of opportunity were carried out with triple radiometer system (L_u , L_d , E_d).

The boat reflectance measurements were carried out with two TriOS RAMSES sensors, where RAMSES-ACC-VIS measured sky irradiance and RAMSES-ARC upwelling radiance.

The downwelling irradiance sensor was looking straight up and the upwelling radiance sensor was looking straight down. Reflectance was calculated as L_u/E_d . Reflectance measurements were carried out both in the air and under water. The methodology, which also includes glint-free measurements, was described in more detail in [34]. RAMSES measures with 3.3 nm spectral interval at the wavelength range of 350–900 nm. In order to avoid errors in reflectance spectra that occur due to the slight wavelength differences between the two sensors, both radiance and irradiance values were interpolated to a 2-nm step before calculating the reflectance.

The R/V Salme measurements were carried out just below the water surface using a RAMSES-ACC hyperspectral radiometer. The RAMSES used measures with a 3.3 nm spectral interval at the wavelength range of 305.9–1142.8 nm (wavelength range from 350 nm to 900 nm was used in current analysis). Downwelling (E_d) irradiance was measured when the sensor was looking straight up, upwelling (E_u) irradiance was measured by turning the device face down and measuring at the same height/depth. Irradiance reflectance was calculated as E_u/E_d .

The ship of opportunity reflectance measurements were carried out with Rflx systems [29] that consists of three Ramses sensors and a moving platform with software that keeps the sensor package at optimal viewing angles proposed by [35]. It measures with a 3.3 nm spectral interval at the wavelength range of 320–947 nm.

2.3. Sentinel-3 OLCI Data

Sentinel-3 OLCI full resolution (FR) Level-1 and Level-2 data products with 300 m spatial resolution were used for analyses. Sentinel-3 OLCI cloud free images were available on 9 May, 21 May, 26 July, 3 August (with system vicarious calibration), 14 September and 10 October (without system vicarious calibration) 2016. Spectral bands of Sentinel-3 OLCI are brought out in Table 1.

Sentinel-3 Toolbox Kit Module (S3TBX) version 5.0.1 in Sentinel Application Platform (SNAP) version 5.0. On Windows 10 was used to process the images. Cloud free pixel values corresponding to the locations of sampling points were extracted from OLCI imagery. To get the Level-1 Top of Atmosphere (TOA) and Level-2 (L2) Bottom of Atmosphere (BOA) reflectance images (derived from the associated L1 products) Case-2 Regional/Coast Colour (C2RCC) atmospheric correction (AC) module version 0.15 for Sentinel-3 OLCI was applied. Output products of the C2RCC are: BOA reflectance, inherent optical properties (absorption coefficient of phytoplankton pigments, detritus, coloured dissolved organic carbon and total absorption at 443 nm, scattering coefficient of marine and white particles at 443 nm), chlorophyll, TSM and CDOM, which were compared with appropriate in situ measurements.

Table 1. Spectral bands, central wavelengths (nm) and bandwidths (nm) of Sentinel-3 OLCI.

Band Number	Central Wavelength (nm)	Bandwidth (nm)
Oa1	400	15
Oa2	412.5	10
Oa3	442.5	10
Oa4	490	10
Oa5	510	10
Oa6	560	10
Oa7	620	10
Oa8	665	10
Oa9	673.75	7.5
Oa10	681.25	7.5
Oa11	708.75	10
Oa12	753.75	7.5
Oa13	761.25	2.5
Oa14	764.375	3.75
Oa15	767.5	2.5
Oa16	778.75	15

Table 1. Cont.

Band Number	Central Wavelength (nm)	Bandwidth (nm)
Oa17	865	20
Oa18	885	10
Oa19	900	10
Oa20	940	20
Oa21	1020	40

In addition to the standard processor (C2RCC), common empirical algorithms were tested (Table 2).

Table 2. List of empirical algorithms tested in this study.

Algorithm (Wavelength)	Algorithm (OLCI Bands)	Reference
Chlorophyll <i>a</i> and Other Pigments		
R560/R665	B6/B8	[36]
R665/R709	B8/B11	[21]
R665/R754	B8/B12	
R674/R709	B9/B11	[37]
R674/R754	B9/B12	
R709/R754	B11/B12	[38]
$(1/R6651/R709) \times R754$	$(1/B8 - 1/B11) \times B12$	[39]
$(R490 - R665)/R560$	$(B4 - B8)/B6$	[40]
$R709 - ((R665 + R754)/2)$	$B11 - ((B8 + B12)/2)$	[41]
$R709 - R754$	$B11 - B12$	
Total Suspended Matter		
R665/R560	B8/B6	[42]
R709	B11	[43]
Coloured Dissolved Organic Matter		
R665/R490	B8/B4	[21]
R665/R560	B8/B6	[44]
Secchi		
$(R560/R709)^{0.788} \times 1.125$	$(B6/B11)^{0.788} \times 1.125$ (turbid waters)	[45]
$(R490/R709)^{0.697} \times 2.137$	$(B4/B11)^{0.697} \times 2.137$ (clear waters)	[45]

3. Results

3.1. In Situ Data

The in situ data used in this study come from three different sources, as described above. Therefore, the number and type of parameters varies. Table 3 summarises the results of the measurements.

The boat measurements included absorption and scattering that are also products of the C2RCC processing chain. The absorption, attenuation and scattering coefficient measurements were hyperspectral and backscattering measurements were carried out at six wavelengths. Some total absorption coefficient spectra are shown in Figure 2 together with data from our other Baltic Sea study sites to demonstrate how the results of this study fit within the range of optical properties we have observed previously.

Table 3. In situ data of chlorophyll *a* (Chl *a*), phycocyanin, total suspended matter (TSM), the inorganic fraction of suspended matter (SPIM), the organic fraction of suspended matter (SPOM), turbidity, *a*_{CDOM(412)}, Secchi disc depth (Secchi), total absorption at 443 nm (*a*_{tot}), total attenuation at 443 nm (*c*_{tot}), total scattering at 443 nm (*b*_{tot}), and total backscattering at 470 nm (*b*_{b_{tot}}) collected during three different field campaigns on 24 May, in on 14 September and on 12 October 2016 (Boat), on board the R/V Salme on 26 July and 3 August 2016 (R/V Salme stations), by Ferrybox installed on board research vessel R/V Salme on 26 July and 3 August 2016 (R/V Salme Ferrybox) and measured in the frame of the FerryScope project on 10 May 2016 (FerryScope).

	Chl <i>a</i> (mg m ⁻³)	Phycocyanin (ppb)	TSM (mg L ⁻¹)	SPIM (mg m ⁻³)	SPOM (mg m ⁻³)	<i>a</i> _{CDOM(412)} (m ⁻¹)	Turbidity (NTU)	Secchi (m)	<i>a</i> _{tot} (m ⁻¹)	<i>c</i> _{tot} (m ⁻¹)	<i>b</i> _{tot} (m ⁻¹)	<i>b</i> <i>b</i> _{tot} (m ⁻¹)
Boat	Mean	1.53	1.52	1.14	2.23	-	-	5.18	0.55	1.61	1.07	0.02
	Min	0.38	0.11	0.13	1.20	-	-	2.20	0.39	0.69	0.29	0.01
	Max	2.95	2.93	1.44	4.53	-	-	12.7	0.80	2.33	1.76	0.05
	N	17	17	8	16	-	-	17	15	15	15	15
R/V Salme stations	Mean	4.33	1.14	1.14	2.23	-	-	3.32	0.64	2.12	1.48	-
	Min	1.81	0.13	0.13	1.20	-	-	2.50	0.58	1.84	1.2	-
	Max	6.02	1.44	1.44	4.53	-	-	4.00	0.75	2.79	2.2	-
	N	16	8	8	16	-	-	16	16	15	15	-
R/V Salme Ferrybox	Mean	1.12	0.35	0.35	-	-	0.66	-	-	-	-	-
	Min	0.00	0.00	0.00	-	-	0.24	-	-	-	-	-
	Max	2.63	1.81	1.81	-	-	12.8	-	-	-	-	-
	N	822	299	299	-	-	771	-	-	-	-	-
FerryScope	Mean	1.60	-	-	-	-	0.29	-	-	-	-	-
	Min	0.82	-	-	-	-	0.19	-	-	-	-	-
	Max	2.48	-	-	-	-	0.36	-	-	-	-	-
	N	385	-	-	-	-	385	-	-	-	-	-

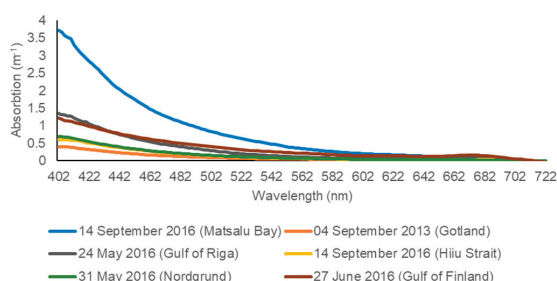


Figure 2. Selected total absorption coefficient spectra of the Baltic Sea. The Gotland spectrum is from our other field study [46] to show typical absorption we have measured in the open parts of the Baltic Sea and Swedish Archipelago waters during our previous field campaigns.

3.2. Atmospheric Correction and Reflectance Spectra

In situ reflectance spectra were recalculated into Sentinel-3 OLCI bandwidths and compared with the C2RCC corrected reflectance. The comparison between OLCI bottom of atmosphere reflectance spectra and FerryScope project Rflex system results are shown in Figure 3, with R/V Salme underwater irradiance reflectance in Figure 4 and with glint-free remote sensing reflectance measured from a boat in Figure 5.

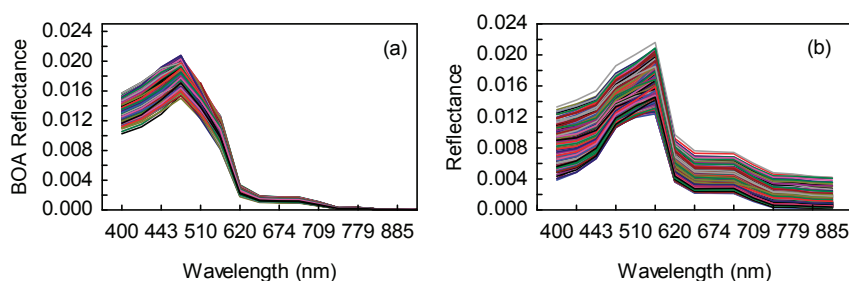


Figure 3. Reflectance spectra of the open Baltic Sea area: (a) Bottom of Atmosphere (BOA) reflectance of Sentinel-3 OLCI after correction with C2RCC (9 May 2010); and (b) FerryScope reflectance spectra measured on 10 May 2016 and recalculated to match Sentinel-3 OLCI bands.

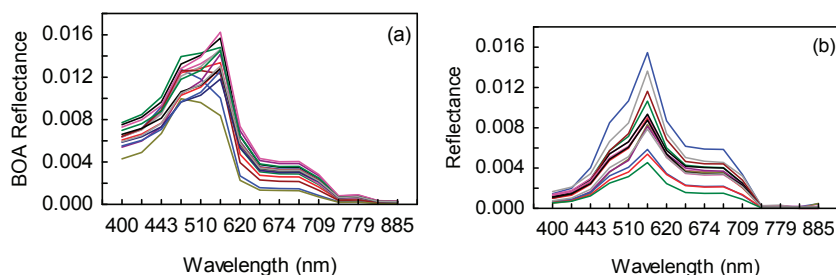


Figure 4. Reflectance spectra of the coastal waters of Baltic Sea: (a) Bottom of Atmosphere (BOA) reflectance of Sentinel-3 OLCI after correction with C2RCC (26 July and 3 August 2016); and (b) R/V Salme. Reflectance spectra measured on board the research vessel R/V Salme on 26 July and 3 August 2016 and recalculated into Sentinel-3 bands.

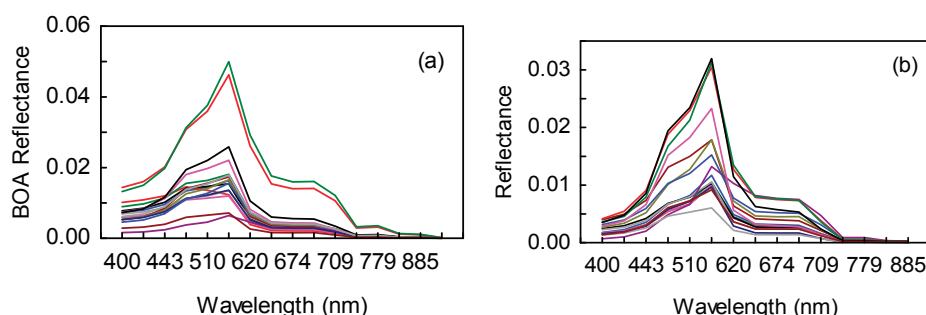


Figure 5. Reflectance spectra of the coastal waters of the Baltic Sea: (a) Bottom of Atmosphere (BOA) reflectance of Sentinel-3 OLCI after correction with C2RCC (21 May, 14 September and 10 October 2016); and (b) boat. Glint-free reflectance spectra measured with the methodology described in [35] during three different field campaigns (24 May, 14 September, 12 October 2016) and recalculated into Sentinel-3 OLCI bands.

We also calculated band by band correlations between the atmospherically corrected OLCI data and three different types of in situ reflectance. The correlation coefficients are given in Table 4.

Table 4. Correlation (and corresponding p -values) between bottom of atmosphere (BOA) reflectance of Sentinel-3 OLCI after correction with C2RCC and in situ reflectance. Reasonably good correlations are highlighted in bold. R, correlation coefficient; P , p -value.

Central Wavelength (nm)/Band	FerryScope		R/V Salme		Field	
	R	P	R	P	R	P
400 (B1)	0.06	0.25	0.55	0.03	0.51	0.04
413 (B2)	0.06	0.26	0.56	0.03	0.55	0.02
443 (B3)	0.07	0.20	0.66	0.01	0.67	0.00
490 (B4)	0.31	0.00	0.65	0.01	0.77	0.00
510 (B5)	0.59	0.00	0.38	0.16	0.81	0.00
560 (B6)	0.77	0.00	−0.16	0.58	0.82	0.00
620 (B7)	0.71	0.00	−0.48	0.07	0.77	0.00
665 (B8)	0.68	0.00	−0.47	0.08	0.68	0.00
674 (B9)	0.69	0.00	−0.49	0.06	0.68	0.00
681 (B10)	0.69	0.00	−0.51	0.05	0.68	0.00
709 (B11)	0.64	0.00	−0.41	0.13	0.58	0.02
754 (B12)	0.60	0.00	−0.18	0.51	0.43	0.09
779 (B16)	0.60	0.00	0.06	0.82	0.37	0.14
865 (B17)	0.60	0.00	0.07	0.82	0.61	0.01
885 (B18)	0.59	0.00	−0.63	0.01	0.71	0.00

The height of the peak between 700 and 710 nm has been used as a proxy of phytoplankton biomass (chlorophyll a) for a long time [41]. The NIR part of spectrum is also important for detecting surface scum, as was mentioned above [4]. Therefore, the correct representation of the 709 nm band height and NIR signal are especially important for the Baltic Sea. Our own observations, as well as published results [46], suggest that most atmospheric correction procedures had problems in retrieving the 709 nm peak properly (compared to in situ data), especially in the earlier phases of MERIS mission. There was dense cyanobacterial bloom slightly outside the R/V Salme route on 26 July 2016. We chose a few pixels from the image where it was sure that there is at least a very dense subsurface bloom if not surface scum present and checked how the C2RCC performs in such situation. The comparison between TOA and BOA reflectance is given in Figure 6, which indicates that the C2RCC atmospheric correction provides unrealistic reflectance spectra in cyanobacterial bloom situations.

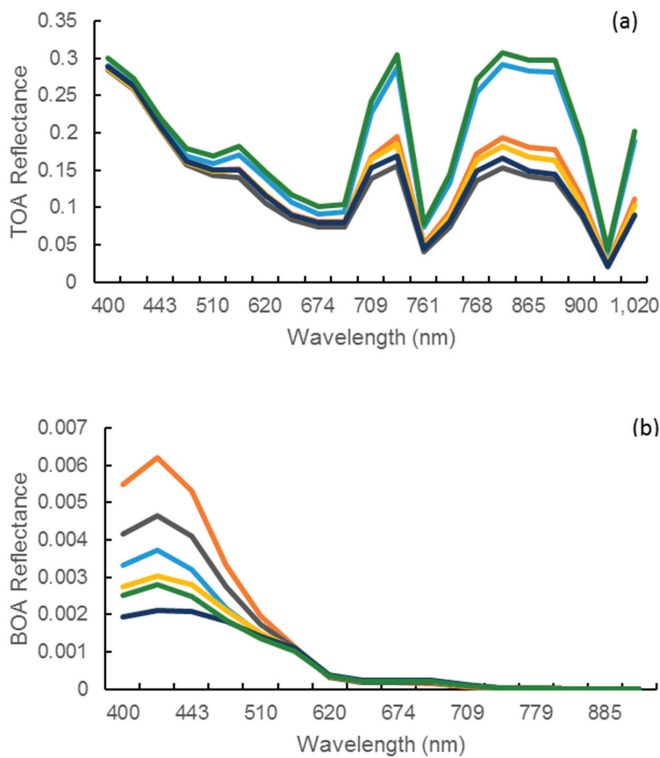


Figure 6. Sentinel-3 OLCI reflectance spectra from the bloom area near the R/V Salme route (26 July 2016): (a) top of atmosphere (TOA) reflectance of OLCI; and (b) bottom of atmosphere (BOA) reflectance of OLCI after correction with C2RCC.

3.3. Results of the Remote Sensing Products vs. In Situ Data

The C2RCC processor retrieves first inherent optical properties, such as absorption and scattering coefficients, and then estimates the concentrations of optically active substances from the IOPs. It is seen in Figure 7 that none of the OLCI products had statistically significant correlation ($p > 0.05$) with in situ measured values.

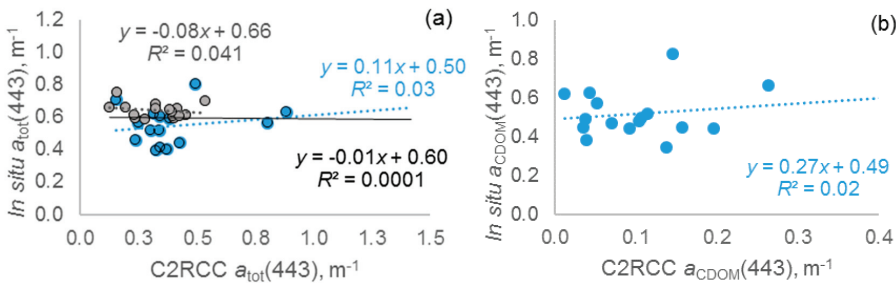


Figure 7. Cont.

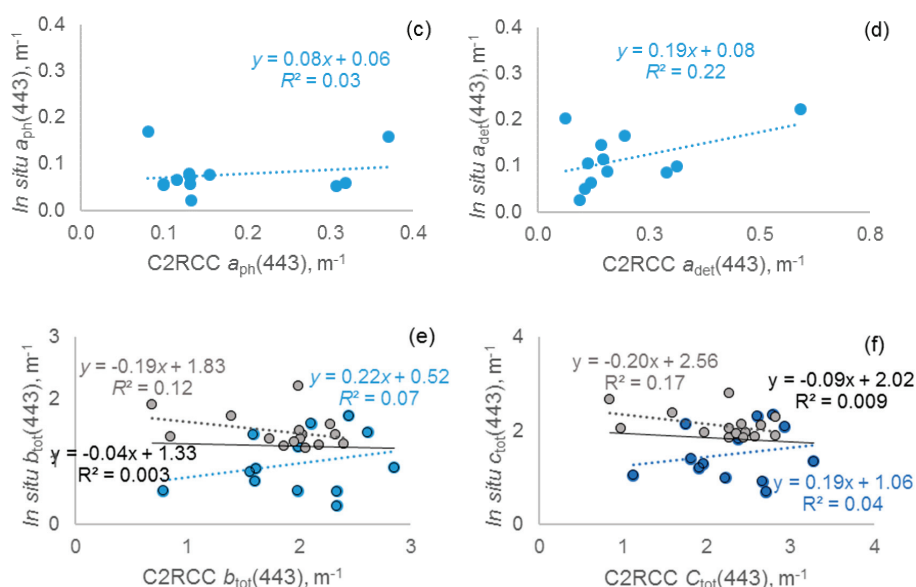


Figure 7. Comparison of inherent optical properties of C2RCC and appropriate in situ measurements: (a) $a_{\text{tot}}(443)$, (b) $a_{\text{CDOM}}(443)$, (c) $a_{\text{ph}}(443)$, (d) $a_{\text{det}}(443)$, (e) $b_{\text{tot}}(443)$, (f) $c_{\text{tot}}(443)$. Grey dots, R/V Salme; blue dots, boat; and black regression line, R/V Salme + boat.

OLCI chlorophyll a and TSM products are calculated from estimated IOP values (pigment absorption and total scattering products at 443 nm respectively). Therefore, it is surprising that the concentration products have slightly better correlation with in situ data than the IOPs they were derived from (Figure 8a,b), although the highest correlation ($R^2 = 0.25$) is still very low. The correlations were even higher when we used in situ data collected with ferrybox flow through systems (Figure 8c,d). However, it is clearly seen that the scatter of the results is very high despite the correlation coefficients in the range of 0.4–0.5. For example, C2RCC chlorophyll a varies between 0 and 11 mg m^{-3} when the ferrybox concentration is around 2.5 mg m^{-3} and for C2RCC concentrations 6 mg m^{-3} ferrybox values range between 1.5 and 6 mg m^{-3} (Figure 8c). It must be noted that there are no in situ IOP data for the points where ferrybox data were collected.

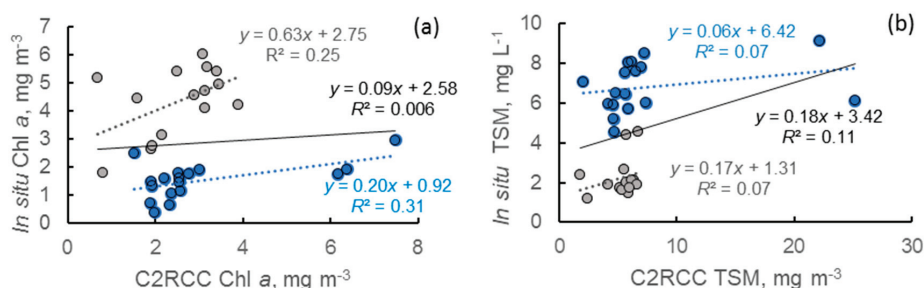


Figure 8. Cont.

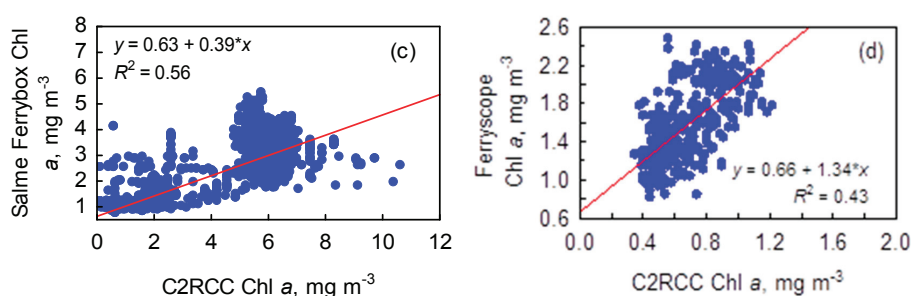


Figure 8. Comparison of output products of C2RCC: (a,c,d) chlorophyll *a* (Chl *a*), and (b) total suspended matter (TSM) and appropriate (a,b) in situ, (c) R/V Salme ferrybox and (d) FerryScope measurements: (a,b) grey dots, R/V Salme; blue dots, boat; and black regression line, R/V Salme + boat.

3.4. Results of the Empirical Remote Sensing Algorithms vs. In Situ Data

The IOPs and concentrations of optically active substances retrieved with the C2RCC processor did not provide reasonable results. On the other hand, reflectance spectra produced by the C2RCC were quite realistic in non-bloom situations both in shape and magnitude (Figures 3–5). Therefore, we decided to test whether simple empirical algorithms perform better than the neural network approach included in the C2RCC. The algorithms used are given in Table 2 and some better results are shown in Figures 9–13.

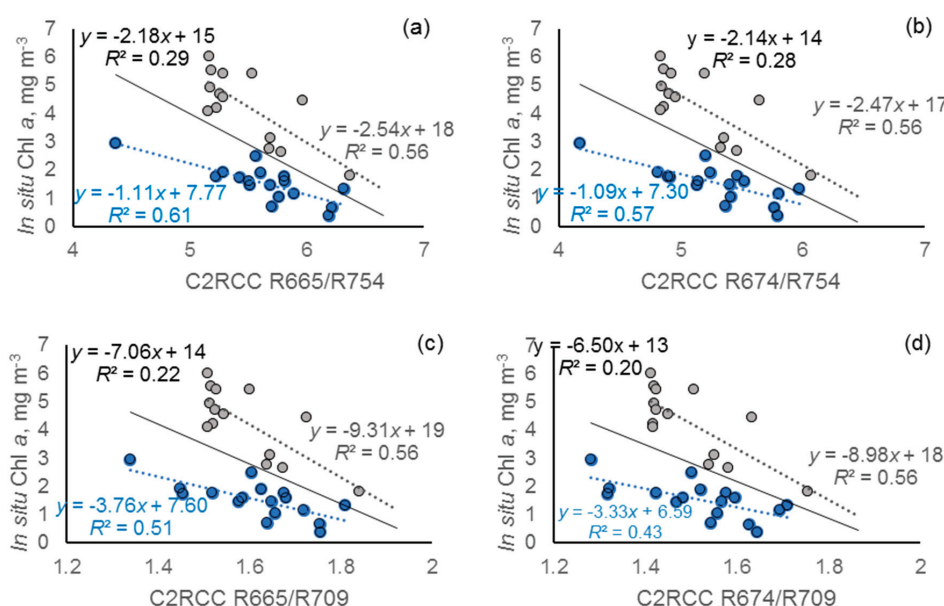


Figure 9. Correlation between the empirical algorithm calculated from the bottom of atmosphere data of Sentinel-3 OLCI (atmospherically corrected with C2RCC) and chlorophyll *a* (Chl *a*): grey dots, R/V Salme; blue dots, boat; and black regression line, R/V Salme + boat.

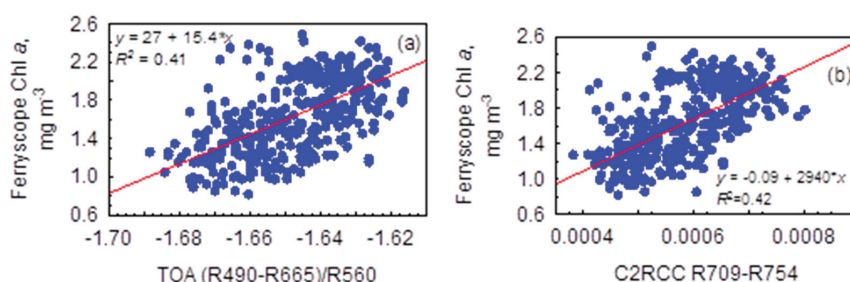


Figure 10. Correlation between the empirical algorithm calculated from the Sentinel-3 OLCI data and chlorophyll *a* (Chl *a*) measured in the frame of the FerryScope project: (a) empirical algorithm calculated from the top of atmosphere reflectance; and (b) band ratio calculated from the bottom of atmosphere reflectance (atmospherically corrected with C2RCC).

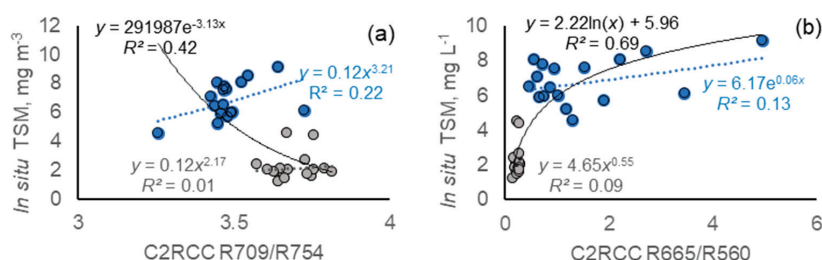


Figure 11. Correlation between the empirical algorithm calculated from the bottom of atmosphere data of Sentinel-3 OLCI (atmospherically corrected with C2RCC) and total suspended matter (TSM): grey dots, R/V Salme; blue dots, boat; and black regression line, R/V Salme + boat.

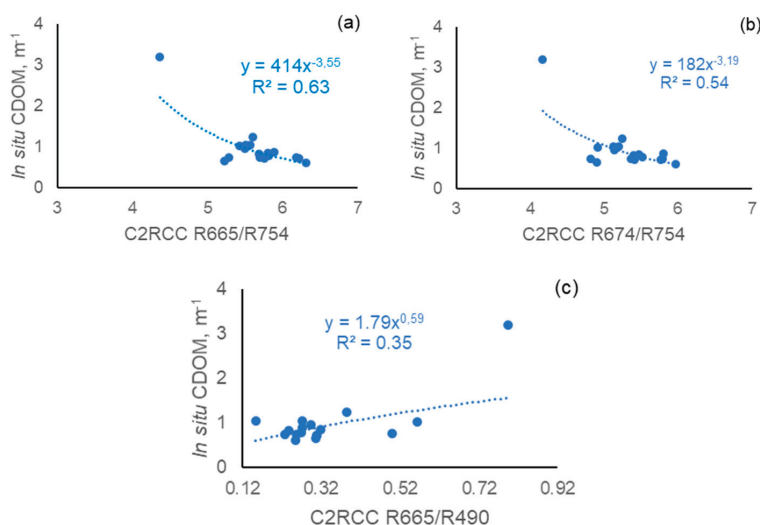


Figure 12. Correlation between the empirical algorithm calculated from the bottom of atmosphere data of Sentinel-3 OLCI (atmospherically corrected with C2RCC) and coloured dissolved organic matter (CDOM) measured from boat.

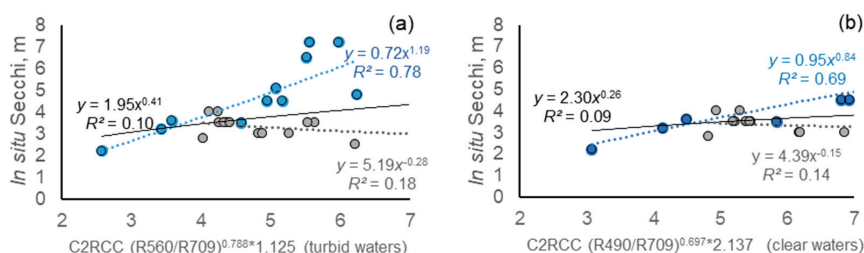


Figure 13. Correlation between the empirical algorithms [45] calculated from the bottom of atmosphere data of Sentinel-3 OLCI (atmospherically corrected with C2RCC) and Secchi disc depth: grey dots, R/V Salme; blue dots, boat; and black regression line, R/V Salme + boat.

4. Discussion

Optical properties of the studied waters varied over a quite wide range. Our previous results [46] and the current study (Figure 2) demonstrated that the absorption coefficient varies over an order of magnitude in the coastal waters of the Baltic Sea. Many rocky and relatively deep archipelago waters (e.g., Sweden) are often optically similar to open parts of the Baltic Sea, whereas shallow sandy coastal and archipelago waters (e.g., Estonia and Latvia) are much more absorbing and scattering by resuspended from the sea bottom particles may play significant role in windy days as extensive areas are just a few meters deep. The range of observed absorption coefficients is demonstrated in Figure 2. It is seen that the absorption in the clearest sites was only by about 45–65% higher than typical central Baltic Sea absorption values. On the other hand, the absorption coefficient was almost by an order of magnitude higher in Matsalu Bay, which is a typical estuary with CDOM-rich inflow from nearby wetlands. Thus, we may say that the study covers a reasonable range of optical variability.

The reflectance spectra produced by C2RCC processing chain from OLCI data for non-bloom conditions are quite reasonable, in both shape and magnitude (Figures 3–5). In the case of R_{flex} systems on ships of opportunity, the corrected OLCI spectra have too high values in the blue part of spectrum whereas the in situ data has high and variable reflectance in NIR part of spectrum that suggest presence of glint or some other artefact in the reflectances measured from moving ship (Figure 3). Comparison of OLCI reflectance and R/V Salme subsurface irradiance reflectance measurements (Figure 4) also suggest that the BOA OLCI reflectances are too high in blue part of spectrum. The best match between the in situ and OLCI reflectances was observed in the case of boat measurements (Figure 5). It must be noted that the reflectances measured from the boat do not contain any surface reflection (sky and sun glint), as they were measured keeping upwelling radiance sensor just below the water surface [34]. C2RCC is supposed to remove these components from the measured signal as well. Probably, the B1 and B2 values are slightly too high in the OLCI BOA reflectance spectra, but in general the atmospherically corrected spectra are very realistic in non-bloom conditions.

The problems in atmospheric correction are the highest in the blue part of spectrum, as is seen in Figures 3–5 and Table 4. ESA also has ongoing activities to improve OLCI calibration in shorter wavelengths bands, but atmospheric correction of blue bands is very difficult anyway as atmospheric and glint effects are higher in the blue part of spectrum. Water leaving signal in the Baltic Sea is typically close to zero in the blue part of spectrum [11,25] and in coastal waters may be low also at longer wavelengths. This makes atmospheric correction of the Baltic Sea imagery especially difficult. The errors in retrieving correct reflectance do affect results obtained by neural networks as all spectral bands are taken into account in the processing. On the other hand, these errors in both instrument calibration and atmospheric correction do not affect results obtained by means of empirical algorithms as blue wavelengths are not used in empirical algorithms developed for optically complex waters and there are no issues in calibrations and atmospheric correction of green to NIR bands.

Cyanobacterial blooms cover up to 200,000 km² of the Baltic Sea every summer [15] and the duration of the blooms may be quite long. Therefore, in the Baltic Sea the performance of any atmospheric correction procedure and water quality retrieval algorithm is especially critical during the cyanobacterial season in the Baltic Sea. The C2RCC atmospheric correction does not provide realistic reflectance in cyanobacterial bloom situations as is seen in Figure 6. The top of atmosphere spectra have significant signal at 709 nm band (critical for the retrieval of chlorophyll *a* [42]) and further in NIR part of spectrum (necessary to separate surface scum from dense subsurface bloom). All this useful information is removed by the C2RCC. Ten years ago, there were problems with MERIS atmospheric correction and therefore it was suggested to retrieve chlorophyll *a* by using the height of the 709 nm peak taken from the TOA signal instead of BOA [47]. Later atmospheric correction procedures preserved the 709 nm peak better [48], but still not completely. Thus, the C2RCC has made a step backwards in correcting OLCI data compared to the latest developments in MERIS processing. Some atmospheric correction procedures, such as FLAASH (Fast Line-of-sight Atmospheric Analysis of Hypercubes), produce very realistic subsurface bloom and surface scum reflectance spectra [4]. C2RCC is a neural network approach that requires training data to perform well and produce realistic water reflectances. Thus, there is a strong need for in situ reflectance data from bloom conditions to train the C2RCC processor in order to retrieve realistic reflectance both in the Baltic Sea and large lakes where optically similar blooms do occur. The training data should include surface scum and subsurface blooms with different biomass and different vertical structure as, unlike other types of phytoplankton, cyanobacteria can move in the water column themselves and the vertical distribution of biomass has significant impact on the remote sensing signal [16].

The next step in the C2RCC processing chain, after retrieving water reflectance, is estimating IOPs (absorption and scattering coefficients). For example, the total absorption at 443 nm is retrieved and is then split into contributions by CDOM, phytoplankton and detritus. Our earlier lake remote sensing studies with MERIS [49] have shown that the total absorption coefficient is retrieved better than its components (a_{ph} , a_{CDOM} , etc.). We measured absorption, scattering and backscattering coefficients during our boat sampling campaigns. Comparisons of the OLCI products with the in situ data showed that the neural network approach used in the C2RCC does not allow yield accurate estimates of IOPs in the Baltic Sea (Figures 7 and 8). Neural networks as such require extensive amount of training data to perform well. The C2RCC processor was trained with simulated reflectance data [50] and was developed to cope better with highly scattering coastal waters such as coccolithophore blooms, which do not occur in the Baltic Sea. However, the Baltic Sea waters in general are highly absorbing [4,11,25] except in very shallow areas with high resuspension during strong wind or some river estuaries that bring higher amount of sediments to the coastal waters. For example, CDOM absorption in several of our sampling sites goes beyond the normal maximum training range of C2RCC. On the other hand, the extreme maximum training range of the C2RCC goes even an order of magnitude higher. Despite that we see no correlation between the measured and estimate from OLCI data IOPs.

It is obvious that the correlations between measured and C2RCC processor estimated water products (chlorophyll *a*, TSM) are close to zero if the retrieved IOPs did not have correlation with in situ values. The best results were obtained when comparing ferrybox data from FerryScope database and the R/V Salme ferrybox measurements with C2RCC chlorophyll (Figure 8). The r^2 was up to 0.56 in coastal waters (R/V Salme measurements) and 0.43 in the open parts of the Baltic Sea (FerryScope measurements). This is obviously not satisfactory for any remote sensing product that could be used in quantitative monitoring of phytoplankton biomass not speaking about long time trend studies.

It is seen in the Figure 9 that chlorophyll *a* estimates made with different empirical algorithms (band ratios) vary for boat sampling and the R/V Salme measurements and the difference is quite consistent for different algorithms. The first potential explanation could be that the C2RCC has some kind of stability problems as the boat and the R/V Salme measurements were made on different dates. However, this cannot be the case, whereas both boat measurements and ship measurements

were made on multiple dates and the consistency within these two groups of data (boat and ship) is good. Therefore, this difference must come from in situ data. The R/V Salme measurements were carried out during cyanobacterial bloom (July–August), whereas boat measurements were carried out in May, September, and October when other groups of phytoplankton dominated in the water column. Extracting pigments from cyanobacteria is a complicated problem [51]. Consequently, some of the chlorophyll *a* remains in the cells and is not measured in the spectrophotometer. As a result the measured chlorophyll *a* values are lower than the actual chlorophyll *a* concentrations (what remote sensing can detect) in cyanobacterial cells. This should produce the opposite difference between boat and R/V Salme measurements compared to what we observe now.

One of the possible explanations may be differences between the chlorophyll *a* values obtained in different institutes as problems in the bad performance of C2RCC or dominance of different phytoplankton assemblages should have caused different discrepancies than we observe now. Water samples from R/V Salme and boat cruises were carried out with the same methodology—surface samples were used in both cases. The laboratory methodology used in both institutes is also the same, however, the results we observe are different. Ruling out potential effect of different laboratories would require analysing parallel samples taken from the same stations. This is a topic that needs further analysis.

It is assumed in all remote sensing studies that the in situ values are the “truth” when actually the in situ values have their own errors which may be quite large. HELCOM has carried out intercalibration measurements of chlorophyll *a* around the Baltic Sea (analysis of water from the same sample) that showed large discrepancies between different institutes. With trainings and further intercalibration experiments, these errors were taken down to 14% [52]. However, the laboratory analysis error is still quite large. The errors resulting from taking the water samples may be even larger. HELCOM protocol [52] requires taking integral water sample (subsamples taken at different depths are mixed together). This is fine when algae dominate in the phytoplankton community as these are passive particles that are uniformly mixed in the top layer of water (10–20 m in the Baltic Sea). However, cyanobacteria can regulate their buoyancy and in calm weather (wind less than 2 m s^{-1}) tend to move to water depth most optimal for their growth. The main biomass of cyanobacteria may be condensed in relatively narrow (a few meters) layer. Thus, it may happen that all subsamples taken for the integral water sample are actually from depths which are very low in cyanobacterial biomass. In that case there is no correlation between the bloom satellites are detecting and the clear water sample analysed in laboratory. On the other hand, one or several subsamples for the integral sample may come from exactly this or these depth(s) where the cyanobacterial bloom was. In that case, the laboratory results will show higher values than remote sensing can detect. During both the boat measurements and R/V Salme measurements all water samples were taken from the surface layer (top 0.5 m). Thus, the discrepancies in in situ values due to different sample collection strategies may be ruled out.

The issue of quality of in situ data is one that needs stronger attention. In the situation of general lack of data for algorithm development and validation, remote sensing scientists use whatever is available not knowing how the water samples were collected and how they have been analysed. Using exactly the same sampling and laboratory analysis methodologies can result concentration errors in the order of ten(s) of per cent. On the other hand, differences in sample collection methods and strategies (i.e., sampler type, depth(s), how much care was taken to preserve the natural state of the bloom, etc.) may cause variability in measured biomass that can be in the orders of magnitude. It is obvious that developing and/or validating remote sensing products with such inconsistent data is problematic.

It must be noted that there were no IOP data available for the continuous autonomous measurements of chlorophyll *a* carried out from moving ships. Therefore, it was not possible to check whether the C2RCC IOP products would have produced reasonable results for the open parts of the Baltic Sea or not.

It must also be noted that the chlorophyll *a* fluorometers cannot provide reasonable results when cyanobacteria dominate in water as in cyanobacteria chlorophyll *a* is in the non-fluorescing photosystem [53]. Meaning that phycocyanin fluorometers have to be used to describe cyanobacterial biomass. R/V Salme cruises were carried out during cyanobacterial bloom, but only in the relatively low biomass edge of the bloom where the biomass of other cells of phytoplankton was probably not very low. Slightly elevated phycocyanin values (up to 1.8 ppb) were registered by the ferrybox system onboard R/V Salme in the Gulf of Finland while phycocyanin concentration values of ~1.2 ppb were observed in the Moonsund (Väinameri) area. It is seen in Figure 10 that scattering of data points is very high despite the relatively high correlation coefficient. For example, if the C2RCC estimate of chlorophyll *a* is 0.5 mg m^{-3} then the fluorometer values varied between 0.5 and 4; for C2RCC chlorophyll 6 mg m^{-3} the fluorometer values varied between 1.5 and 6; or for fluorometer values of 3 mg m^{-3} C2RCC estimated values between 0 and 11 mg m^{-3} . Reflectance spectra produced by the C2RCC were realistic as was shown on Figures 3–5 above. Therefore, it was logical to try simple empirical algorithms in water quality parameter retrieval when C2RCC failed to do this. We did not undertake a full empirical algorithm testing study, as the aim was to test C2RCC as one of the main processors for OLCI data. Nevertheless, several empirical (band ratio) algorithms produced good estimates of chlorophyll *a*, CDOM, TSM, and Secchi depth (Figures 9–12). The result for chlorophyll *a* retrieval was already described above. As was expected the algorithms utilizing green to red (and NIR) part of spectrum performed the best as the impact of phytoplankton on the blue part of spectrum is usually negligible in CDOM-rich waters such as the Baltic Sea.

Performance of the TSM algorithms was relatively poor. It is not surprising considering that the TSM samples were collected and analysed during the R/V Salme and the boat cruises in near coastal waters. Most of the TSM collected during the R/V Salme measurements were of organic nature (cyanobacterial cells), while boat measurements were carried out in relatively shallow waters, where resuspension of inorganic particles plays significant role, and closer to rivers, which may bring inorganic material into coastal waters. SPIM and SPOM were measured separately only from the boat cruises data and the dominance of inorganic particles is seen also in the Table 3.

Unfortunately, there was only one sampling station where the CDOM value was relatively high compared to the majority of sampled values. Therefore, the conclusion about the performance of CDOM retrieval algorithms using C2RCC corrected OLCI data is not very strong. However, the single high value (3.2 m^{-1}) of this study is not very high for the coastal parts of the Baltic Sea. In our recent study [11], we had $a_{\text{CDOM}}(412)$ range between 0.28 m^{-1} and 13.46 m^{-1} . Satellite estimates [54] have shown that CDOM absorption may go over 30 m^{-1} near some rivers bringing highly absorbing waters from wetlands. Nevertheless, the regression equations that are heavily influenced by one data-point should be used with caution.

OLCI Secchi depth estimates showed also some dependency on the source of in situ data. There may be differences in Secchi depth estimates between measurements carried out from an altitude of a few meters (research vessel) or from a boat (observer a meter or two above the water surface). However, most of the discrepancies between the two data sources seem to come from the fact that the Secchi depth varied very little during R/V Salme measurements while it was varying significantly during the boat measurements.

The results of the study showed that there is strong need in developing the Baltic-Sea-specific C2RCC processor. The current one provides reasonable reflectance results in non-bloom conditions, but fails in cyanobacterial blooms while the IOP and other products do not have correlation with in situ data. On the other hand, there is also strong need in improving the consistency of in situ data used in calibration and validation of satellite data products. Usually, it is assumed that in situ data are the truth against which satellite products are validated. It must be remembered that the in situ data also (even if measured with the same methods, such as chlorophyll *a* analysis in the lab) have errors that are relatively large. We combined reflectance from different sources measured using three different methods and analysis performed in different laboratories. Our study showed that this had also had

an effect on the results. Comparing point measurements with large (300 m) pixel values is problematic in coastal waters and in cyanobacterial blooms where dramatic changes in water properties occur at meter scales. Combining this with the methodological problems and measurement errors of in situ data described above makes improving remote sensing products extremely difficult.

5. Conclusions

Combining the BOA reflectance spectra obtained by means of C2RCC processor with the in situ reflectance spectra shows that the atmospheric correction part of the neural network performs quite well in non-bloom conditions. In the case of dense subsurface blooms and surface scum of cyanobacteria, the atmospheric correction removes the most valuable piece of information—signal at wavelengths longer than 700 nm.

Several empirical algorithms using green to NIR part of spectrum performed relatively well in retrieval of different water quality parameters. This also suggests that the performance of atmospheric correction part of the C2RCC is robust for this part of spectrum.

No correlation between measured and retrieved IOPs was observed. Consequently, there was also no correlation between the retrieved parameters (such as chlorophyll *a*) and in situ data. To a certain degree, this result may have been caused by the suboptimal performance of atmospheric correction at shorter wavelengths, as the neural network uses all spectral bands not just green to NIR part like the empirical algorithms. However, the main problem is that the C2RCC is not trained with sufficient amount of data from the Baltic Sea. Significantly more in situ data from different parts of the Baltic Sea collected during different seasons are needed to train the neural network and produce reasonable IOP estimates for the Baltic Sea.

The data collection and analysis methodology may also need improvement in order to develop robust remote sensing products that perform well in optically complex waters. Horizontal, vertical and temporal variabilities of water properties, especially during cyanobacterial blooms or near river estuaries make it challenging to acquire reliable in situ data. Inter calibration of laboratory methods between different institutions is advisable to ensure validation of satellite products against data with well characterized accuracy.

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Appendix 3

Publication III

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Article

Optical Water Type Guided Approach to Estimate Optical Water Quality Parameters

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Abstract: Currently, water monitoring programs are mainly based on in situ measurements; however, this approach is time-consuming, expensive, and may not reflect the status of the whole water body. The availability of Multispectral Imager (MSI) and Ocean and Land Colour Instrument (OLCI) free data with high spectral, spatial, and temporal resolution has increased the potential of adding remote sensing techniques into monitoring programs, leading to improvement of the quality of monitoring water. This study introduced an optical water type guided approach for boreal regions inland and coastal waters to estimate optical water quality parameters, such as the concentration of chlorophyll-a (Chl-a) and total suspended matter (TSM), the absorption coefficient of coloured dissolved organic matter at a wavelength of 442 nm (aCDOM(442)), and the Secchi disk depth, from hyperspectral, OLCI, and MSI reflectance data. This study was based on data from 51 Estonian and Finnish lakes and from the Baltic Sea coastal area, which altogether were used in 415 in situ measurement stations and covered a wide range of optical water quality parameters (Chl-a: 0.5–215.2 mg·m⁻³; TSM: 0.6–46.0 mg·L⁻¹; aCDOM(442): 0.4–43.7 m⁻¹; and Secchi disk depth: 0.2–12.2 m). For retrieving optical water quality parameters from reflectance spectra, we tested 132 empirical algorithms. The study results describe the best algorithm for each optical water type for each spectral range and for each optical water quality parameter. The correlation was high, from 0.87 up to 0.93, between the in situ measured optical water quality parameters and the parameters predicted by the optical water type guided approach.

Keywords: optical water type; chlorophyll-a; total suspended matter; CDOM; Secchi disk depth; Sentinel-3 OLCI; Sentinel-2 MSI; lakes; Baltic Sea

1. Introduction

Remote sensing offers effective ways to observe spatial and/or temporal variations in water quality, which is vital for the comprehensive assessment and management of water bodies [1]. Currently, water monitoring programs are mainly based on in situ measurements; however, considering that water bodies are dynamic in nature, this method may not reflect the status of the whole water body. Therefore, it is important to implement techniques that allow more effective monitoring of the aquatic environment. However, remote sensing of inland and coastal waters can be challenging as they are independently influenced by different optically significant constituents (OSC)-coloured dissolved organic matter (CDOM), phytoplankton, and total suspended matter (TSM). All of these OSCs shape the spectral characteristics that are measured by the remote sensor.

Phytoplankton consists of single-celled, free-floating, photosynthetic organisms that form the base of the aquatic food web, being an important component of the carbon cycle. Seasonal phytoplankton

blooms are natural processes in the aquatic environment [2]. However, a rise in phytoplankton biomass may also be a sign of eutrophication, which indicates increased nutrient inputs [3,4], all of which, in turn, leads to drastic changes in the aquatic ecosystem (e.g., altered species composition, hypoxia, decreased water transparency, toxins, problems for fishes) [5,6]. The photosynthetic phytoplankton pigment chlorophyll-a (Chl-a) is typically used as a proxy for phytoplankton biomass [7]. Chl-a absorbs strongly in the blue (440–500 nm) and red (650–680 nm) regions of the visible spectrum and reflects in the green (550 nm) [8]. Remote sensing algorithms for the retrieval of Chl-a are based on the ratios of reflectance, such as the blue-green ratio [9], which are empirically related to the Chl-a concentration. However, this is not valid for optically complex waters, where CDOM and TSM also affect the optical properties of water. Several studies have suggested the use of various combinations of near-infrared (NIR) and red band combinations instead [10–12].

TSM is used as an indicator of physical forcing, for instance, wind-driven resuspension, land runoff, as well as dredging operations, which lead to much higher TSM concentrations in the area [13,14]. TSM is divided into suspended particulate organic matter (SPOM) and suspended particulate inorganic matter (SPIM). SPOM contains a mixture of planktonic organisms (e.g., phytoplankton, bacterioplankton, etc.) and non-living organic matter, and the optical properties are similar to those of CDOM [15]. The presence of terrigenous particles in the water often accounts for the bulk of SPIM. SPIM scatters light, whereas the scattering depends on the size and shape of the particles—particles $< 1 \mu\text{m}$ scatter more strongly at shorter wavelengths, while in the case of larger particles, the wavelength dependence is weak [15,16]. This limits the accuracy of algorithms for estimating TSM. The use of red and/or NIR wavelengths is suggested to quantify the SPIM part due to strong water absorption in the NIR wavelengths [17].

CDOM is an optically active fraction of dissolved organic matter [18]. It may have a local origin, for instance, from degradation of phytoplankton cells, or it may be advected from a distant source, for example, from organic-rich rivers. CDOM can be used as a proxy for assessing dissolved organic carbon dynamics, identifying organic pollution in agricultural and urban catchments, and detecting influences of anthropogenic activities (e.g., land-use change) [19]. Light absorption by CDOM tends to be the strongest at shorter wavelengths (350–450 nm) of the electromagnetic spectrum. Absorbance increases exponentially with decreasing wavelengths and diminishes to near-zero in the red wavelength region [20]. Therefore, the water-leaving reflectance at 440 nm is often used to estimate CDOM from remote sensing data [21,22].

Secchi disk depth (ZSD) is a measure of water transparency or of the depth of penetration of visible light in the aquatic environment, which is relevant for primary production [23]. The lower the Secchi disk depth value, the more turbid and less clear the water. Substances that influence the transparency of water include phytoplankton, CDOM, and suspended matter (i.e., OSCs). Therefore, changes in the ZSD also reflect variations in the water properties. Many regional algorithms have been developed to estimate ZSD from remote sensing reflectance. For optically complex waters, different spectral band combinations between blue, green, and red bands are often used [24,25].

The launches of Multispectral Imager (MSI) and Ocean and Land Colour Instrument (OLCI) on board Sentinel-2 and Sentinel-3, respectively, have increased the potential for improved monitoring of water quality. MSI was primarily designed to support land monitoring for Europe's environmental monitoring Copernicus programme, but owing to its high spatial resolution (10, 20, and 60 m), with 13 spectral bands [26], it has opened new opportunities to investigate smaller water bodies [27] and different phenomena in more detail (e.g., filaments and eddies of biological activity) [28,29]. OLCI, on the other hand, is specially designed for water quality monitoring. It is a follow-up of the MERIS (Medium Resolution Imaging Spectrometer) mission, with improved capabilities. It has a 300 m spatial resolution with 21 spectral bands optimised to measure ocean colour over optically complex water bodies [26].

Different approaches have been used to evaluate water quality products from these sensors [30–33]. In the case of optically complex waters, where optical properties are more diverse and can vary over

short spans of time and space, standard remote sensing products often fail [30,34–36], which has led to the development of regionally specific algorithms [37]. However, regional algorithms also do not show consistency in terms of changes in their optical properties [30]. The possible solution could be to use remote sensing algorithms based on the classification of the optical water types (OWTs). For instance, a similar OWT-based solution was also used to interpret data from the first satellite ocean color sensor Coastal Zone Color Scanner (CZCS) [38,39], where the classification of OWTs by Morel and Prieur [40] was used for the separation of water masses. Using remote sensing to classify waters according to their optical properties will help to identify relationships between different OSCs and to understand the biogeochemical processes therein. Several studies have developed optical pre-classification schemes to select regional algorithms for water quality parameters [41–44]. Uudeberg et al. [45] developed an OWT classification based on reflectance spectral features for boreal inland and coastal waters. This classification divides waters into five OWTs dominated by Chl-a, TSM, or CDOM, and the classification is compatible with data from OLCI and MSI. This OWT classification forms the base of this study.

The main aim was to find a solution for boreal region inland and coastal waters to estimate optical water quality parameters from reflectance spectra as an alternative to standard algorithms that do not work in this region. For this, we chose the OWT guided approach and tested various published empirical algorithms to find the best algorithm for every OWT for different spectral ranges for different optical water quality parameters. Our study included optical water quality parameters, such as the concentration of Chl-a and TSM, the absorption coefficient of CDOM at a wavelength of 442 nm ($a_{CDOM(442)}$), the Secchi disk depth; and spectral ranges, such as in situ measured hyperspectral reflectance with 1 nm steps, the OLCI, onboard the Sentinel-3 satellite, bands, and the MSI, onboard the Sentinel-2 satellite, bands. Since there are still many problems associated with the removal of the atmospheric influence from satellite imagery; this work is based on in situ measured reflectance spectra and in situ measured reflectance spectra convolved into OLCI and MSI bands using sensor spectral response functions. Furthermore, the OWT guided approach was later applied to OLCI images to map the OWT guided approach and selected algorithms' strengths and weaknesses.

2. Materials and Methods

2.1. Study Sites and In Situ Dataset

This study was based on data from 415 in situ measurement stations gathered from the boreal region inland and coastal waters from April to September in 2012–2019. Data were collected from 51 different Estonian and Finnish lakes and from three coastal locations in the Baltic Sea (Figure 1). The first area in the Baltic Sea was Pärnu Bay, located on the west coast of Estonia, where the mean depth is 4.7 m (maximum 8 m) and the water is well mixed. Since Pärnu Bay is shallow, open to winds, and has sandy, clayey, and muddy bottom, wind-derived resuspension can lead to quite high and changeable TSM concentrations. The second area is located in the Gulf of Finland region, where the mean depth is 37 m, with a maximum of 123 m (Paldiski Deep), and where the water column is vertically stratified [16]. The area is prone to upwelling and downwelling events in the summer and autumn [46,47]. The third area is located in the Western Gotland Basin close to the coast of Sweden. The Baltic Sea reaches its greatest depth in the Western Gotland Basin, Landsort Deep (459 m), but in our measurement stations, the water depth was up to 30 m. In situ lake data were mainly collected from Estonian lakes (42 lakes), from small lakes, such as Lake Holstre (0.04 km²), to large lakes, such as Lake Peipsi (3555 km²); from lakes with highly transparent water, such as Lake Nohipalo Valgjärv (Secchi disk depth 5 m), to lakes with very brown-water, such as Nohipalo Mustjärv (Secchi disk depth 0.3 m) (Figure 2).

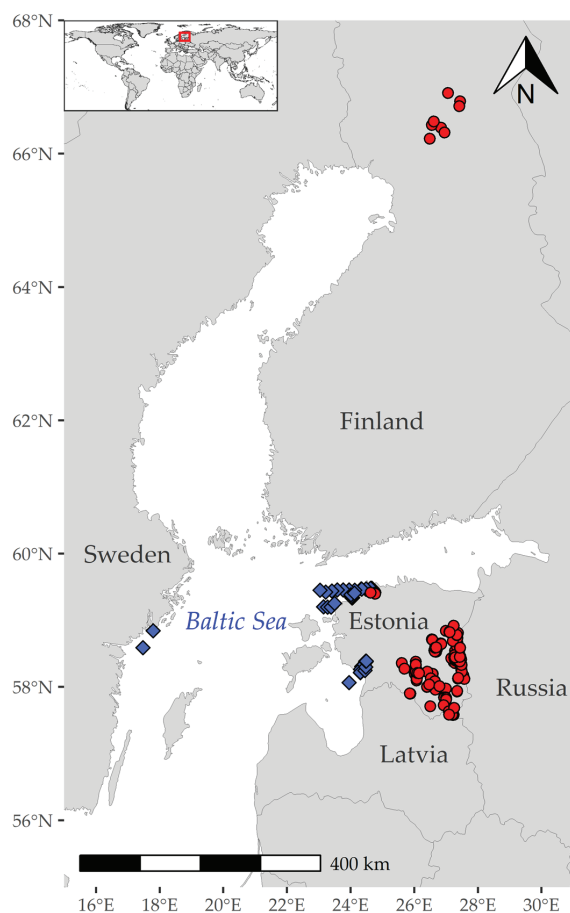


Figure 1. Locations of the in situ measurement stations. Measurement stations of inland waters are marked with red circles and measurement stations of coastal waters with blue diamonds.

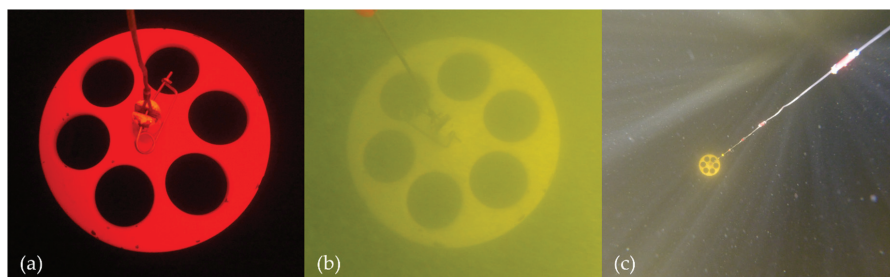


Figure 2. Examples of the colour of water photographed in different Estonian lakes: (a) reddish-brown water in Nohipalo Mustjärv (Secchi disk depth 0.3 m; aCDOM(442) 41.1 m⁻¹); (b) greenish water in Lake Tamula (Secchi disk depth 0.5 m); and (c) highly transparent water in lake Nohipalo Valgjärv (Secchi disk depth 5 m).

The in situ dataset contains data from measurements of water-leaving reflectance ($R(\lambda)$), concentrations of OSC (such as the concentration of Chl-a and TSM, and aCDOM(442)), Secchi

disk depth, and different environment parameters, such as wind speed, waves heights, cloudiness, and sun condition. The Secchi disk depths were measured on the shadowed side of the vessel with a white disk with a 30 cm diameter or with a 20 cm diameter white disk with holes. The wind speed was measured with a handheld mechanical anemometer. The wave height, cloudiness, and sun condition were estimated by visual inspection.

2.1.1. Water-Leaving Reflectance ($R(\lambda)$)

$R(\lambda)$ was measured with TriOS-RAMSES hyperspectral radiometers using two different setups. The first setup was used in 233 in situ measurement stations and the second setup was used on 182 in situ measurement stations.

For the first setup, the above the water system consisted of three TriOS-RAMSES hyperspectral radiometers: two radiance sensors measuring upwelling radiance ($L_t(\lambda)$) and downwelling radiance ($L_{sky}(\lambda)$) in the same azimuthal plane, and one irradiance sensor measuring downwelling irradiance ($E_d(\lambda)$) [48]. The radiance sensor's nadir/zenith angles of 40° were fixed in the frame. The measured spectral range was 350–900 nm. The recording interval was once per 10-second interval. The solar azimuth angle was kept between 90° and 180° and was adjusted manually during measurements. The calculation of $R(\lambda)$ followed the protocol of REVAMP [48] and included the next steps. First, all measured radiance and irradiance spectra were linearly interpolated to a 1 nm step. Secondly, $R(\lambda)$ was calculated as

$$R(\lambda) = \pi \frac{L_t(\lambda) - \rho(w)L_{sky}(\lambda)}{E_d(\lambda)}, \quad (1)$$

where $\rho(w)$ is the sea surface reflectance as function of wind speed (w , $\text{m}\cdot\text{s}^{-1}$) and calculated as $\rho(w) = 0.0256 + 0.00039w + 0.000034w^2$ [48]. Finally, the median $R(\lambda)$ was calculated and used as the representative of the measurement station.

For the second setup, the profiling system consisted of two TriOS-RAMSES hyperspectral radiometers: one irradiance sensor measuring downwelling irradiance ($E_d(\lambda)$) and one radiance sensor measuring upwelling radiance ($L_u(\lambda)$). Measurements were made above the water, below the water surface, and at different depths in the water column. In this study, only above-the-water measurements were used. The measured spectral range was 350–900 nm. At every depth, five recordings were made. The $R(\lambda)$ calculations included three steps. First, all measured spectra were linearly interpolated to a 1 nm step. Secondly, $R(\lambda)$ was calculated as

$$R(\lambda) = \pi \frac{L_u(\lambda)}{E_d(\lambda)}. \quad (2)$$

Finally, the median $R(\lambda)$ was calculated and used as the representative of the in situ measurement station.

To study the implementation capacity of the OWT guided approach for retrieving water quality parameters, the $R(\lambda)$ spectra representing the in situ measurement stations were also convolved into MSI and OLCI bands using spectral response functions (SRFs) of satellite sensor bands and calculated according to Uudeberg et al. [45]. The SRFs for the MSI and OLCI were taken from [49] and [50], respectively.

2.1.2. Analysis of Water Samples

Water samples for measurements of the concentrations of OSC were collected from the water surface (up to 0.5 m depth) according to ISO 5667-3 [51] and analysed according to ISO 10260 [52]. After the samples were filtered through Whatman GF/F filters that retain fine particles down to $0.7 \mu\text{m}$, and the pigments were extracted with 5 ml of 96% ethanol, the concentrations of Chl-a were measured spectrophotometrically with a Hitachi U-3010 spectrophotometer and calculated according to Jeffrey and Humphrey [53]. After the samples were filtered through a filter with a pore size of $0.2 \mu\text{m}$, CDOM was measured in a 5 cm optical cuvette against distilled water with a Hitachi

U-3010 spectrophotometer and calculated according to Lindell et al. [54]. The concentrations of TSM were measured gravimetrically after the samples were filtered through pre-washed, pre-ashed, and pre-weighed Whatman GF/F filters.

The water samples collected during July 2018 in the Gulf of Finland had some differences in analysis. For TSM, a fixed amount of water (0.750 L) was filtered through pre-combusted and pre-weighed Millipore membrane filters with a pore size of 0.45 μm . For Chl-a, the Thermo Helios γ spectrophotometer was used and the concentrations of Chl-a were calculated according to Lorenzen [55].

2.2. Classification of Optical Water Types (OWTs)

The classification of OWTs introduced by Uudeberg et al. [45] was used to determine the OWT. The classification divides the boreal region inland and coastal waters into five OWTs, each linked to the specific bio-optical condition in order to reflect the dominance of group OSC concentrations. The Clear OWT corresponds to water with the highest transparency and lowest OSC concentrations. In the Moderate OWT, the concentrations of OSC have risen, but none of them dominate. In the Turbid OWT, the TSM is the dominant OSC and the $R(\lambda)$ values are the highest. In the Very Turbid OWT, Chl-a is the dominant OSC. The strong Chl-a peak, which is associated with blooms, occur in the red part of spectra. The Brown OWT water is dominated by CDOM.

The OWT classification is based on reflectance spectra key features, such as the wavelength of the maximum, the slopes, and the amplitude of $R(\lambda)$. The maximum likelihood of individual spectra to reference spectra using a combination of spectral correlation similarity and modified spectral angle similarity was used to determine the OWT for measured $R(\lambda)$ spectra. The OWTs were assigned on each in situ measurement of $R(\lambda)$ and the in situ measurements of $R(\lambda)$ convolved into MSI and OLCI sensor bands.

2.3. Algorithms for Retrieving Water Quality Parameters

OWT guided approach was used for finding models for retrieving water quality parameters, such as the concentration of Chl-a, the concentration of TSM, the aCDOM(442), and Secchi disk depth, from $R(\lambda)$ spectra. Since the inland and coastal waters are optically complex and cover large variations of OSC concentrations, the OWT guided approach allows to find the best model for different bio-optical conditions. In this study, we used 132 previously published algorithms from manuscripts that were available for us, including 60 for Chl-a, 39 for TSM, 21 for CDOM, and 12 for Secchi disk depth. Details of used algorithms are shown in Appendix A Table A1.

Repeated K-fold Cross-validation [56] was the statistical method to build and select the model using published algorithms for optical water quality parameter and the R package caret [57] by Max Kuhn was used for implementation. The Repeated K-fold Cross-validation contains following steps: (1) the data are divided randomly into k folds of equal size; (2) the k-1 folds are used for the model training; (3) the hold-out fold is used for the model validation; and (4) steps (1)–(3) are repeated n times. Finally, based on a selected statistical metric, the model with the best average score is assigned as the final model. Ten folds, ten repeats, and the root mean squared error as metrics were used in this study.

The ranking system used a combination of scaled and threshold-based statistical metrics to select the model for retrieving the optical water quality parameter from $R(\lambda)$ per OWTs. Statistical metrics, such as RMSE, RMSLE, MAE, MAPE, and BIAS, were scaled from 0 (maximum value) to 1 (minimum value); the R^2 was scaled from 0 (minimum value) to 1 (maximum value); and for the p -value, the thresholds were used as 1 for p -value under 0.001, 0.5 for p -value between 0.001 and 0.05, and 0, when p -value was over 0.05. Finally, all values were summed up and the model with the highest score was selected as the model for future retrievals. The following statistical metrics were used in this study and they are described in detail in R package Metrics [58].

- RMSE (Root Mean Squared Error)—represents the average difference between the measured values and the values predicted by the model. This metric indicates the fit of the model to the data. The lower the RMSE, the better the model.

- RMSLE (Root Mean Squared Logarithmic Error)—represents the average difference between the log-transformed measured values and the log-transformed values predicted by the model. This metric does not penalize big differences when both the predicted and the measured values are big numbers. This is useful when the measurement values are in a wide range. The lower the RMSLE, the better the model.
- MAE (Mean Absolute Error)—represents the average absolute difference between the measured and predicted model values. This metric measures the model prediction error and is robust against the effect of outliers. The lower the MAE, the better the model.
- MAPE (Mean Absolute Percentage Error)—measures the average absolute percentage error from the measured value and the values predicted by the model divided by the measured value. This metrics shows the model prediction accuracy. The lower the MAPE, the better the model.
- R^2 —represents the squared correlation between the measured values and the predicted values by the model. This metric shows the percentage of variance explained by the model. The closer to 1 the R^2 , the better the model.
- BIAS—represents the average amount by which the measured value is greater than predicted. The lower the bias, the better the model.
- p -value—tests the null hypothesis and shows if the model is statistically significant or not. A low p -value (<0.05) suggests that the model is statistically significant.

To find the best solutions also for the MSI and OLCI sensors $R(\lambda)$ spectral range, all calculations were made separately on $R(\lambda)$ spectra range with a 1 nm step, $R(\lambda)$ spectra convolved into OLCI sensor bands, and $R(\lambda)$ spectra convolved into MSI sensor bands. Since the OLCI and MSI band locations were sometimes different than the band locations described in algorithms, the closest possible band was selected in case of OLCI or MSI were lacking exact bands.

2.4. Satellite Dataset

To assess the ability of the OWT guided approach to obtain optical water quality parameters from satellite data, the full resolution Level-1 images acquired in 2018 and 2019 by OLCI, onboard the Sentinel-3 satellite, were used. Level-1 images were processed with the Case-2 Regional CoastColour (C2RCC) atmospheric correction processor v1.15, based on the previous study's recommendation [45]. Image primary processing, such as subsetting the region of interest and atmospheric correction processing, and downloading was done using the ESTHub Processing Platform, which is the Estonian Land Board's national mirror site for Copernicus satellite data and processing [59]. After that, the OWT were determined for every pixel of the satellite images. Finally, the OWT-based models described in Tables 2–5 were used to find the optical water quality parameters.

3. Results

3.1. Description of In Situ Dataset

Our in situ dataset from 415 in situ measurement stations covers wide ranges of the OSC concentrations and Secchi disk depth. However, datasets of all four parameters are significantly non-Gaussian. Table 1 shows the skewness of Chl-a and CDOM are 4.3 and 4.1, respectively. This indicates that their distributions are not symmetrical and are skewed strongly towards higher values. Moreover, Table 1 allows us to assume based on the high maximum and median values of the Chl-a, CDOM, and Secchi disk depth, that the dataset includes also measurements from extreme optical conditions for the boreal region. For example, the high transparency (Secchi disk depth up to 12.2 m) was measured in July in the Gulf of Finland during an upwelling event. Therefore, water masses with different properties (low OSC concentrations, high transparencies, and cold temperatures ($\sim 4^\circ\text{C}$)) were present compared to the usual situations. High CDOM values around 40 m^{-1} were measured multiple times through the vegetation period in dark-water small Estonian lakes. Chl-a values of $215.2\text{ mg}\cdot\text{m}^{-3}$

and $168.4 \text{ mg}\cdot\text{m}^{-3}$ were captured during the blooming situation in large Lake Peipsi. However, in the dataset, there is a lack of measurement stations where the TSM was dominated by mineral particles. For instance, the median proportion of suspended particulate organic matter in TSM is 76%.

Table 1. Descriptive statistics of the measured in situ optical water quality parameters.

Parameter	No. of Stations	Mean	Median	Range	Skewness
Chl-a ¹	415	19.0	13.6	0.5–215.2	4.3
TSM ²	415	7.6	5.7	0.6–46.0	1.9
aCDOM(442) ³	415	3.9	2.0	0.4–43.7	4.1
Secchi depth, m	411	1.8	1.4	0.2–12.2	2.1

¹ Concentration of chlorophyll a, $\text{mg}\cdot\text{m}^{-3}$. ² Concentration of total suspended matter, $\text{mg}\cdot\text{L}^{-1}$. ³ Absorption coefficient of coloured dissolved organic matter at a wavelength of 442 nm, m^{-1} .

Figure 3 shows the in situ measured $R(\lambda)$ at 415 stations classified into various OWTs, and Figure 4 shows the range of the variations of the OSC concentrations and Secchi disk depth for OWTs. The OWT for each in situ measured $R(\lambda)$ was determined by the maximum likelihood of the individual spectrum to type averages. The Clear OWT was assigned to the $R(\lambda)$ of 100 measurement stations. The maxima of $R(\lambda)$ were between 540 and 580 nm and the mean maximum value was 0.012. Waters were the most transparent (maximum Secchi disk depth 12.2 m) and with the lowest OSC concentrations. However, in Figure 3, one Clear OWT station has a too high maximum value at 550 nm (0.06) compared to the rest of the Clear OWT spectra, but inspection of the station OSC concentration does not confirm a misclassification. The Moderate OWT was the most frequent in our dataset, with the $R(\lambda)$ of 124 stations being assigned to this OWT. The Turbid OWT was assigned to the $R(\lambda)$ of 98 measurement stations. This OWT is dominated by TSM and the highest TSM values were expected to be in this OWT. However, in this dataset, the highest TSM values were in stations assigned to the Very Turbid OWT. TSM is mainly dominated by SPOM in our dataset, and especially in these high TSM valued Very Turbid OWT stations (88% of TSM was SPOM). These waters are generally dominated by Chl-a, and stations are classified correctly. The Very Turbid OWT was assigned to the $R(\lambda)$ of 51 measurement stations, which were dominated by Chl-a. The Brown OWT was assigned to the $R(\lambda)$ of 42 stations. These stations had very low $R(\lambda)$ values (median value 0.003), with maxima in the red part of the spectrum, and very high aCDOM(442) values with a median at 13.6 m^{-1} .

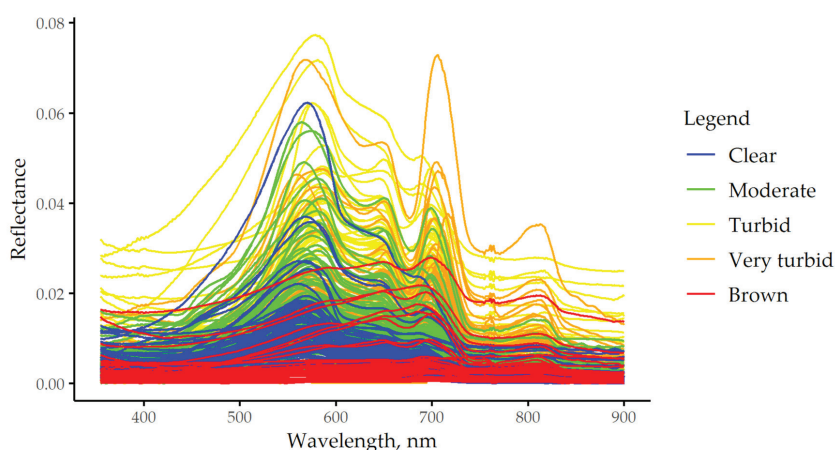


Figure 3. In situ measured $R(\lambda)$ classified into various optical water types by the maximum likelihood of individual spectra to type averages, using the spectral correlation similarity and modified spectral angle similarity.

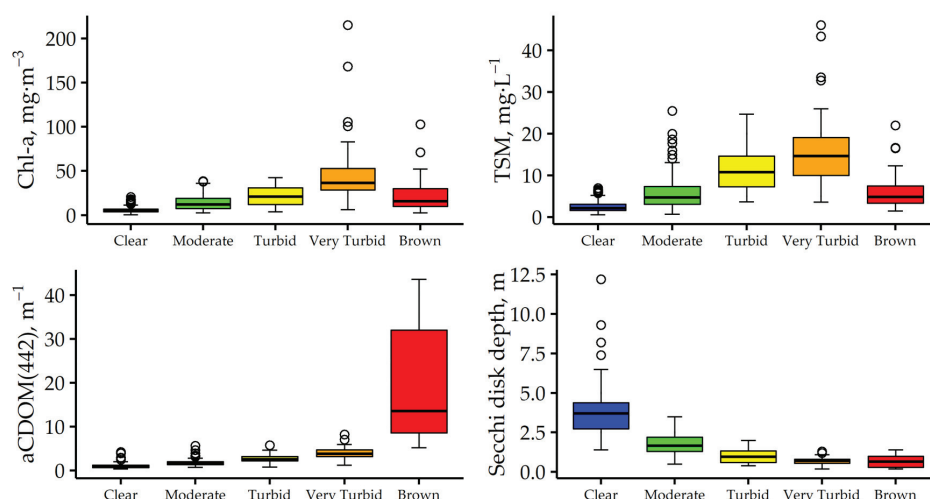


Figure 4. The range of the variation of the concentrations of optically significant constituents, such as chlorophyll-a (Chl-a), total suspended matter (TSM), absorption coefficient of coloured dissolved organic matter at a wavelength of 442 nm (aCDOM(442)), and Secchi disk depth by optical water types.

The accuracies of OWT estimations, based on in situ measurements of $R(\lambda)$ convolved into MSI and OLCI sensor bands using sensor-specific SRFs, were 96% for OLCI and 91% for MSI. As the goal was to use the OWT guided approach to retrieve optical water quality parameters, it was important to understand the capability to assign the same OWT on in situ measurements of $R(\lambda)$ regardless of spectral scale (Ramses with 1 nm step resolution, and distinct bands for OLCI and MSI). Confusion matrices were constructed between the OWTs assigned on in situ measurements of $R(\lambda)$ (set as the true OWT value) and those which were assigned based on in situ measurements of $R(\lambda)$ convolved into various sensor bands (set as the predicted OWT value). As shown in Figure 5, the OLCI confusion matrix demonstrates a strong distinction for Clear and Brown OWTs (100% correct assignment) and the highest rate of misclassification in Very Turbid OWT, with 8% of spectra being misclassified as Brown or Turbid OWT. The MSI confusion matrix illustrates a strong distinction for Very Turbid, and Brown OWTs (100% and 98% correct assignment respectively); however, 16% of Moderate OWT spectra were misclassified.

3.2. Predictive Models for Concentration of Chlorophyll-a (Chl-a)

The best models to retrieve the concentration of Chl-a from the $R(\lambda)$ spectra for each OWT and each spectral ranges, such as Ramses with 1 nm step, and OLCI and MSI bands, are defined in Table 2. We tested 60 published empirical algorithms to retrieve the Chl-a values and the best ones for all the cases were chosen based on our model ranking system described in paragraph 2.3. As a result, the four best models for each OWT and each spectral range are shown on radar plots in Appendix B Figure A1. The linear regression models showed a better performance for all the cases.

For the Clear OWT, in the case of Ramses and OLCI, the model CHL69 using the Gitelson et al. [60] algorithm had the highest score, and, for MSI, the model using the MERIS maximum chlorophyll index by Gower et al. [61] was the most suitable. The model CHL97 using the Mishra and Mishra [62] algorithm was the best for Moderate OWT for Ramses and in Very Turbid OWT, for all the different spectral ranges. For Turbid OWT, all three spectral ranges were described best with different models with different approaches: for Ramses, the model using the Kutser et al. [63] algorithm based on two-band ratio approach; for OLCI, the model using the Gitelson et al. [64] algorithm based on a three-band approach, and for MSI, the model using the Zimba and Gitelson [11] four-band approach.

For Brown OWT, retrieving the concentration of Chl-a from $R(\lambda)$ was the most difficult and the coefficient of determination suggested that the regression model explained about 40% of the variance observed in the in situ measured data. However, all models were statistically significant based on the p -values.

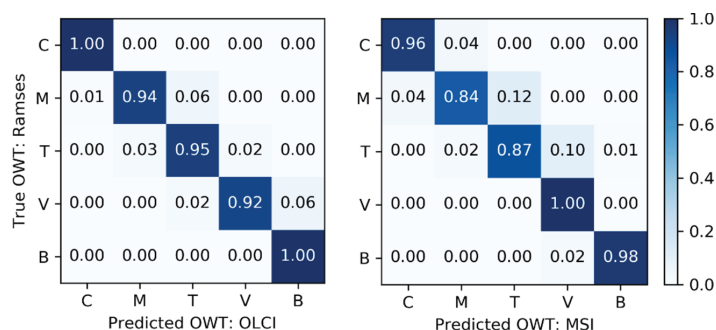


Figure 5. The accuracy of the optical water type (OWT) assignment using in situ measurements of $R(\lambda)$ convolved into Ocean and Land Colour Instrument (OLCI) and Multispectral Imager (MSI) bands by normalized confusion matrices. The rows show the true OWTs determined from in situ measurements of $R(\lambda)$ using Ramses, and the columns show the predicted OWTs determined from the convolved $R(\lambda)$. The diagonal elements represent the situation where the predicted OWT is the same as the true OWT (i.e., the correct classification).

The correlations shown in Figure 6, between the concentration of Chl-a predicted using OWT based models and in situ measured concentration of Chl-a, were strong, such as 0.93 for Ramses and OLCI, and 0.92 for MSI. Overall, the predicted concentrations of Chl-a were the most accurate compared to other optical water quality parameters explored in this study.

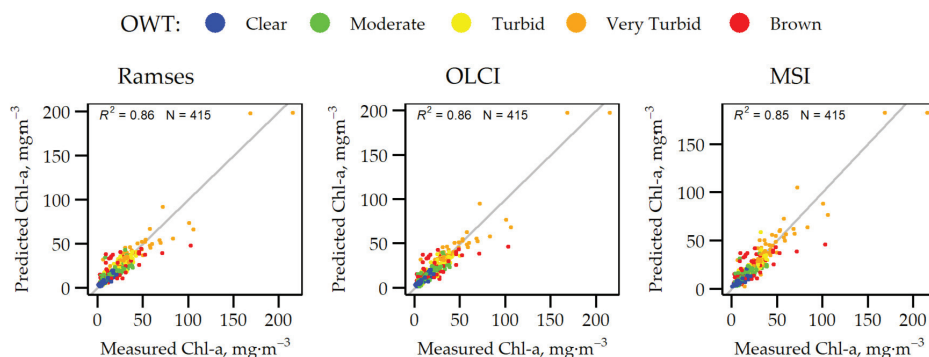


Figure 6. Comparison of concentrations of Chl-a estimated from in situ measured $R(\lambda)$ spectra using the optical water type (OWT) guided approach and in situ measured concentrations of Chl-a for different spectral scales: (left to right) Ramses with 1 nm resolution, OLCI, and MSI. OWTs are indicated by colours and the line shows 1:1 relationship.

Table 2. The best published chlorophyll-a (Chl-a) predictive models tested in this study for each optical water types (OWT) and for sensors with different spectral scales. Descriptions of the algorithms used for these models are found in Table A1, and the acronyms and abbreviations are in Table A2. The band central wavelength is used to mark the Ocean and Land Colour Instrument (OLCI) and Multispectral Imager (MSI) models bands.

OWT	Model	Model Formula	ST ¹	R ²	p-value
Ramses					
Clear	CHL69	$Chla = 5956.0 \cdot \left(\frac{R709 - \frac{R665 + R754}{2}}{R705 - R665} \right) + 3.84$	LR	0.79	< 2.2E-16
Moderate	CHL97	$Chla = -84.42 \cdot \left(\left(\frac{1}{R705} - \frac{1}{R665} \right) / \left(\frac{1}{R705} + \frac{1}{R665} \right) \right) + 18.69$	LR	0.62	< 2.2E-16
Turbid	CHL88	$Chla = 55.85 \cdot \left(\frac{R702}{R674} \right) - 43.08$	LR	0.79	< 2.2E-16
Very Turbid	CHL97	$Chla = -180.6 \cdot \left(\left(\frac{1}{R705} - \frac{1}{R665} \right) / \left(\frac{1}{R705} + \frac{1}{R665} \right) \right) + 19.89$	LR	0.88	< 2.2E-16
Brown	CHL67	$Chla = 46.56 \cdot \left(\frac{R748}{R667} \right) - 8.310$	LR	0.41	4.3E-06
OLCI					
Clear	CHL69	$Chla = 6097.2 \cdot \left(\frac{R708.75 - \frac{R665 + R753.75}{2}}{R708.75} \right) + 3.998$	LR	0.78	< 2.2E-16
Moderate	CHL65	$Chla = -33.91 \cdot \left(\frac{R673.75}{R708.75} \right) + 54.07$	LR	0.67	< 2.2E-16
Turbid	CHL98	$Chla = 177.4 \cdot \left(\frac{1}{\frac{R673.75}{R708.75} - \frac{1}{R753.75}} \right) \cdot R753.75 + 20.68$	LR	0.79	< 2.2E-16
Very Turbid	CHL97	$Chla = -173.6 \cdot \left(\left(\frac{1}{R708.75} - \frac{1}{R665} \right) / \left(\frac{1}{R708.75} + \frac{1}{R665} \right) \right) + 25.6$	LR	0.89	< 2.2E-16
Brown	CHL67	$Chla = 42.96 \cdot \left(\frac{R753.75}{R665} \right) - 5.470$	LR	0.38	5.9E-06
MSI					
Clear	CHL101	$Chla = 4367.1 \cdot \left(\frac{R705 - R665 - \frac{705 - 665}{740 - 665} \cdot (R740 - R665)}{R705} \right) + 2.658$	LR	0.61	< 2.2E-16
Moderate	CHL65	$Chla = -40.83 \cdot \left(\frac{R665}{R705} \right) + 61.71$	LR	0.60	< 2.2E-16
Turbid	CHL57	$Chla = -184.1 \cdot \left(\frac{R740}{R705} - \frac{R740}{R665} \right) + 21.20$	LR	0.63	< 2.2E-16
Very Turbid	CHL65	$Chla = -171.4 \cdot \left(\frac{R665}{R705} \right) + 183.6$	LR	0.89	< 2.2E-16
Brown	CHL67	$Chla = 46.98 \cdot \left(\frac{R740}{R665} \right) - 9.360$	LR	0.40	6.0E-06

¹ Statistical technique.

3.3. Predictive Models for Concentration of Total Suspended Matter (TSM)

The best models to retrieve the concentrations of TSM from $R(\lambda)$ spectra for each OWT and for each spectral range are defined in Table 3. We tested 39 published empirical algorithms to retrieve the concentrations of TSM. The model TSM18 using the Kutser et al. [65] algorithm based on the reflectance spectra peak at 810 nm was the most well represented based on our models ranking system results. This model suited well for the MSI sensor, where it had the highest score for Turbid, Very Turbid, and Brown OWTs and according to Figure A2, for the Moderate OWT, it had the second place due to its low bias contribution. Model TSM18 had high scores for Ramses and the OLCI spectral scale for Turbid, Very Turbid, and Brown OWTs. For the Clear OWT, the model TSM39 using Zhang et al. [66] developed log-transformed multiple linear regression algorithm, based on a combination of 488, 555, and 645 nm information, was the best for all sensors. The Moderate OWT had the lowest coefficient of determination for all the spectral ranges from all the OWTs; however, all models were statistically significant based on p -values.

The correlations between concentrations of TSM predicted using OWT based models and in situ measured concentrations of TSM values were strong: 0.87, 0.89, 0.88 for Ramses, OLCI, and MSI respectively. However, Figure 7 shows that model tends to underestimate strongly points with high TSM values (from 15 to 25 mg·L⁻¹), present in Moderate OWT.

3.4. Predictive Models for Absorption Coefficient of Coloured Dissolved Organic Matter (CDOM)

The best models to retrieve the aCDOM(442) from the $R(\lambda)$ spectra for each OWT and for each spectral range, are defined in Table 4. We tested 21 published empirical algorithms to retrieve the CDOM values. The power regression models (referred also as a log–log regression model) of the reflectance ratio showed better performance for all the spectral ranges in Clear, Moderate, and Turbid OWTs. For instance, the reflectance ratio 665/560 nm described by Menken et al. [67] was the best for OLCI and MSI; however, for Ramses, the model using the ratio 560/660 nm had the highest score. For the Very turbid OWT, the linear regression model CDOM119, using the Ammenberg et al. [68]

algorithm, was the best for all spectral ranges. Furthermore, this model received high scores also in Clear, Moderate, and Turbid OWTs for OLCI and MSI, as shown in Figure A3. For the Brown OWT, the log-transformed multiple linear regression models had the best performance; however, this time the model for MSI used different reflectances compared to other spectral ranges. The *p*-value showed that all models were statistically significant, but only the Clear OWT coefficient of determination suggested that the regression model explained 74% of the variance observed in the in situ measured data.

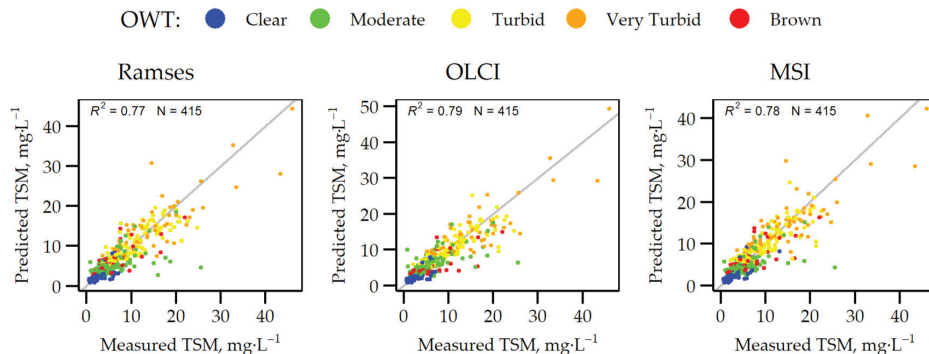


Figure 7. Comparison of concentrations of TSM estimated from in situ measured reflectance spectra using the optical water type (OWT) guided approach and in situ measured concentrations of TSM for sensors with different spectral scales: (from left) Ramses with 1 nm resolution, OLCI, and MSI. OWTs are indicated by colours and the line shows 1:1 relationship.

Table 3. The best published total suspended matter (TSM) predictive models tested in this study for each optical water type (OWT) and for sensors with different spectral scales. Descriptions of the algorithms used for these models are found in Table A1, and acronyms and abbreviations, in Table A2. The band central wavelength is used to mark the Ocean and Land Colour Instrument (OLCI) and Multispectral Imager (MSI) models bands.

OWT	Model	Model Formula	ST ¹	R ²	<i>p</i> -value
Ramses					
Clear	TSM39	$\log TSM = -30.20 \cdot R_{555} + 74.14 \cdot R_{645} - 0.991 \cdot \frac{R_{488}}{R_{555}} + 0.784$	LT-MLR	0.47	5.7E-13
Moderate	TSM38	$\log TSM = 0.264 \cdot \log R_{555} + 14.71 \cdot R_{645} - 0.189 \cdot \log \frac{R_{488}}{R_{555}} + 0.941$	LT-MLR	0.36	1.5E-11
Turbid	TSM20	$\ln TSM = 0.685 \cdot \ln \frac{R_{620} \cdot R_{681}}{R_{510}} + 4.852$	LLR	0.69	< 2.2E-16
Very Turbid	TSM18	$TSM = 3748.6 \cdot \left(R_{810} - \frac{R_{770} + R_{840}}{2} \right) + 5.515$	LR	0.68	9.8E-14
Brown	TSM18	$TSM = 5673.9 \cdot \left(R_{810} - \frac{R_{770} + R_{840}}{2} \right) + 2.178$	LR	0.61	8.4E-10
OLCI					
Clear	TSM39	$\log TSM = -24.36 \cdot R_{560} + 80.66 \cdot R_{665} - 1.096 \cdot \frac{R_{490}}{R_{560}} + 0.840$	LT-MLR	0.47	3.5E-13
Moderate	TSM18	$TSM = -8090.1 \cdot \left(R_{865} - \frac{R_{778.75} + R_{865}}{2} \right) + 1.825$	LR	0.45	< 2.2E-16
Turbid	TSM18	$TSM = -7664.9 \cdot \left(R_{865} - \frac{R_{778.75} + R_{865}}{2} \right) + 3.250$	LR	0.69	< 2.2E-16
Very Turbid	TSM38	$\log TSM = -0.249 \cdot \log R_{560} + 26.20 \cdot R_{665} - 0.483 \cdot \log \frac{R_{490}}{R_{560}} + 0.095$	LLR	0.60	4.0E-09
Brown	TSM31	$\ln TSM = 311.8 \cdot \left(R_{708.75} - \frac{R_{753.75} + R_{665}}{2} \right) + 1.165$	LT-LR	0.49	2.0E-07
MSI					
Clear	TSM39	$\log TSM = -24.0 \cdot R_{560} + 79.02 \cdot R_{665} - 1.152 \cdot \frac{R_{490}}{R_{560}} + 0.892$	LT-MLR	0.49	4.0E-14
Moderate	TSM38	$\log TSM = 0.279 \cdot \log R_{560} + 16.24 \cdot R_{665} - 0.215 \cdot \log \frac{R_{490}}{R_{560}} + 0.958$	LT-MLR	0.36	3.4E-10
Turbid	TSM18	$TSM = 7037.6 \cdot \left(R_{783} - \frac{R_{783} + R_{865}}{2} \right) + 3.464$	LR	0.64	< 2.2E-16
Very Turbid	TSM18	$TSM = 5416.1 \cdot \left(R_{783} - \frac{R_{783} + R_{865}}{2} \right) + 6.259$	LR	0.68	< 2.2E-16
Brown	TSM18	$TSM = 7573.5 \cdot \left(R_{783} - \frac{R_{783} + R_{865}}{2} \right) + 2.748$	LR	0.54	1.8E-08

¹ Statistical technique.

The correlations between the predicted aCDOM(442), using OWT based models, and the in situ measured aCDOM(442) were strong, 0.88 for Ramses and 0.87 for both OLCI and MSI. Still, as shown in

Figure 8, the capability to estimate the Brown OWT high CDOM values over 20 m^{-1} was non-existent and needs future investigation.

Table 4. The best published coloured dissolved organic matter (CDOM) predictive models tested in this study for each optical water type (OWT) and for sensors with different spectral scales. Descriptions of the algorithms used for these models are found in Table A1, and the acronyms and abbreviations, in Table A2. The band central wavelength is used to mark the Ocean and Land Colour Instrument (OLCI) and Multispectral Imager (MSI) models bands.

OWT	Model	Model Formula	ST ¹	R ²	p-value
Ramses					
Clear	CDOM131	$\ln \text{CDOM} = -1.4124 \cdot \ln\left(\frac{R_{560}}{R_{660}}\right) + 1.042$	LLR	0.74	< 2.2E-16
Moderate	CDOM124	$\ln \text{CDOM} = -1.470 \cdot \ln\left(\frac{R_{570}}{R_{655}}\right) + 1.111$	LLR	0.36	1.4E-13
Turbid	CDOM124	$\ln \text{CDOM} = -2.187 \cdot \ln\left(\frac{R_{570}}{R_{655}}\right) + 1.225$	LLR	0.45	4.2E-14
Very Turbid	CDOM119	$\text{CDOM} = 3.063 \cdot \frac{R_{664}}{R_{550}} + 1.096$	LR	0.42	2.3E-07
Brown	CDOM117	$\ln \text{CDOM} = -107.8 \cdot R_{485} - 0.245 \cdot \frac{R_{485}}{R_{830}} + 3.371$	LT-MLR	0.38	8.1E-05
OLCI					
Clear	CDOM122	$\ln \text{CDOM} = 1.352 \cdot \ln\left(\frac{R_{665}}{R_{560}}\right) + 1.070$	LLR	0.74	< 2.2E-16
Moderate	CDOM122	$\ln \text{CDOM} = 1.108 \cdot \ln\left(\frac{R_{665}}{R_{560}}\right) + 1.070$	LLR	0.33	7.1E-12
Turbid	CDOM122	$\ln \text{CDOM} = 1.490 \cdot \ln\left(\frac{R_{665}}{R_{560}}\right) + 1.265$	LLR	0.32	6.8E-10
Very Turbid	CDOM119	$\text{CDOM} = 3.128 \cdot \frac{R_{665}}{R_{560}} + 1.266$	LR	0.38	2.3E-06
Brown	CDOM117	$\ln \text{CDOM} = -127.6 \cdot R_{485} - 0.140 \cdot \frac{R_{485}}{R_{830}} + 3.377$	LT-MLR	0.41	1.6E-05
MSI					
Clear	CDOM122	$\ln \text{CDOM} = 1.429 \cdot \ln\left(\frac{R_{665}}{R_{560}}\right) + 1.059$	LLR	0.74	< 2.2E-16
Moderate	CDOM122	$\ln \text{CDOM} = 1.330 \cdot \ln\left(\frac{R_{665}}{R_{560}}\right) + 1.086$	LLR	0.42	1.6E-14
Turbid	CDOM122	$\ln \text{CDOM} = 1.338 \cdot \ln\left(\frac{R_{665}}{R_{560}}\right) + 1.151$	LLR	0.31	1.9E-09
Very Turbid	CDOM119	$\text{CDOM} = 3.292 \cdot \frac{R_{665}}{R_{560}} + 0.947$	LR	0.39	8.7E-08
Brown	CDOM133	$\ln \text{CDOM} = -62.93 \cdot R_{665} - 0.020 \cdot \frac{R_{560}}{R_{490}} + 3.107$	LT-MLR	0.41	2.2E-05

¹ Statistical technique.

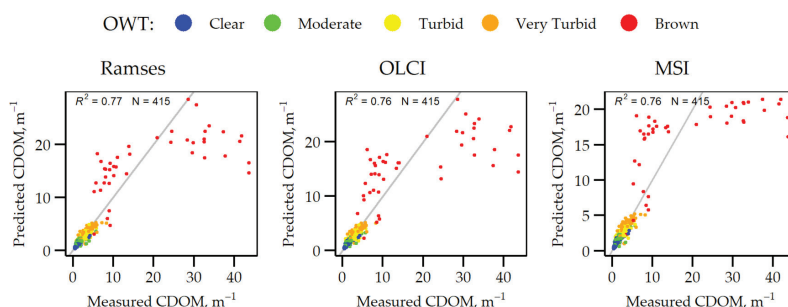


Figure 8. Comparison of the absorption coefficients of coloured dissolved organic matter (CDOM) at a wavelength of 442 nm estimated from the in situ measured reflectance spectra using the optical water type (OWT) guided approach and in situ measured absorption coefficients of CDOM at a wavelength of 442 nm, for sensors with different spectral scales: (from left) Ramses with 1 nm resolution, OLCI, and MSI. OWTs are indicated by colours and the line shows a 1:1 relationship.

3.5. Predictive Models for Secchi Disk Depth

The best models to retrieve the Secchi disk depth value from $R(\lambda)$ spectra for each OWT and for each sensor with different spectral ranges are defined in Table 5. We tested 12 published empirical algorithms to retrieve the Secchi disk depth. The model ZSD104, using the Kloiber et al. [69] algorithm based on log-transformed multiple regression of form 485/660 nm ratio and the additional 485 nm, had the best performance based on our ranking system. In all spectral ranges, the ZSD104 model was the best for Clear, Moderate, and Turbid OWTs and was also in the top four models for Very Turbid and

Brown OWTs, as shown in Figure A4. For Very Turbid OWT, the model ZSD112 using Wu et al. [70] algorithm, based on multiple linear regression of five variables, had the highest score for all spectral ranges. For the Brown OWT, retrieving the Secchi disk depth from $R(\lambda)$ was the most difficult and the highest correlation of all tested models was with ZSD109 using Hellweger et al. [71] algorithm, based on the reflectance at 660 nm. However, the coefficient of determination was around 0.28, but a p -value lower than 0.0005 shows that the model is still statistically significant.

Correlations between the Secchi disk depth predicted using OWT based models and the in situ measured Secchi disk depth values were strong, 0.91 for all the tested spectral ranges. However, as shown in Figure 9, some higher Clear OWT Secchi disk depth estimations from the $R(\lambda)$ spectra had a lower accuracy. These in situ measurements were made during an upwelling event in the Gulf of Finland.

Table 5. The best Secchi disk depth predictive models using published algorithms tested in this study for each optical water types (OWT) and for sensors with different spectral scales. Descriptions of the algorithms used for building models are found in Table A1, and the acronyms and abbreviations, in Table A2. The band central wavelength is used to mark the Ocean and Land Colour Instrument (OLCI) and Multispectral Imager (MSI) models bands.

OWT	Model	Model Formula	ST ¹	R ²	p-value
Ramses					
Clear	ZSD104	$\ln SDD = 0.617 \cdot \frac{R_{485}}{R_{660}} - 43.58 \cdot R_{485} + 0.759$	LT-MLR	0.60	< 2.2E-16
Moderate	ZSD104	$\ln SDD = 1.685 \cdot \frac{R_{485}}{R_{660}} - 63.01 \cdot R_{485} - 0.265$	LT-MLR	0.64	< 2.2E-16
Turbid	ZSD104	$\ln SDD = 2.98 \cdot \frac{R_{485}}{R_{660}} - 41.32 \cdot R_{485} - 1.294$	LT-MLR	0.74	< 2.2E-16
Very Turbid	ZSD112	$SDD = -5.63e^{-07} \cdot \ln \frac{R_{555}}{R_{488}} - 0.018 \cdot \frac{R_{645} + R_{858}}{R_{469}} - 15.57 \cdot R_{555} + 1.07$	MLR	0.48	9.6E-07
Brown	ZSD109	$\ln SDD = 0.268 \cdot \ln R_{660} + 1.024$	LLR	0.27	0.0005
OLCI					
Clear	ZSD104	$\ln SDD = 0.573 \cdot \frac{R_{490}}{R_{665}} - 42.89 \cdot R_{490} + 0.742$	LT-MLR	0.62	< 2.2E-16
Moderate	ZSD104	$\ln SDD = 1.801 \cdot \frac{R_{490}}{R_{665}} - 60.42 \cdot R_{490} - 0.510$	LT-MLR	0.65	< 2.2E-16
Turbid	ZSD104	$\ln SDD = 2.960 \cdot \frac{R_{490}}{R_{665}} - 39.95 \cdot R_{490} - 1.451$	LT-MLR	0.69	< 2.2E-16
Very Turbid	ZSD112	$SDD = -7.03e^{-06} \cdot \ln \frac{R_{560}}{R_{490}} - 0.027 \cdot \frac{R_{645} + R_{858}}{R_{469}} - 14.63 \cdot R_{555} + 1.08$	MLR	0.48	1.6E-06
Brown	ZSD109	$\ln SDD = 0.269 \cdot \ln R_{665} + 1.037$	LLR	0.28	0.0003
MSI					
Clear	ZSD104	$\ln SDD = 0.602 \cdot \frac{R_{490}}{R_{665}} - 45.09 \cdot R_{490} + 0.728$	LT-MLR	0.64	< 2.2E-16
Moderate	ZSD104	$\ln SDD = 1.821 \cdot \frac{R_{490}}{R_{665}} - 63.25 \cdot R_{490} - 0.478$	LT-MLR	0.68	< 2.2E-16
Turbid	ZSD104	$\ln SDD = 2.784 \cdot \frac{R_{490}}{R_{665}} - 38.22 \cdot R_{490} - 1.367$	LT-MLR	0.63	< 2.2E-16
Very Turbid	ZSD112	$SDD = -6.81e^{-06} \cdot \ln \frac{R_{560}}{R_{490}} - 0.030 \cdot \frac{R_{645} + R_{858}}{R_{469}} - 17.11 \cdot R_{555} + 1.14$	MLR	0.51	9.7E-09
Brown	ZSD109	$\ln SDD = 0.271 \cdot \ln R_{665} + 1.033$	LLR	0.29	0.0002

¹ Statistical technique.

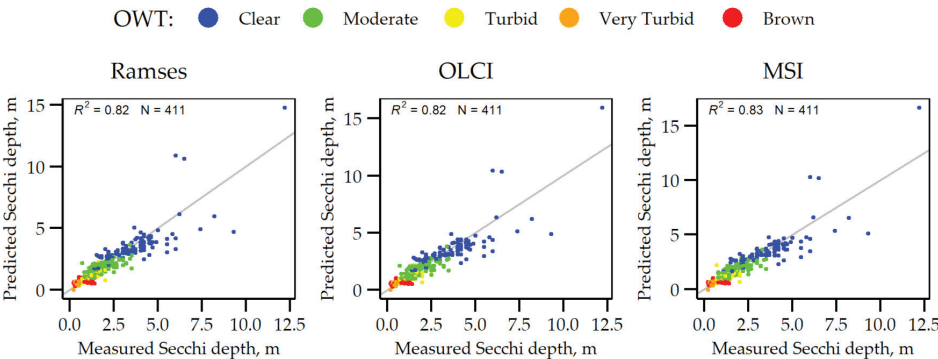


Figure 9. Comparison of the Secchi disk depth estimated from in situ measured reflectance spectra using the optical water type (OWT) guided approach and in situ measured Secchi disk depth for sensors with different spectral scales: (from left) Ramses with 1 nm resolution, OLCI, and MSI. OWTs are indicated by colours and the line shows a 1:1 relationship.

4. Discussion

Our OWT guided approach to estimate optical water quality parameters, such as Chl-a, TSM, CDOM, and Secchi disk depth, from $R(\lambda)$ spectra, can be the solution to monitor boreal region inland and coastal waters health operatively. Water bodies can vary in shape, size, depth, and also by water colour. As shown in Table 1, our in situ dataset from 52 different water bodies demonstrates that the optical water quality parameters can vary largely. For example, the concentration of the Chl-a range was from 0.5 to 215.2 $\text{mg}\cdot\text{m}^{-3}$, the TSM range was from 0.6 to 46.0 $\text{mg}\cdot\text{L}^{-1}$, the range for aCDOM(442) was 0.4 to 43.7 m^{-1} , and for the Secchi disk depth the range was from 0.2 to 12.2 m. Therefore, to assume to find one algorithm per optical water quality parameter to fit with a good accuracy for all the water bodies may be a bit too optimistic.

Optically complex waters are independently influenced by Chl-a, TSM, and CDOM [8]. Therefore, these can be the reasons why standard remote sensing algorithms often fail in optically complex waters [72,73], and there are many regional or waterbody based [25,65,70,74,75] empirical algorithms. However, optical properties can vary strongly even inside one waterbody, for instance, during the one day in Lake Peipsi the concentration of Chl-a varied from 16.8 to 215.2 $\text{mg}\cdot\text{m}^{-3}$, and in addition there is seasonal and interannual variability; therefore, studies have suggested, that more detailed approach would be beneficial [76,77]. The use of OWT guided approach, which first classifies water into different OWTs, reflecting different bio-optical conditions, and then applies that OWT specific algorithm to estimate the optical water quality parameters, may be one of the possible solutions.

In the context of selecting the best empirical algorithm for predicting the optical water quality parameter from $R(\lambda)$ spectra, this study showed, as expected, that the choice depends on the OWT and also the sensor spectral range. As the $R(\lambda)$ spectra are the basis for all the future calculations and developments, the error in $R(\lambda)$ may multiply in the final product or lead to incorrect conclusions [78]. Moreover, it is known that atmospheric correction over inland and coastal areas is difficult [79–81] and the result still can contain large errors [30,45,77,82,83]. Therefore, in this study, to eliminate as many errors as possible and focus on finding the best algorithm, we used in situ measured $R(\lambda)$ spectra with 1 nm step and for OLCI and MSI we recalculated in situ measured $R(\lambda)$ using SRFs into OLCI and MSI bands. The same approach has been used before [65]. However, it is still important to remember that in situ measured $R(\lambda)$ is not the absolute truth and can contain large errors for example due to variable weather conditions [45,84–86]. For example, $R(\lambda)$ measurements are difficult to perform well in CDOM-rich waters, which often leads to strong overestimation in the blue region of the spectrum [45,65]. Moreover, the presence of sunlight increases the $R(\lambda)$ values in the blue part of the spectrum.

Linear regression models were used for predicting the concentration of Chl-a. Compared to other optical water quality parameter model selections, Chl-a varies the most between OWTs and the spectral range. The widely used [10,63,68,87–92] ratio 700/670 nm with a high correlation for high-biomass waters, was the best model only for Turbid OWT with a Ramses spectral range. However, the two variables ratio approach was the best for all the spectral ranges in Brown OWT, OLCI and MSI Moderate OWT, Ramses Turbid OWT, and MSI Very Turbid OWT. Matthews [93] suggests for lower Chl-a concentrations to use the ratio of the blue and green. In our best-performing models, all variables were selected from the red and NIR spectral range, with different combinations. Moreover, broadly used [10,30,61,87,94,95] algorithms that include chlorophyll fluorescence information using values of reflectance spectra around 681 nm were not the best for any cases. The Brown OWT retrieving models coefficients of determination were about 40%, thus needing future investigation and improvement.

From the 39 tested empirical algorithms to retrieve the concentration of TSM, the model TSM18 using the Kutser et al. [65] algorithm based on a reflectance peak at 810 nm was the best for MSI for Turbid, Very Turbid, and Brown OWTs. It also suited well for Ramses and OLCI Turbid, Very Turbid, and Brown OWTs. The authors of the algorithm pointed out the usefulness of NIR spectral part for retrieving the TSM in turbid waters was already known from previous studies [96,97]. Similarly, Matthews [93] discussed the potential of NIR spectral part for retrieving the concentration of TSM in

the empirical algorithms overview article. However, despite being developed in waters with high mineral particles, Kutser et al. [65] showed the usefulness of NIR part of the spectra in waters, where the majority of TSM was organic, as in our dataset. Often, algorithms use the knowledge that near 560 nm is the phytoplankton absorption minimum; therefore, the reflectance is sensitive to changes in the TSM [93]. However, Zhang et al. [66] demonstrated that reflectance at 550 nm is sensitive to TSM changes in less turbid waters and reflectance at 645 nm is sensitive in turbid waters. For Clear OWT, the model TSM39 using Zhang et al.'s [66] developed log-transformed multiple linear regression algorithm, based on a combination of 488, 555, and 645 nm information, was the best for all sensors.

For the aCDOM(442) the power regression predictive models of the reflectance ratio showed better performances for all the spectral ranges in Clear, Moderate, and Turbid OWTs. For instance, the reflectance ratio of 665/560 nm was the best for OLCI and MSI; however, for Ramses, the model using the ratio of 560/660 nm was preferred. These ratios are quite commonly used for predictions; however, as shown in Table A1, they are used with different statistical techniques, such as linear regression [67,68,91,98,99], and power regression [67,75,98,99]. For Brown OWT, the log-transformed multiple linear regression model using the Brezonik et al. [100] algorithm, using 488 nm and 830 nm, showed the highest results for all spectral ranges. However, Figure 8 shows that the Brown OWT model is not sensitive for higher than 20 m^{-1} values and strongly underestimates in situ measured values in that region. Details of the algorithm in Table A1 also show that the algorithm development range was up to 19.7 m^{-1} . Overall, none of these tested CDOM algorithms' data ranges were up to 42 m^{-1} as were the in situ measurements present in our dataset. Therefore, future work is needed to find or develop algorithms that are suitable for these kinds of humic lakes. Additionally, reflectance measurements, both in situ and satellite, are difficult to perform well for these very dark lakes. Since uncertainties are higher in the blue part, the longer wavelengths are preferred for algorithms from the reflectance measurement side.

The predictive models for the Secchi disk depth analysis showed that the model ZSD104, using the Kloiber et al. [69] algorithm based on log-transformed multiple regression of form 485/660 nm ratio and the additional 485 nm, was the best model for all spectral ranges in Clear, Moderate, and Turbid OWTs. As shown in Table A1, this algorithm was developed for data ranges up to 5 m; and from Clear, Moderate, and Turbid OWTs, 96% of measurements fit within the limits. Furthermore, in the Clear OWT the maximum measured Secchi disk depth is 12.2 m and Figure 9 shows a lower accuracy predicting high Secchi disk depths. However, studies using the same algorithm have demonstrated that this can be used up to 15 m [101,102]. Therefore, it may be that upwelling and optically extreme conditions are the main reason for the lower prediction accuracy. For the Very Turbid OWT, the model ZSD112 using Wu et al. [70] algorithm, based on multiple linear regression of five variables, was the best. For the Brown OWT, the best model was based on reflectance at 660 nm. Matthews [93] also suggested, that for humic lakes, a single band algorithm may work; however, the blue part of spectrum was suggested. Overall, the Brown OWT best model was not good enough and needs future work.

The presented OWT guided approach to estimate optical water quality parameters was applied to OLCI images acquired in the Pärnu Bay region to investigate ecosystem seasonal and spatial changes and responses to weather effects. As shown in Figure 10, the left column includes OWT estimations and optical water quality parameters derived images during the most common situations, when higher values were present close to coast; however, the bay was mainly classified into Clear OWT. There was a storm event with a daily average wind speed of $11.2 \text{ m}\cdot\text{s}^{-1}$ and the gusts over $21 \text{ m}\cdot\text{s}^{-1}$ at 22th June 2018. The image captured the day after the storm showed the changes in the bay. As the bay is shallow with a soft bottom, the wind caused resuspension of sediments into the water column and as a result the bay was then classified into Turbid or Moderate OWTs. Derived images (Figure 10) showed an increase of TSM concentration (due to both inorganic and organic part) and drastic decrease in Secchi disk depth. This indicates changes in the underwater light field. The Chl-a values rose, but we do not have a reason to believe that this was actually true in this case, and we assume the overprediction of the Chl-a due to TSM side-effect. Firstly, finding empirical algorithms that effectively separate the

signals from TSM and Chl-a can be challenging [93], and secondly, our datasets mainly include TSM dominated by SPOM in situ measurements. In the future, it is necessary to add more SPIM dominated in situ measurements to train our Turbid OWT models. Five days later (right column of Figure 10) conditions had returned to near those on the 17th, though with higher Chl-a values, possibly due to the added nutrients from the sediments. These changes are quick in nature and remain often uncaptured by traditional monitoring programs, adding more value to remote sensing possibilities.

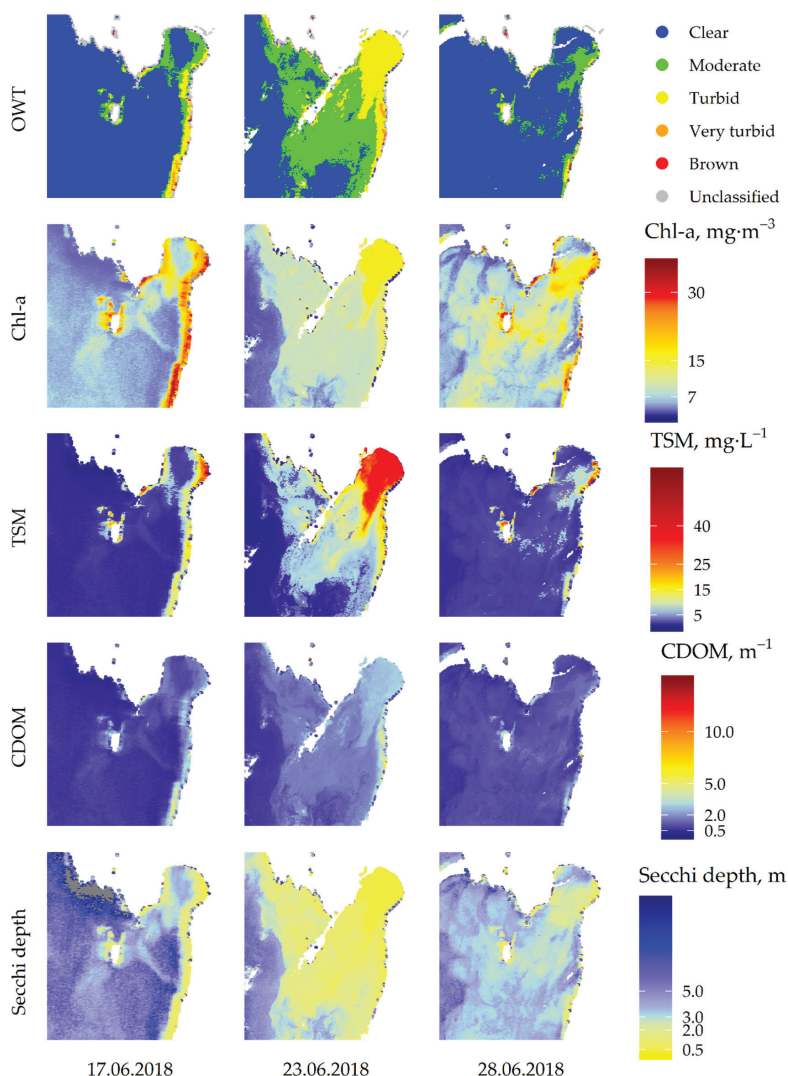


Figure 10. Changing the optical water types (OWTs) and optical water quality parameters (such as the Chl-a, TSM, CDOM, and Secchi disk depth) before and after a strong wind (day average wind speed $11.2 \text{ m}\cdot\text{s}^{-1}$ and the gust over $21 \text{ m}\cdot\text{s}^{-1}$) event on 22 June 2018 in Pärnu Bay captured by OLCI images processed with the C2RCC AC processor. Water quality parameters are estimated from $R(\lambda)$ using OWT based algorithms.

Additionally, exploring our OWT guided approach applied to OLCI images, we discovered that sometimes artificial lines emerged as a transition from one OWT model to another OWT model.

As changes in natural water are usually continuous, but we are trying to push these into very strict limits, then these lines are expected to happen. In another study, fuzzy logic is often used to blend algorithms for optical water quality parameter algorithms [41,103,104]. Since the OWT classification we used uses similarity calculations, each pixel had a similarity assessment for every OWT. For the purpose of blending OWT models, the combination of similarities as weights and the threshold for the selection of when to add another OWT's model in blending calculations was giving promising results, but are in need of more detailed studies in the future.

5. Conclusions

Currently, water monitoring programs are mainly based on in situ measurements; however, considering that water bodies are dynamic in nature, this method may not reflect the status of the entire water body. Remote sensing offers effective ways to observe the spatial and temporal variations in water quality. Moreover, the launch of MSI and OLCI, and the free availability of their data with high spectral, spatial, and temporal resolution, have increased the potential to add remote sensing techniques into monitoring programs and to improve the quality of monitoring water. However, remote sensing of inland and coastal waters can be challenging as they are independently influenced by Chl-a, TSM, and CDOM. In this study, we introduce an OWT guided approach to estimate the optical water quality parameters, such as the concentration of Chl-a and TSM, the aCDOM(442), and the Secchi disk depth from the $R(\lambda)$ spectra with different spectral ranges. We focused our study on the boreal region inland and coastal waters; however, we showed the large variation of optical water quality parameters.

We tested 132 previously published empirical algorithms to find the best existing solution for each OWT (Clear, Moderate, Turbid, Very Turbid, and Brown) and for different spectral ranges, such as Ramses with a 1 nm step, OLCI bands, and MSI bands. We demonstrated that the suitability of the algorithm depends on the OWTs and spectral ranges. It is necessary to select an appropriate algorithm for the region of interest; therefore, using only one algorithm for optically complex waterbodies does not work, and we suggest using the OWT guided approach as the possible of pre-selection method for choosing right algorithm. The OWT guided approach can provide a basis for understanding the seasonal and spatial variabilities of water bodies and can be an additional technique in water monitoring programs to improve the quality of monitoring the optical water quality parameters.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. The algorithms used to retrieve the optical water quality parameters, such as chlorophyll-a (Chl-a), total suspended matter (TSM), absorption coefficient of coloured dissolved organic matter (CDOM), and Secchi disk depth (ZSD). In algorithms that were designed for satellite sensors, the central wavelength is used to the mark sensor band. Descriptions of acronyms and abbreviations are found in Appendix C Table A2. The data range is given in parametric units: for Chl-a $\text{mg}\cdot\text{m}^{-3}$, for TSM $\text{mg}\cdot\text{L}^{-1}$, for the absorption coefficient of CDOM at wavelength shown in brackets m^{-1} , and for Secchi disk dept m.

Model	Algorithm	Stat. Tech.	Sensor	Data Range	Waterbody	Country	Reference
TSM1	R858	P2R	MODIS	0.3–145.6	Bay of Biscay	France	Petus et al. (2010) [105]
TSM2	R858/R645	LR	MODIS	77–2182	Gironde Estuary	France	Chavula et al. (2009) [106]
TSM3	R645	LR	MODIS	1–55	Gulf of Mexico	USA	Miller, McKee (2004) [107]
TSM4	R850/R550	P3R	Radiometric	13–985	Gironde Estuary	France	Doxaran et al. (2002) [108]
TSM5	(R485–R830)/(R660–R830)	LT-LR	LS TM	0.7–23	Southern Finland lakes	Finland	Härmä et al. (2001) [109]
TSM6	R702	LR	AlSA	0.7–32	Finnish lakes	Finland	Kallio et al. (2001) [110]
TSM7	R709/5)	LR	AlSA	0.7–32	Finnish lakes	Finland	Kallio et al. (2001) [110]
TSM8	R551	LR	MODIS	1.2–110.3	Southern North Sea	France	Nechad et al. (2010) [111]
TSM9	R850/R550	LR	Radiometric	13–985	Gironde Estuary	France	Doxaran et al. (2002) [108]
TSM10	R702-R751	LR	AlSA	0.7–32	Finnish lakes	Finland	Kallio et al. (2001) [110]
TSM11	(R560-R520)/(R560+R520)	LLR	Radiometric	1–66	Hungarian, Bulgarian, Germany lakes	Finland	Gietelson et al. (1993) [112]
TSM12	R709-R779	LR	MERIS	0.7–23	Finnish lakes	Finland	Härmä et al. (2001) [109]
TSM13	R490/R645	LLR	Radiometric		Baltic Sea - southern	Poland	Wozniak (2014) [113]
TSM14	R555/R645	LLR	Radiometric		Baltic Sea - southern	Poland	Wozniak (2014) [113]
TSM15	(R545+R645)/2	LLR	SPOT, LS TM		Frisian lakes	Netherlands	Dekker et al. (2002) [114]
TSM16	(R545+R645)/2	LR	SPOT, LS TM		Frisian lakes	Netherlands	Dekker et al. (2002) [114]
TSM17	max(R700–R720)-(R646+R770)/2	LR	Radiometric	0.75–63.33	Estonian lakes	Estonia	Kutser et al. (2016) [65]
TSM18	R810-(R770+R840)/2	LR	Radiometric	0.75–63.33	Estonian lakes	Estonia	Kutser et al. (2016) [65]
TSM19	R635	LR	SEVIRI	2–100	North Sea – Belgian coast	Belgium	Neukermans et al. (2009) [115]
TSM20	R620-R681/R510	LLR			New Caledonia lagoon, Cienfuegos Bay, Suva Harbour and Laucala Bay	New Caledonia, Cuba, Fiji	Outilon et al. (2008) [116]
TSM21	R620-R681/R412	LLR			New Caledonia lagoon, Cienfuegos Bay, Suva Harbour and Laucala Bay	New Caledonia, Cuba, Fiji	Outilon et al. (2008) [116]
TSM22	R681	P2R			New Caledonia lagoon, Cienfuegos Bay, Suva Harbour and Laucala Bay	New Caledonia, Cuba, Fiji	Outilon et al. (2008) [116]
TSM23	R443/R670	LLR			New Caledonia lagoon, Cienfuegos Bay, Suva Harbour and Laucala Bay	New Caledonia, Cuba, Fiji	Outilon et al. (2008) [116]
TSM24	R560, R660, R830	MLR	LS TM	11.5–33.5	Lake Reelfoot	USA	Wang et al. (2006) [74]
TSM25	R709/R754	LT-LR	OLCI	1.2–9.14	Baltic Sea	Estonia	Toming et al. (2017) [30]

Table A1. Cont.

Model	Algorithm	Stat. Tech.	Sensor	Data Range	Waterbody	Country	Reference
TSM26	R745/R490	LT-LR	GOCI	8–5275	Lake Taihu	China	He et al. (2019) [117]
TSM27	R560	LR	MSI	5–38.76	Gorky Reservoir	Russia	Molokov et al. (2019) [118]
TSM28	R560	P2RR	MSI	5–38.76	Gorky Reservoir	Russia	Molokov et al. (2019) [118]
TSM29	R740	P2R	MSI	5–38.76	Gorky Reservoir	Russia	Molokov et al. (2019) [118]
TSM30	R740/R705	P2R	MSI	5–38.76	Gorky Reservoir	Russia	Molokov et al. (2019) [118]
TSM31	R705-(R740+R665)/2	LT-LR	MSI	5–38.76	Gorky Reservoir	Russia	Molokov et al. (2019) [118]
TSM32	R908	LR	WV 2	>820	inland waters in Deqing County	China	Shi et al. (2018) [119]
TSM33	R427	LR	WV 2	>820	inland waters in Deqing County	China	Shi et al. (2018) [119]
TSM34	R658	LR	WV 2	>820	inland waters in Deqing County	China	Shi et al. (2018) [119]
TSM35	R840/R545	LT-LR	SPOT	35–2000	Gironde estuary	France	Doxaran et al. (2002) [108]
TSM36	R840/R645	LT-LR	SPOT	35–2000	Gironde estuary	France	Doxaran et al. (2002) [108]
TSM37	(R550+R670)/(R550/R670)	LT10-LR					Han et al. (2006) [120]
TSM38	log(R555), R645, log(R488/R555)	LT10-MLR			Gulf of Naples	Italy	Tassan (1993) [121]
TSM39	R555, R645, R488/R555	LT10-MLR			Yellow Sea	China	Zhang et al. (2010) [66]
CHL40	R443/R551	LR	MODIS	0.1–0.4	Lake Malawi	Malawi	Chavula et al. (2009) [106]
CHL41	R688/R674	LR	AISA	1.0–100	Finnish lakes	Finland	Kallio et al. (2001) [110]
CHL42	(1/R665-1/R708)/R753	LR	MERS	0.63–45.51	Taganrog Bay, Azov Sea	Russia	Moses et al. (2009) [122]
CHL43	R705/R664	LR	CASI	2.5–18.9	Lake Mälaren	Sweden	Amnenberg et al. (2002) [68]
CHL44	R550	LR	CASI	2.9–50.6	Lakes Erken and Mälaren	Sweden	Flink et al. (2001) [87]
CHL45	R708/R678	LR	CASI	2.9–50.6	Lakes Erken and Mälaren	Sweden	Flink et al. (2001) [87]
CHL46	R708/R678, R643/R628	MLR	CASI	2.9–50.6	Lakes Erken and Mälaren	Sweden	Flink et al. (2001) [87]
CHL47	R700/R670	LLR	Radiometric	6.3–58.2	Lake Chagan	China	Duan et al. (2007) [88]
CHL48	R560/R660	LLR	LS TM	~5–50	New York Harbour	USA	Hellwegger et al. (2004) [71]
CHL49	(R485-R660)/R560	LR	LS TM	3.0–6.0	Lake Garda	Italy	Brivio et al. (2001) [123]
CHL50	ln(R485), ln(R560)	LT-MLR	LS TM	3.0–6.0	Lake Garda	Italy	Brivio et al. (2001) [123]
CHL51	R485/R560	LLR	LS TM		Arabian Sea		Dwivedi, Narain (1987) [124]
CHL52	R660/R485	LLR	LS TM	2.0–70.0	Haifa Bay	Israel	Gitelson et al. (1996) [125]
CHL53	max(R400–R900)/R670	LR	Radiometric	5.1–185	Lake Kinneret	Israel	Yacobi et al. (1995) [126]
CHL54	R830/R660	LR	LS TM	5.1–185	Lake Kinneret	Israel	Yacobi et al. (1995) [126]
CHL55	R560	LLR	LS TM	1.0–50.3	Lake Michigan	USA	Lathrop, Lillesand (1986) [127]
CHL56	R710/R670	LT-LR	CASI-2	~4–63	Barton Broad	UK	Hunter et al. (2008) [128]
CHL57	(1/R650-1/R710)/R740	LR	Radiometric	107–3078	Tamar Estuary	UK	Zimba, Gitelson (2006) [111]
CHL58	R704/R672	LR	Radiometric	3–185	Inland waters	Netherlands	Gons (1999) [90]
CHL59	sum(R670–R850)	LR		21.0–280	Carter Lake	USA	Schalles et al. (1998) [129]
CHL60	sum(R670–R730)	LR	Radiometric	3.1–7.3	Lake Kinneret	Israel	Gitelson et al. (1994) [130]

Table A1. Cont.

Model	Algorithm	Stat. Tech.	Sensor	Data Range	Waterbody	Country	Reference
CHL61	R700/R680	LR	AMMS	2–79	Tennessee Valley	USA	Dierberg, Carricker (1994) [89]
CHL62	R688/R681	LR	AISA	10–100	Finnish lakes	Finland	Kallio et al. (2001) [110]
CHL63	R702/R664	LR	AISA	22–130	Gulf of Finland	Finland	Koponen et al. (2007) [91]
CHL64	R665/R754	LR	OLCI	0–6.02	Baltic Sea		Toming et al. (2017) [30]
CHL65	R674/R709	LR	OLCI	0–6.02	Baltic Sea		Toming et al. (2017) [30]
CHL66	R674/R754	LR	OLCI	0–6.02	Baltic Sea		Toming et al. (2017) [30]
CHL67	R748/R667	LR	MODIS		Dnieper River, Sea of Azov	Russia	Moses et al. (2009) [92]
CHL68	(R490-R665)/R560	LR	LS TM	3–7	Lake Kinneret	Israel	Mayo et al. (1995) [131]
CHL69	R709-(R665+R754)/2	LR					Gitelson et al. (1992) [60]
CHL70	R709-R754	LR					Gitelson et al. (1992) [60]
CHL71	R705-(R665+R740)/2	LR	MSI	3.6–72.9	Estonian lakes	Estonia	Toming et al. (2016) [27]
CHL72	R709/R681	LR	OLCI	5.99–117.54	Mangaba	Brazil	Lins et al. (2017) [10]
CHL73	R709/R665	LR	OLCI	5.99–117.54	Mangaba	Brazil	Lins et al. (2017) [10]
CHL74	R705/R665	LR	MSI	5.99–117.54	Mangaba	Brazil	Lins et al. (2017) [10]
CHL75	(1/R661-1/R709)/R674	LR	OLCI	5.99–117.54	Mangaba	Brazil	Lins et al. (2017) [10]
CHL79	(1/R650-1/R710)/R740	LR		4.4–3078	National Warm-water Aquaculture Center, Stonevill	USA	Zimba, Gitelson (2006) [11]
CHL80	(R485-R660)/R560	LR	LS TM	3.0–7.0	Lake Kinneret	Israel	Mayo et al. (1995) [131]
CHL81	log(R710/R670)	LR	CASI-2		Barton Broad	UK	Hunter et al. (2008) [128]
CHL82	log(R483)/log(R660)	LR	LS ETM+	1.14–23.23	Pensacola Bay	Florida	Han, Jordan (2005) [132]
CHL83	R483/R660	LT-LR	LS TM	2.1–183	Minnesota lakes	USA	Brezonik et al. (2005) [102]
CHL84	R483/R660	LR	LS TM	2.1–183	Minnesota lakes	USA	Brezonik et al. (2005) [102]
CHL85	R830/(R485+R560+R830)	LR	LS TM	1.8–18		Sweden	Lindell et al. (1999) [54]
CHL86	R660/R565	LR	LS TM	66.0–188.59	Lake Reelfoot	USA	Wang et al. (2006) [74]
CHL87	R700/R670	LR	Radiometric	2–79	Tennessee	USA	Dierberg, Carricker (1994) [89]
CHL88	R702/R674	LR	AISA	2.6–100	Finnish lakes	Finland	Kutser et al. (1999) [63]
CHL89	R681-R665-(R709-R665)/((681-665)/(709-665))	LR	MERS				Gower et al. (1999) [94]
CHL90	(1/R662-1/R693)/(1/R740-1/705)	LR		0.98–89.23	Lake Taihu	China	Le et al. (2009) [12]
CHL91	R708/R665	LR	MERS	1.0–100	Finnish lakes	Finland	Kallio et al. (2001) [110]
CHL92	R710/R688	LR	AISA	1.0–100	Finnish lakes	Finland	Kallio et al. (2001) [110]
CHL93	R719/R667	LR	Radiometric	0–0.2	Lake Tai	China	Jiao et al. (2006) [133]
CHL94	R550/R590	LR	Radiometric	0.6–70	Baltic Sea		Darecki et al. (2003) [72]
CHL95	R555/R645	LR	MODIS	1–100	Baltic Sea		Wozniak (2014) [113]
CHL96	(1/R681-1/R709)/(1/R753-1/R709)	LR	MERS				Zhou (2011) [95]

Table A1. Cont.

Model	Algorithm	Stat. Tech.	Sensor	Data Range	Waterbody	Country	Reference
CHL97	(1/R705-1/R665)/(1/R705+1/R665)	LR	MERIS	1–60	Fremont State lakes	USA	Mishra, Mishra (2012) [62]
CHL98	(1/R670-1/R710)/R750	LR	Radiometric	2.07–183.5			Grielson et al. (2009) [64]
CHL99	log(max(R443/R360, R490/R560, R510/R560))	P4R	MERIS				OC4E for MERIS
CHL100	log(max(R443/R547, R488/R547))	P4R	MODIS		Lake Carter	USA	OC3M for MODIS
CHL101	R709-R681-(709-681)/(759-681)-(R753-R681)	LR	MERIS				Gower et al. (2008) [61]
CHL102	max(R670-R850)	LR	Radiometric	20–280			Schalles et al. (1998) [129]
ZSD103	R560	LLR	LS TM	0.5–9.0	Lake Michigan	USA	Lathrop, Lillesand (1986) [127]
ZSD104	R485/R660, R485	LR-MLR	TS TM	~0.5–5	Minnesota lakes	USA	Kloiber et al. (2002) [69]
ZSD105	R485/R560	LR	LS TM	4.6–6.8	Lake Iseo	Italy	Giardino et al. (2001) [134]
ZSD106	(R488-R748)/(R667-R748)	LR	LS TM	0.4–7.0	Southern lakes	Finland	Härma et al. (2001) [109]
ZSD107		MLR	LS TM	0.16–0.33	Reelfoot Lake	USA	Wang et al. (2006) [74]
ZSD109		LLR	LS TM	0.45–2	New York Harbour	USA	Hellweger et al. (2004) [71]
ZSD110	R485/R660	LR	LS ETM+	0.5–5.5	Southern Lakes	Finland	Kallio et al. (2008) [99]
ZSD111	R660/R560	LT-LR	LS TM	0.22–0.79	Lake Chagan, Xinmiao, Kuli	China	Duan et al. (2009) [135]
ZSD112	ln(R555)/R488, (R645+R858)/R469, R555	MLR	MODIS	0.25–1.2	Chaohu Lake	China	Wu et al. (2009) [70]
ZSD113	R490/R620	LT-LR	MERIS	3.0–6.0	Himmerf-järden Bay	Sweden	Kratzer et al. (2008) [24]
ZSD114	R560/R709	LLR	OLCI	(turbid waters)	Baltic Sea	Estonia	Alikas, Kratzer (2017) [25]
ZSD115	R490/R709	LLR	OLCI	(clear waters)	Baltic Sea	Estonia	Alikas, Kratzer (2017) [25]
CDOM116	R670/R412	LR	Radiometric	0.1–1.5 (440 nm)	Clyde Sea	Scotland	Bowers et al. (2000) [136]
CDOM117	R485, R485/R530	LT-MLR	LS TM	0.6–19.4 (440 nm)	Minnesota lakes	USA	Brezonik et al. (2005) [102]
CDOM118	R443/R510	LTLR	SeaWiFS	0.07–1.1 (412 nm)	Gulf of Mexico	USA	D'Sa, Miller (2003) [137]
CDOM119	R664/R550	LR	MERIS	1.13–2.07 (420 nm)	Lake Mälaren	Sweden	Amnenberg et al. (2002) [68]
CDOM120	R565/R660	LR	ALI	0.68–11.1 (420 nm)	Finnish and Sweden lakes		Kutser et al. (2005) [98]
CDOM121	R565/R660	LLR	ALI	0.68–11.1 (420 nm)	Finnish and Sweden lakes		Kutser et al. (2005) [98]
CDOM122	R670/R550	LLR		0.35–11.9 (440 nm)	Minnesota lakes	USA	Menken et al. (2006) [67]
CDOM123	R700/R670	LR		0.35–11.9 (440 nm)	Minnesota lakes	USA	Menken et al. (2006) [67]
CDOM124	R570/R655	LLR	Radiometric	0.23–17.4 (440 nm)	Pomeranian lakes, Baltic Sea	Poland	Fieck et al. (2011) [75]

Table A1. Cont.

Model	Algorithm	Stat. Tech.	Sensor	Data Range	Waterbody	Country	Reference
CDOM125	R412/R510	LLR	SeaWiFS	0.07–1.1 (412 nm)	Gulf of Mexico	USA	D'Sa, Miller (2003) [137]
CDOM126	R510/R590	LLR	SeaWiFS	0.07–1.1 (412 nm)	Gulf of Mexico	USA	D'Sa, Miller (2003) [137]
CDOM127	R400/R600	LLR	Radiometric	0.1–1.9 (440 nm)	Tamar Estuary	UK	Doxaran et al. (2005) [97]
CDOM128	R665/R490	LR	AISA	1.29–2.61 (400 nm)	Gulf of Finland	Finland	Koponen et al. (2007) [91]
CDOM129	R560/R660	LR	LS ETM+	1.1–12.2 (400 nm)	Finnish lakes and rivers	Finland	Kallio et al. (2008) [99]
CDOM130	(R480-R700/R675-R520)/(R480-R700/R675+R520)	LLR	Radiometric	0.1–12 (580 nm)	Hungarian, Bulgarian, German lakes		Gitelson et al. (1993) [112]
CDOM131	R560/R660	LLR	LS ETM+	1–12.2 (400 nm)	Finnish lakes	Finland	Kallio et al. (2008) [99]
CDOM132	R412+R700/R670	MLR		0.35–11.9 (440 nm)	Minnesota lakes	USA	Menken et al. (2006) [67]
CDOM133	R660, R560/R485	LT-MLR	LS TM	1.38–6.45 (400 nm)	Kolyma River	Russia	Griffin et al. (2011) [138]
CDOM134	log(R490/R550)	LT-P2R	MODIS; MERIS, SeaWiFS	0.4–2 (400 nm)	Baltic Sea	Poland	Kowalczyk et al. (2005) [139]
CDOM135	R510/R753.75	LLR	OLCI	0.51–25.1 (440 nm)	Lakes and rivers	USA	Brezonik et al. (2015) [100]
CDOM136	R490/R740	LLR	MSI	0.51–25.1 (440 nm)	Lakes and rivers	USA	Brezonik et al. (2015) [100]

Appendix B

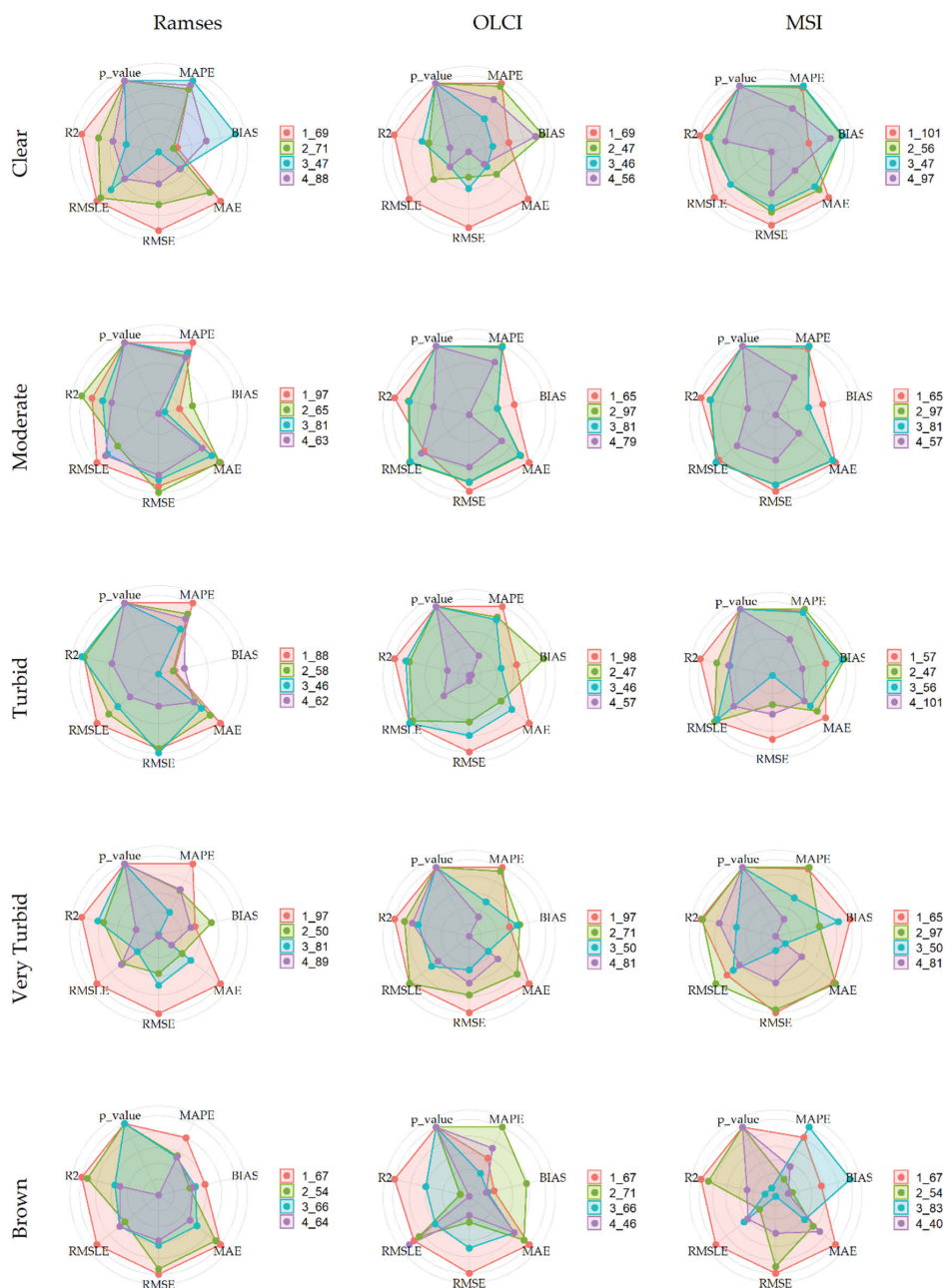


Figure A1. On radar plots, four Chl-a predictive models with the highest score from our ranking system are plotted for each optical water type and spectral range. The statistical metrics that were used to rank the model are displayed on each axis. The center of the radar plot indicates a low score. The legend includes information about model position (1 to 4) and model number, without parametric specifications.

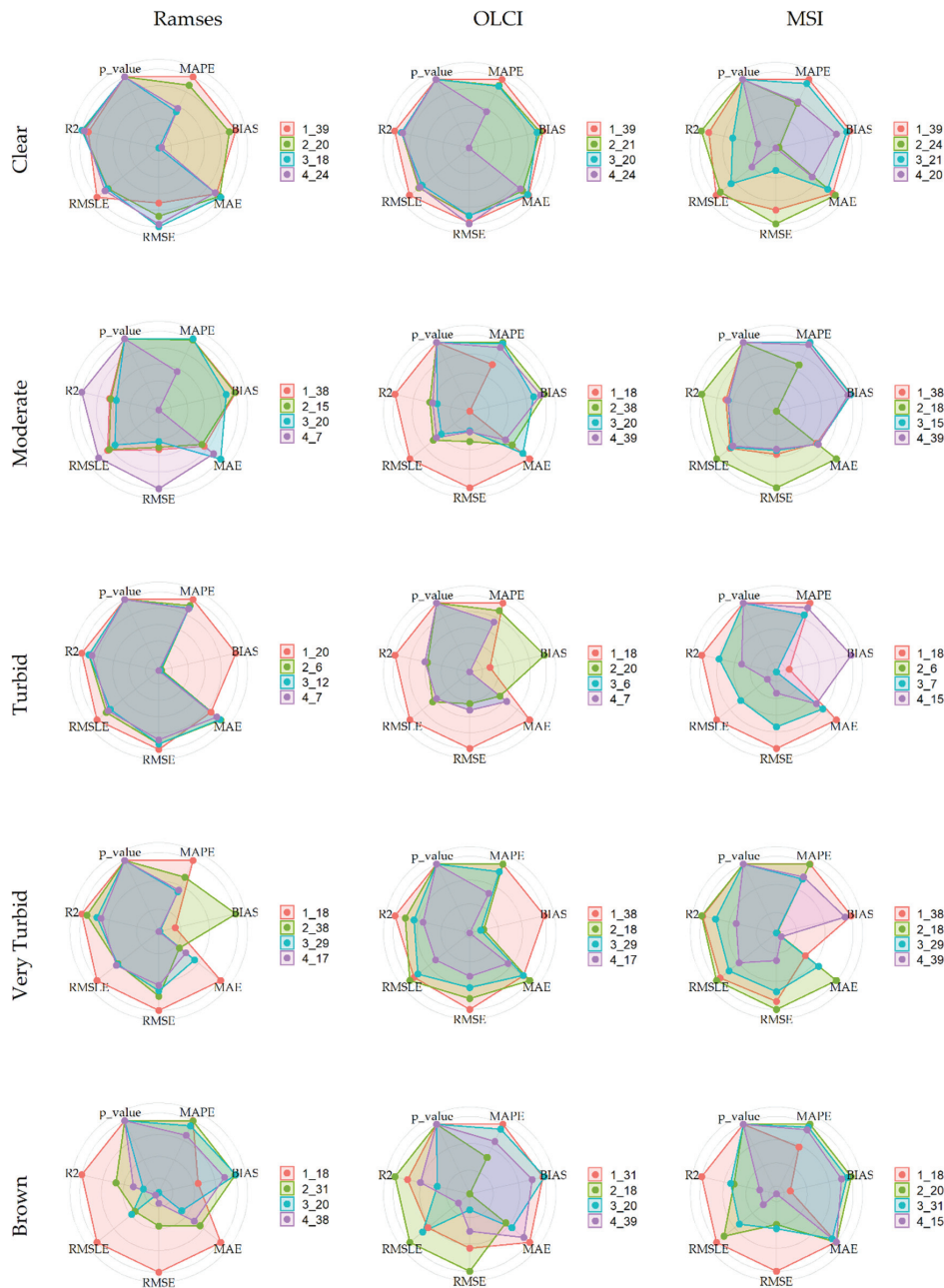


Figure A2. On radar plots, four TSM predictive models with the highest score from our ranking system are plotted for each optical water type and spectral range. The statistical metrics that were used to rank the model are displayed on each axis. The center of the radar plot indicates a low score. The legend of the radar plots includes information about the model position (1 to 4) and model number, without parametric specifications.

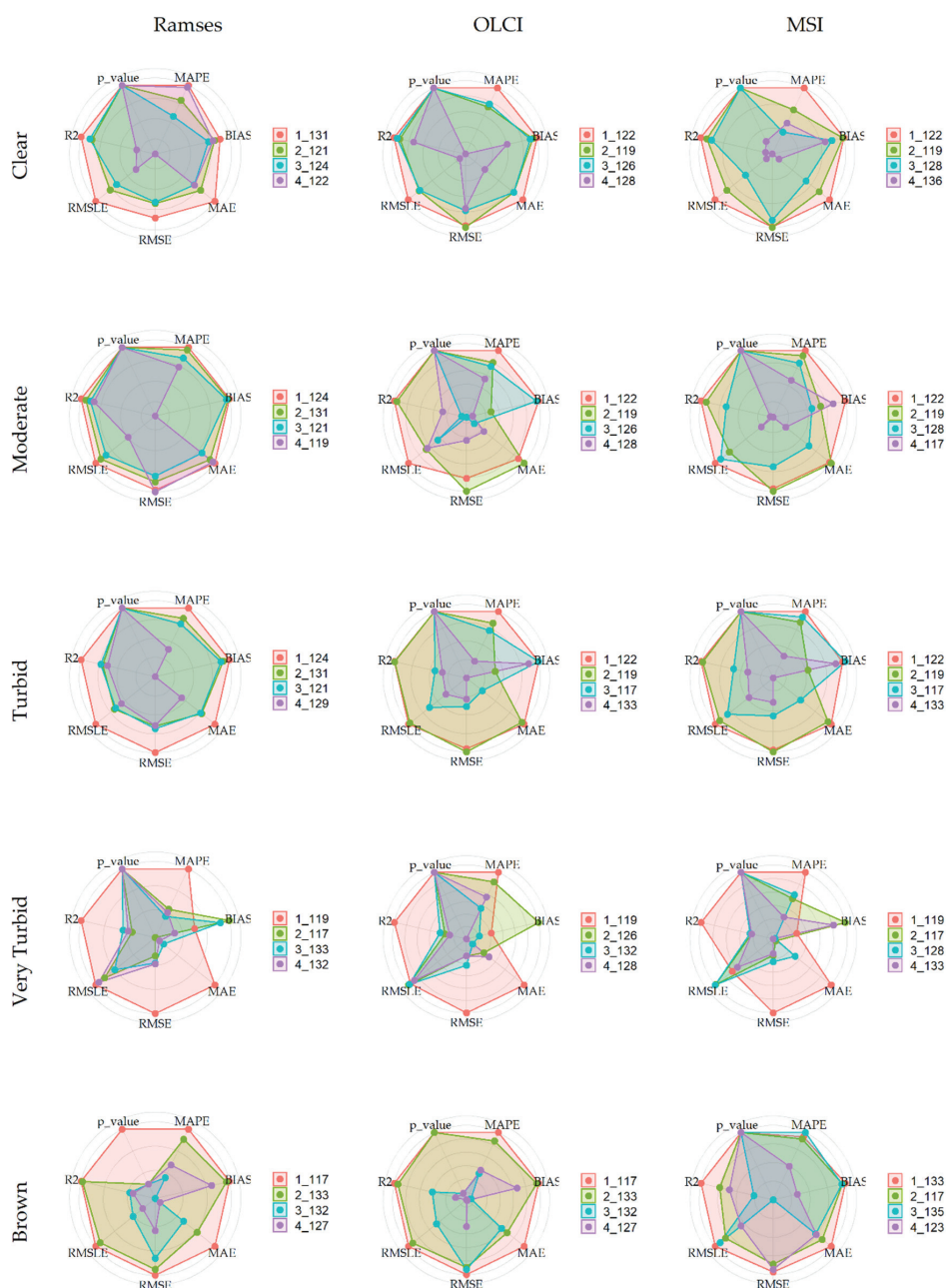


Figure A3. On radar plots, four absorption coefficients of CDM at a wavelength of 442 nm predictive models with the highest score from our ranking system are plotted for each optical water type and spectral range. The statistical metrics that were used to rank the model are displayed on each axis. The center of the radar plot indicates a low score. The legend of the radar plots includes information about the model position (1 to 4) and the model number, without parametric specifications.

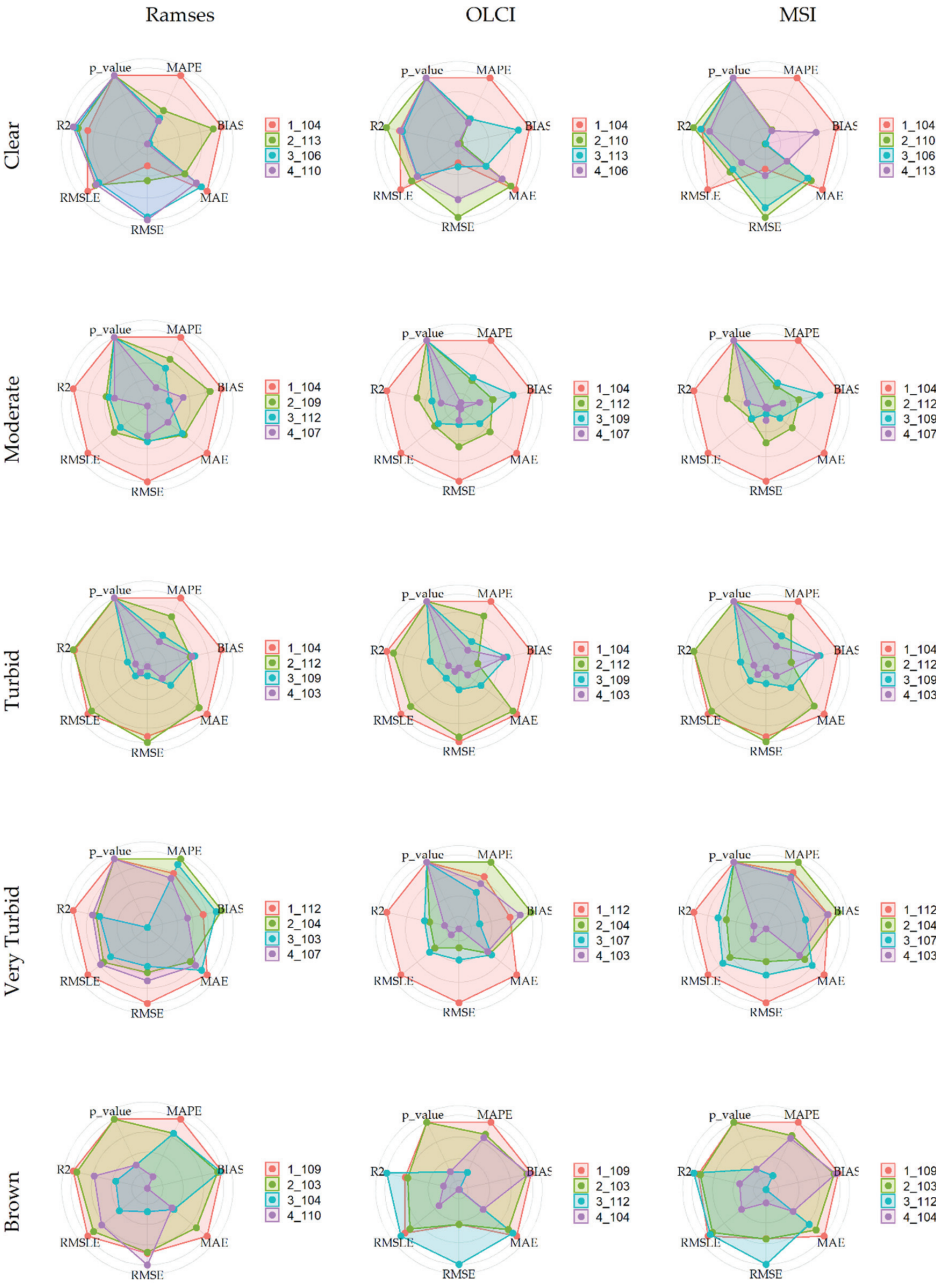


Figure A4. On radar plots, four Secchi disk depth predictive models with the highest score from our ranking system are plotted for each optical water type and spectral range. The statistical metrics that were used to rank the model are displayed on each axis. The center of the radar plot indicates a low score. The legend of the radar plots includes information about the model position (1 to 4) and model number, without parametric specifications.

Appendix C

Table A2. Acronyms and abbreviations used in this study.

Symbol	Meaning
OWT	Optical water type
OSC	Optically significant constituent
$R(\lambda)$	Water-leaving reflectance
TSM	Total suspended matter, $\text{mg}\cdot\text{L}^{-1}$
SPIM	Suspended particulate inorganic matter, $\text{mg}\cdot\text{L}^{-1}$
SPOM	Suspended particulate organic matter, $\text{mg}\cdot\text{L}^{-1}$
CDOM	Coloured dissolved organic matter
aCDOM(442)	Absorption coefficient of CDOM at a wavelength of 442 nm, m^{-1}
Chl-a	Chlorophyll-a, $\text{mg}\cdot\text{m}^{-3}$
ZSD	Secchi disk depth, m
NIR	Near-infrared
SRF	Spectral response function
MSI	Multispectral Instrument
OLCI	Ocean and Land Colour Instrument
MERIS	Medium Resolution Imaging Spectrometer
MODIS	Moderate Resolution Imaging Spectroradiometer
ALI	Advanced Land Imager
LS TM	Landsat Thematic Mapper
LS ETM ⁺	Landsat Enhanced Thematic Mapper Plus
AISA	The Airborne Imaging Spectrometer for Applications
SPOT	Satellite Pour l’Observation de la Terre (in French)
SEVIR	Spinning Enhanced Visible and Infrared Imager
GOCI	Geostationary Ocean Color Imager
WV2	WorldView-2
CASI	Compact Airborne Spectrographic Imager
AMMS	Airborne Multispectral Measurement System
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
LR	Linear regression
MLR	Multiple linear regression
LT-LR	Log-transformed linear regression
LT-MLR	Log-transformed multiple linear regression
LLR	Log-log regression
P2R	Polynomial regression (number indicated degree of polynomial)
LT10-LR	Log-transformed linear regression with base 10
LL10R	Log-log regression with base 10
LT-P2R	Log-transformed polynomial regression

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Appendix 4

Publication IV

Sipelgas, L., Uiboupin, R., Arikas, A., Siitam, L., 2018. Water quality near Estonian harbours in the Baltic Sea as observed from entire MERIS full resolution archive. *Marine Pollution Bulletin*, 126, 565–574.



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Water quality near Estonian harbours in the Baltic Sea as observed from entire MERIS full resolution archive

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ABSTRACT

Variations and trends in water quality parameters (total suspended matter and coloured dissolved organic matter) were examined in five harbours in the eastern Baltic Sea using satellite imagery collected from 2002 to 2011 by the Medium Resolution Imaging Spectrometer (MERIS) at full spatial resolution (300 × 300 m). In the eastern Gulf of Finland harbours (Sillamäe, Kunda) the TSM monthly variations were related to monthly mean wind speed. In Tallinn harbour, which operates > 6000 vessels annually, evidence of anthropogenic impacts was identified through inter-annual TSM variations. The vessel traffic footprint was ascertained from the significant correlation ($R = 0.66$; $p = 0.035$) between the number of annual vessel visits and mean annual TSM concentration. In the harbour of Pärnu, located close to the river mouth, inter-annual water quality variations in terms of the CDOM concentrations were affected by the mean annual river discharge levels of the Pärnu River.

1. Introduction

The coastal area of the Baltic Sea is heavily populated and there are over 200 ports in the Baltic Sea, producing intense marine traffic in the area (HELCOM, 2010). Water quality in harbour areas are influenced by various human-induced and natural processes. In shallow coastal seas, waves and currents resuspend sediments (e.g., Raudsepp et al., 2011). Human induced sediment resuspension caused by shipping (Briciu-Burghina et al., 2014; Rapaglia et al., 2015) and dredging operations (Sipelgas et al., 2006; Raag et al., 2014) is also known to have negative economic and environmental effects. Sediment re-suspension increases concentrations of total suspended matter (TSM) in water column and therefore decreases light penetration depths, resulting in reduced light availability for aquatic plants. Furthermore, fish and wildlife disturbances are known concerns (Hayes and Landis, 2004).

In the Baltic Sea, harbours are primarily located at the river mouths, and thus the water quality in these harbours is influenced by riverine inputs. Using remote sensing imagery and numerical modelling, Soosaar et al. (2016) showed that river water affects coastal water suspended sediment concentrations in the Gulf of Riga of the Baltic Sea. Using MERIS imagery time series Vaičiūtė et al. (2015) showed the influence of river discharge on coastal coloured dissolved organic matter (CDOM) concentrations in Curonian Lagoon of the Baltic Sea. Sipelgas et al. (2004) demonstrate the river water gradients of CDOM along the Estonian coastline based on in situ measurements.

To develop and manage harbour areas, long-term background

datasets on water quality are needed to evaluate the environmental impacts of harbour operations and maintenance. The Central Dredging Association (CEDA) has noted that the impacts of dredging-induced turbidity should be evaluated as increases from background levels and not as absolute values (CEDA Information Paper, 2011).

Optical Remote sensing data (SeaWiFS, MODIS) have been used for routine monitoring of optically active substances such as chlorophyll *a* (Chl *a*), TSM and CDOM concentrations over two decades. However, in optically complex coastal waters such as the Baltic Sea, the accuracy of these retrievals has been poor (Darecki and Stramski, 2004; Reinart and Kutser, 2006). In 2002, the European Space Agency (ESA) launched MERIS (Medium Resolution Imaging Spectrometer) instrument on-board the ENVISAT platform with a spectral band combination specially designed for studying complex case II waters (Doerffer et al., 1999). The reliability of different algorithms and processors for estimating the TSM, Chl *a*, and CDOM concentrations in the coastal Baltic Sea from MERIS data has been evaluated in several publications and water quality product retrieval improvements have been reported (Kratzer et al., 2008; Kratzer and Vinterhav, 2010; Vaičiūtė et al., 2012; Attila et al., 2013; D'Alimonte et al., 2014; Beltran-Abauza et al., 2014; Raag et al., 2014; Woźniak et al., 2014; Alikas et al., 2015; Harvey et al., 2015).

Several studies have been conducted on water quality algorithm calibration/validation and on short-term processes. However, long-term trends and changes in ecological parameters in the Baltic Sea based on remote sensing data have been examined only in few papers.

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Kahru and Elmgren (2014) studied cyanobacterial bloom occurrence patterns over three decades based on data acquired by several ocean colour sensors (AVHRR, MODIS, SeaWiFS, VIIRS). A similar study was conducted by Bresciani et al. (2014) for the Curonian lagoon along the Lithuanian coast using MERIS data. Vaičiūtė et al. (2015) studied CDOM changes in the same lagoon over a shorter time period (2005–2011). Suominen and Tolvanen (2016) also analysed time series of remotely sensed turbidity retrieved from MERIS imagery in a coastal archipelago in 2005, 2008 and 2011.

MERIS full resolution (FR) data have been used to study TSM trends over a decade in coastal waters of Vietnam that are under the influence of the Mecong River (Loisel et al., 2014). Shen et al. (2013) studied suspended sediment concentration responses over a period of continuous and long-term river discharge decline in the Yangtze estuary from 2003 to 2010. Zhao et al. (2015) used MERIS FR data for characterization of harmful algae blooms in the Arabian Gulf and the Sea of Oman.

No studies on the Baltic Sea region have focused on relating hydrometeorological conditions and vessel traffic intensity with water quality variations in a harbour area based on time series of remote sensing imagery.

The main objectives of our study were:

- To analyse the potential of MERIS FR data to monitor inter annual variability of water quality parameters (TSM, CDOM) in harbours along the Eastern Baltic Sea coastline.
- To assess trends in TSM and CDOM concentrations over a decade (2002–2011) near harbours.
- To evaluate the impacts of wind regime changes/variations and riverine inflows on water quality parameters (TSM, CDOM) in the vicinity of harbours.
- To analyse the effect of shipping intensity to water quality in harbours using MERIS imagery.

2. Data and methods

2.1. Study site description

The coastline of Estonia is ~1200 km long and there are 26 harbours located along the coastline. Only 10 of those harbours handle > 1 million ton of goods or > 200,000 passengers annually and are considered as main ports according to Directive 2009/42/EC of the European Parliament and of the Council. Our study focuses on five harbours: Tallinn, Kunda, Sillamäe, Virtsu and Pärnu (Fig. 1). Tallinn and Virtsu harbours operate regular passenger ferries and represent intense ship traffic levels (over 6000 vessel visits per year). Harbours of Kunda and Sillamäe in Eastern Gulf of Finland and port of Pärnu in the Gulf of Riga mainly operate cargo and the ship traffic in those harbours remains below 1000 vessel visits per year. The water area of harbours under investigation is shown in Table 1.

2.2. Satellite data

Full resolution data from MERIS mission (which lasted from May 2002 until April 2012) provides better overall understanding of coastal processes compared to other remote sensing data like Landsat or MERIS reduced resolution data (Kratzer et al., 2014). The main advantage of MERIS FR imagery compared to other available ocean colour sensors (e.g. MODIS or VIIRS) is its higher spatial resolution. For the decade (2002–2011) we studied there is also Landsat satellite remote sensing data with high spatial resolution (30 m) available but the revisit time (16 days at northern latitudes) and spectral resolution (designed for terrestrial studies) of Landsat instrument reduce the possibility to acquire sufficient amount of cloud free images (Kratzer et al., 2014). The use of MERIS FR imagery provides us larger amount of cloud free images (because of frequent revisit time) with suitable spatial and

spectral resolution to catch the water quality variations in the coastal sea.

We used MERIS FR level-1 data from 2002 to 2011 (April–October) (<http://www.coastcolour.org/data/archive/>). The pixel size of MERIS FR data is 300 × 300 m and revisit time 2–3 days. In total, 470 sufficiently cloud free MERIS images were used in the study. The number of used images for each month is shown in Table 2.

2.2.1. Satellite data processing

In the present study, level-2 water quality products (TSM and CDOM) were retrieved from level-1 MERIS imagery using the Case II Regional (C2R) algorithm (Doerffer and Schiller, 2007). The C2R algorithm was developed for coastal waters and involves two procedures that are based on a neural network approach: atmospheric correction and the conversion of inherent optical properties to water quality parameters. All quality flags and masks provided in the level-1 Coast Colour product and level-2 C2R product were used in data processing. The C2R algorithm was preferred as in our previous study (Raag et al., 2014), the algorithm enabled to retrieve TSM concentrations more accurately in our study area (coefficient of determination $R = 0.78$, root mean square error $RMSE = 0.82 \text{ mg L}^{-1}$, standard deviation $SD = 0.77 \text{ mg L}^{-1}$, mean bias $MB = -0.28 \text{ mg L}^{-1}$) than other algorithms designed for turbid and optically complex coastal waters.

Although we used CDOM retrievals obtained from the C2R algorithm, we did not validate the C2R processor for estimating CDOM in our study sites. Nevertheless, the reliability of the C2R for estimating the CDOM in the Baltic Sea has been evaluated in Vaičiūtė et al. (2012) and Attila et al. (2013). Vaičiūtė et al. (2012) showed that in Lithuanian coastal seas (conditions similar to harbours in the Gulf of Riga and Moonsund area) the C2R processor explains > 50% of variations in CDOM ($R = 0.8$). Attila et al. (2013) demonstrated that in Finnish coastal seas (where conditions are similar to the harbours of the Gulf of Finland), the C2R processor explains CDOM variations at a reliability level of $R = 0.66$. As both studies report that the C2R algorithm is capable of detecting > 50% CDOM variations we assume that it can be implemented on uniform MERIS dataset to analyse CDOM trends in the coastal zone of the Baltic Sea.

2.2.2. Statistics used in analysis of inter annual variability and trends in TSM and CDOM

Inter-annual variations of TSM and CDOM concentrations in five harbours located along Estonian coastline (Fig. 1) were examined from MERIS images as follows:

- By calculating the annual mean and standard deviation (SD) of TSM and CDOM for 2002–2011 at each site.
- By calculating monthly mean and standard deviation (SD) of TSM and CDOM for July in years 2002–2011 at each site. The analysis of monthly mean was done as a reference to the annual mean. July was chosen as reference month for the analysis as the number of MERIS images obtained in July was the highest (Table 2).

TSM and CDOM trends for the decade were evaluated by applying a linear regression analysis to identify systematic increases or decreases in TSM and CDOM levels for different harbours over the examined decade. The trend was characterised by the coefficient of the determination (R) and the trend were considered significant at confidence level (p) 0.05.

2.3. Vessel traffic, river flow rates and wind data

2.3.1. Vessel traffic

The number of annual vessel visits for the harbours of Tallinn, Kunda, Pärnu, Sillamäe and Virtsu was obtained from the Statistics Estonia database (<http://www.stat.ee/en>). As the Port of Tallinn operates the harbours of Tallinn, Muuga and Paldiski, the vessel visit data

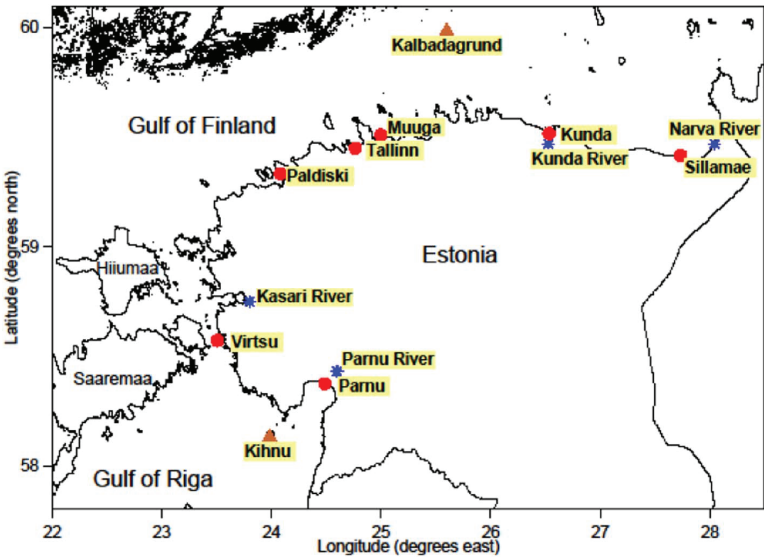


Fig. 1. Study site. Harbours locations are marked as red circles, meteorological stations (wind data) are marked as brown triangles and hydrological stations (river flow rate) are marked as blue stars. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Water area of harbours under investigation.

Port	Water area (ha)
Tallinn	93
Virtsu	17.5
Sillamäe	390.5
Kunda	76
Pärnu	225.68

Table 2
Number of sufficiently cloud-free images per month from 2002 to 2011.

Year	Month							Total number of images per year
	April	May	June	July	August	September	October	
2002	0	0	2	3	11	4	0	20
2003	5	4	6	14	8	7	6	50
2004	9	10	11	12	10	6	5	63
2005	9	10	10	11	9	5	7	61
2006	6	11	10	11	7	5	0	50
2007	11	9	10	6	9	2	2	49
2008	5	12	8	10	5	5	3	48
2009	9	10	8	7	7	5	2	48
2010	9	10	9	11	9	2	4	54
2011	3	7	8	4	3	2	0	27
Total number of images per month	66	83	82	89	78	43	29	

includes the summed values of all three harbours. According to Port of Tallinn data, Tallinn Harbour accommodates approximately 2/3 of all vessel visits and the Paldiski and Muuga Harbours accommodate 1/3 of all vessel visits. The number of vessel visits for the Sillamäe and Virtsu harbours was only available for 2010 and 2011. Therefore, the two ports could not be used in statistical analysis. The vessel visit number was used to estimate the effects of changing transportation patterns on water quality parameters.

2.3.2. River flow rate data

Mean monthly and mean annual flow rates (Q , $m^3 s^{-1}$) were measured for the Narva, Kunda, Pärnu and Kasari Rivers. The flow rates were used to characterize the effects of riverine inflows on coastal water quality near harbours.

2.3.3. Wind data

Wind speed ($m s^{-1}$) and direction ($^{\circ}$) data with of 3-h temporal resolution were measured at the Kihnu (2004–2010) and Kalbadagrund weather stations (2003–2009), which provide representative data on marine wind conditions for the Gulf of Riga and Gulf of Finland, respectively (Fig. 1). Data from the Kalbadagrund station were available for 2003–2009 and data from the Kihnu station were available for 2004–2010. The wind speed measured at Kalbadagrund was recorded at 32 m above the mean sea level while records drawn from the Kihnu station were recorded at 10 m. The Kalbadagrund wind speed was corrected as proposed by Soomere (2005) to synchronize the datasets. Mean annual and mean monthly wind speed values together with wind roses were calculated from data collected from April–October of each year to estimate the effects of wind regime change and directional variations on water quality parameters in the studied harbours.

3. Results

3.1. Annual TSM variations and patterns

The annual mean TSM maps retrieved from MERIS data show the differences in TSM concentration along the Estonian coastline and indicate inter-annual variations of TSM (Fig. 2). The lowest TSM is always in the central Gulf of Finland (GoF) and highest in the Pärnu Bay, Gulf of Riga (GoR). The greatest horizontal variability of TSM concentrations is in Moonsund area which is characterised by high hydrodynamic activity (Fig. 2). The pixel values at the shipping channel inside the harbour water area were extracted from MERIS TSM images for detailed analysis of inter-annual TSM variations (Fig. 3.). The average annual mean TSM concentration ($1.93 mg L^{-1}$) and its inter-annual variation ($SD < 0.38 mg L^{-1}$) were relatively low in the Tallinn harbour located in the central Gulf of Finland (Fig. 3, Table 3). The average annual mean TSM concentrations for harbours locating in the Eastern Gulf of Finland were $3.4 mg L^{-1}$ ($SD = 0.81 mg L^{-1}$) and $3.96 mg L^{-1}$

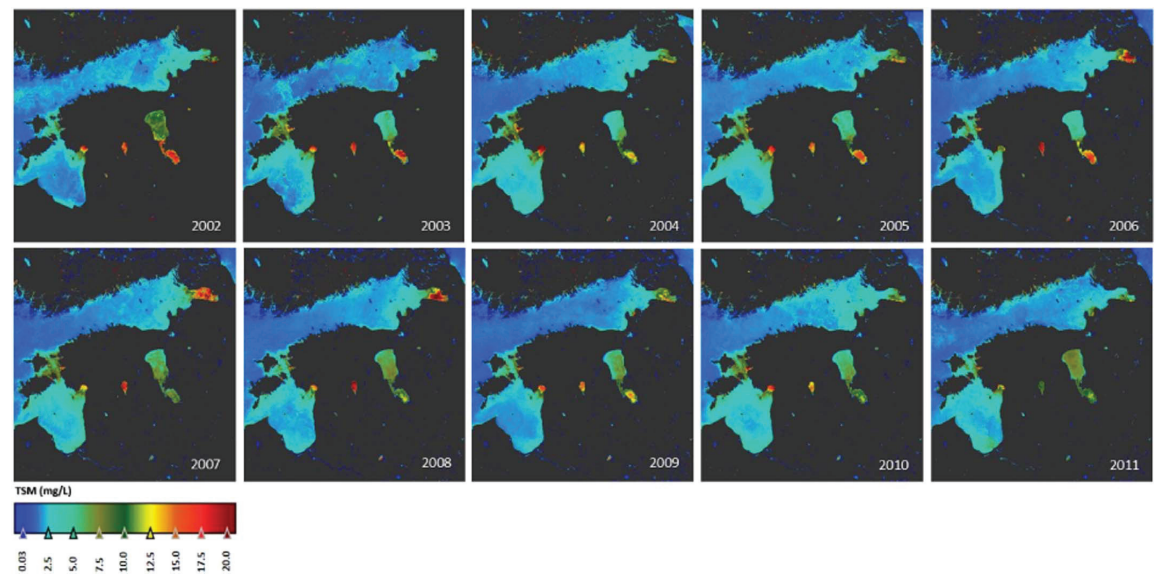


Fig. 2. Maps of annual mean TSM for years 2002–2011 retrieved from MERIS imagery.

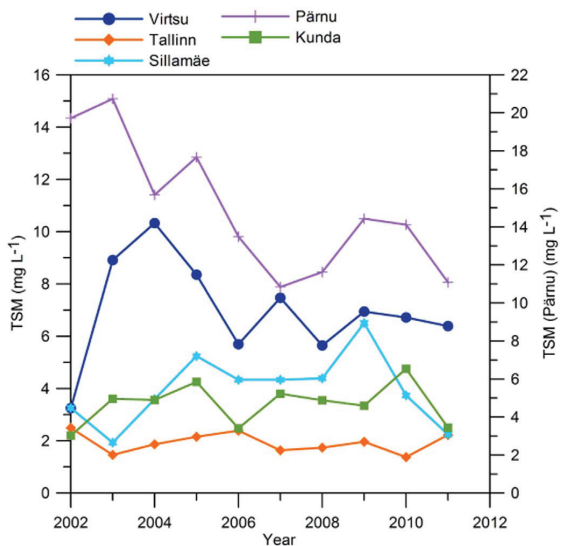


Fig. 3. Mean annual TSM in the studied harbours for 2002–2011. Note the secondary y-axis and separate scale for Pärnu Harbour TSM.

Table 3
TSM trend analysis statistics for 2002–2011 in different harbours.

	Virtsu	Tallinn	Sillamäe	Pärnu	Kunda
Mean annual TSM and SD (mg L ⁻¹)	6.97 (1.97)	1.93 (0.38)	3.96 (1.35)	14.94 (3.50)	3.40 (0.81)
R (annual mean trend)	0.10	0.22	0.21	0.79	0.20
p-level (annual mean trend)	0.79 (0.78)	0.54 (0.52)	0.56 (0.56)	0.01 (0.01)	0.58 (0.59)
Monthly mean TSM and SD in July (mg L ⁻¹)	5.65 (5.13)	1.74 (1.05)	2.95 (1.77)	13.61 (5.67)	1.49 (1.01)
R (monthly mean trend)	0.28	0.09	0.16	0.39	0.10
p-level (monthly mean trend)	0.43 (0.42)	0.82 (0.82)	0.68 (0.68)	0.27 (0.26)	0.79 (0.79)

(SD = 1.35 mg L⁻¹) (Table 3). The high standard deviation of averaged annual mean TSM concentrations 1.97 mg L⁻¹ in the Virtsu harbour denotes larger inter-annual fluctuations compared to harbours located in the Gulf of Finland (Table 3). The highest mean annual TSM concentration of 14.94 mg L⁻¹ and high levels of variability (SD = 3.5 mg L⁻¹) were observed near the Pärnu Harbour located in the Gulf of Riga.

The monthly averaged TSM for July was always smaller compared to annual mean TSM (Table 3). For harbours of Tallinn, Virtsu and Pärnu the average monthly mean TSM for July was about 10% smaller compared to average annual mean TSM. There were larger fluctuations in TSM in Virtsu and Pärnu harbours (SD = 5.13 and 5.67 mg L⁻¹) compared to Tallinn harbour (SD = 1.05 mg L⁻¹) in July (Table 3). In Kunda harbour the average monthly mean TSM for July was considerably (43%) lower compared to annual mean TSM. The difference between monthly average for July and annual mean TSM for Sillamäe harbour was ~25%.

The trend analysis shows that in Pärnu harbour the TSM concentrations decreased over the examined decade and none of the other harbours show positive TSM trends (Table 3). The decreasing trend was found to be significant: R = 0.79 p = 0.01 (at the 95% confidence level) (Table 3). The TSM concentration time series shows that close to the harbours of Pärnu there was a distinct decrease in TSM concentrations in 2006 and 2007 compared to the previous years (Fig. 2). Trend analysis of monthly mean (July) TSM showed that only in Pärnu harbour slightly decreasing TSM trend (R = 0.39) was observed. However, the trend was not significant (p = 0.27). None of the other studied harbours showed any TSM trends over the studied decade. The

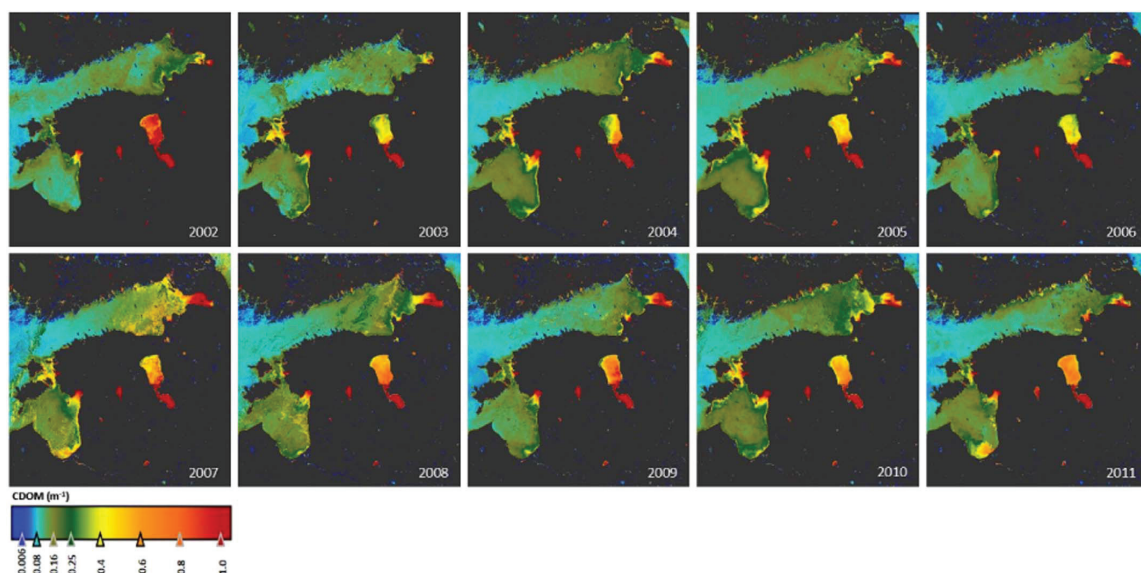


Fig. 4. Maps of annual mean CDOM for years 2002–2011 retrieved from MERIS imagery.

causes of inter-annual variations and of significant TSM concentration trends are analysed in the Discussion section.

3.2. Annual CDOM variations and trends

The annual mean CDOM maps retrieved from MERIS images are shown on Fig. 4. The pixel values of CDOM extracted from MERIS images at each harbour are presented on Fig. 5 and in Table 4. The inter-annual variability of annual mean CDOM was found to be low ($SD < 0.03 \text{ m}^{-1}$) in the harbour of Tallinn with corresponding mean CDOM value of 0.12 m^{-1} (Fig. 5, Table 4). The average annual mean CDOM values were 0.26 m^{-1} and 0.28 m^{-1} in the harbours of Sillamäe

(with $SD = 0.08 \text{ m}^{-1}$) and Kunda ($SD = 0.15 \text{ m}^{-1}$) (Fig. 5 and Table 4). In Virtsu harbour the annual mean CDOM was 0.41 m^{-1} ($SD = 0.13 \text{ m}^{-1}$). Extremely high mean annual CDOM values were found near Pärnu harbour, presenting a maximum value of 2.18 m^{-1} in 2004 and a minimum value of 0.96 m^{-1} in 2006 (averaged annual mean CDOM 1.57 m^{-1}). The average monthly mean CDOM for July was lower than average annual mean CDOM in all study sites (Table 4). The largest difference was in the harbour of Kunda (65%). In Tallinn harbour the difference was 17% and in Virtsu 22%. In Sillamäe and Pärnu harbours the average monthly mean CDOM was about 30% smaller compared to average annual mean CDOM. We could not identify CDOM trends over the decade not in monthly mean or in annual mean data in any of the harbours.

3.3. Annual vessel traffic in harbours

Information on vessel traffic in different harbours shows that the studied harbours present considerable differences in terms of vessel visit levels (Fig. 6.). The numbers range from 30 visits per year in Pärnu in 2008 to 12,500 visits per year in Tallinn Harbour in 2002. In harbours with regular passenger ferry traffic such as the Tallinn and Virtsu harbours, there are > 6000 vessel visits every year. In Tallinn, peak vessel traffic levels occurred in 2002 followed by a rapid decrease (over 50%) in 2003. The number of vessel visits per year remained between 4000 and 7000 during 2003–2012. The harbours of Kunda and Pärnu are characterised by low number of annual vessel visits, which have remained below 1000 until 2012 with strong inter-annual variations. In Pärnu, peak vessel traffic levels occurred in 2002 followed by a drastic decrease in 2003. Annual vessel visit levels in Pärnu remained at < 100 ships per year until 2010 and increased to 572 in 2011. In Kunda, vessel visit levels ranged between 50 and 200 until 2010 and then increased rapidly to 600 in 2011 (Fig. 6).

3.4. Annual flow rates from rivers located close to harbours

The 2002–2011 mean annual flow rates (Q) for the Kunda, Kasari, Pärnu and Narva Rivers (located close to the harbours of Kunda, Virtsu, Pärnu and Sillamäe) were analysed to estimate the effects of riverine inflows on water quality (Fig. 7). The highest mean annual flow rates

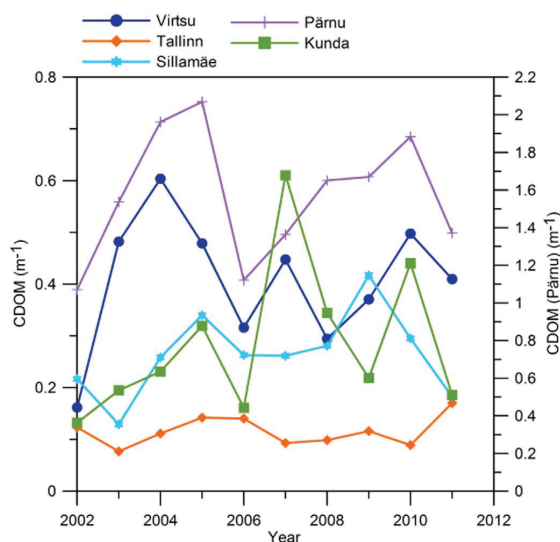


Fig. 5. The mean annual CDOM concentration for the studied harbours for 2002–2011. Note the secondary y-axis and separate scale for Pärnu Harbour.

Table 4
CDOM trend analysis statistics for the decade (2002–2011) in different harbours.

	Virtsu	Tallinn	Sillamäe	Pärnu	Kunda
Mean annual CDOM and SD (mg L^{-1})	0.41 (0.13)	0.12 (0.03)	0.26 (0.08)	1.57 (0.34)	0.28 (0.15)
R (annual mean trend)	0.11	0.22	0.34	0.14	0.33
p-level (annual mean trend)	0.76 (0.77)	0.53 (0.54)	0.34 (0.35)	0.69 (0.71)	0.35 (0.36)
Monthly mean CDOM and SD in July (mg L^{-1})	0.32 (0.34)	0.10 (0.06)	0.18 (0.09)	1.10 (0.61)	0.10 (0.07)
R (monthly mean trend)	0.28	0.09	0.16	0.29	0.005
p-level (monthly mean trend)	0.43 (0.43)	0.83 (0.83)	0.68 (0.69)	0.41 (0.41)	0.99 (0.99)

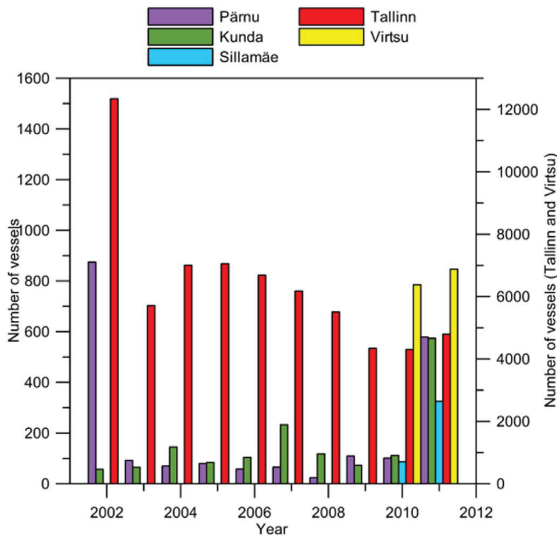


Fig. 6. Annual number of vessel visit for the harbours of Tallinn, Kunda, Pärnu, Sillamäe and Virtsu. Note secondary y-axes for Tallinn and Virtsu.

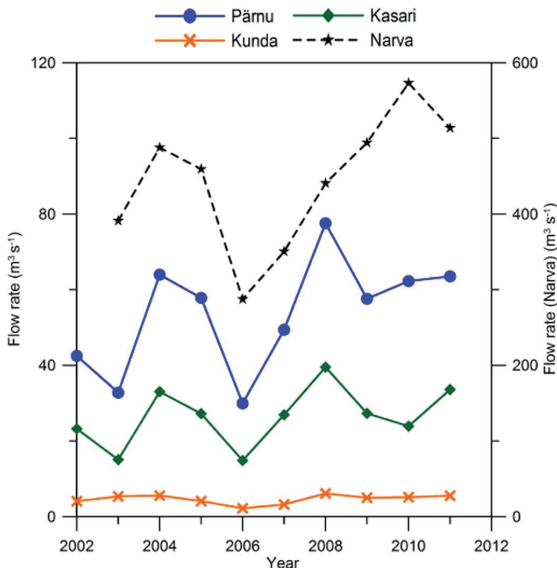


Fig. 7. Mean annual flow rate for the Pärnu, Kunda, Kasari and Narva Rivers for 2002–2011. Note the secondary y-axes for the Narva River flow rate.

between 300 and 600 $\text{m}^3 \text{s}^{-1}$ were recorded in the Narva River that is located near Sillamäe Harbour. The mean annual flow rate of the Pärnu River ranged between 30 and 80 $\text{m}^3 \text{s}^{-1}$ while corresponding values for the Kasari River ranged between 15 and 40 $\text{m}^3 \text{s}^{-1}$. The Kunda River presented a significantly lower mean annual flow rate (approximately 5 $\text{m}^3 \text{s}^{-1}$) compared to other rivers. Inter-annual variations in flow rates follow similar patterns in all four rivers with the lowest values found in 2006. However, the year presenting maximum mean annual flow rates presents some dissimilarity for the analysed decade. In the Pärnu, Kasari and Kunda Rivers, maximum values were reached in 2008 while maximum values were reached in 2010 in the Narva River.

3.5. Wind speed and direction

Wind conditions influence the vertical and horizontal distribution of water constituents. Mean annual and mean monthly wind speeds for Kalbadagrund (describing conditions in the harbours of Sillamäe, Kunda, and Tallinn) and for the Kihnu stations (describing conditions in the harbours of Pärnu and Virtsu) are given in Fig. 8. The monthly average wind speed was between 3.5 and 9 m s^{-1} in Kihnu and between 4.2 and 8.9 m s^{-1} in Kalbadagrund (Fig. 8). Maximum mean monthly wind speed values were recorded in October while lower wind speeds prevailed during the summer (June and July) of each year (Fig. 8).

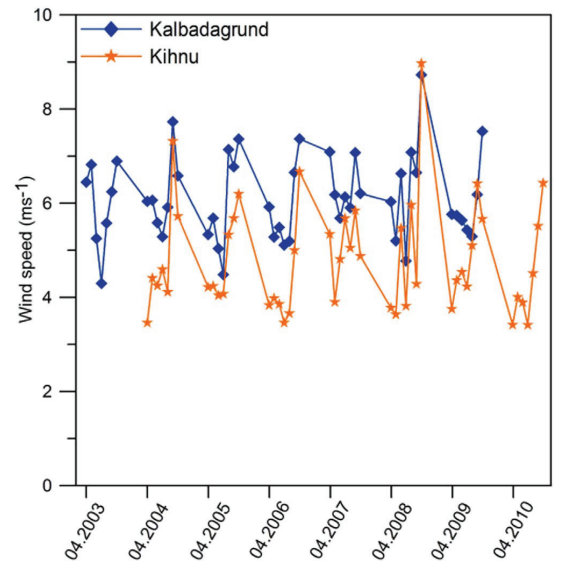


Fig. 8. Monthly mean and annual mean wind speed (m s^{-1}) levels at the Kihnu (2004–2010) and Kalbadagrund (2003–2009) stations.

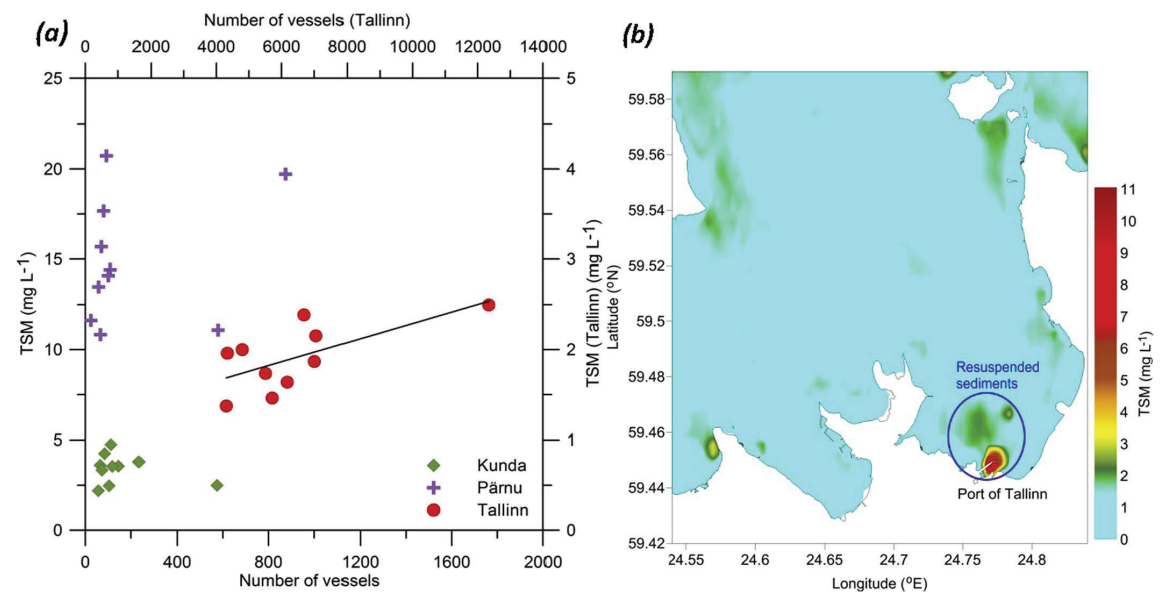


Fig. 9. (a) Scatter plot annual vessel visit level vs. mean annual TSM concentration. Note separate X and Y axes for Tallinn harbour. (b) An example of TSM concentration map derived from a single MERIS image where the elevated TSM concentration (2–7 mg L⁻¹) near the Tallinn harbour can be distinguished from the surrounding area (below 2 mg L⁻¹).

3.6. Comparison between water quality parameters, vessel traffic and hydro-meteorological conditions

A comparison between mean annual TSM and vessel traffic levels for three different harbours using simple regression analysis is shown in Fig. 9a. The vessel traffic footprint was identified in the harbour of Tallinn, where the coefficient of determination (R) between vessel visit levels and mean annual TSM concentrations was 0.66 (*p*-level 0.035). In the harbours of Pärnu and Kunda, the corresponding coincidence was not significant. Example of vessel traffic impact on TSM concentration map over Tallinn Bay area derived from a single MERIS image is shown on Fig. 9b.

Annual mean wind speed was compared against the annual mean TSM. The corresponding coefficients of determination were below 0.3 thus no significant coincidence between these parameters was observed. However, a comparison between monthly average wind speed and monthly averaged TSM concentrations reveals significant correlations for at least one year during the decade in each harbour except for the harbour of Virtsu (Table 5).

We compared annual river inflow and annual TSM and CDOM levels for the harbours of Pärnu, Sillamäe and Kunda located close to the river mouth (Table 6). Fluctuations in annual flow rates were reflected in the inter-annual variations of coastal TSM close to the Pärnu harbour where increased flow rate seemed to decrease the TSM concentration, however

Table 5
Coefficient of determination (R) between monthly mean TSM concentrations and monthly mean wind speed for each year from 2002 to 2010 obtained for different harbour areas. Kalbadagrund wind data were used for the harbours of Tallinn, Kunda and Sillamäe. Kihnu wind data were used for the harbours of Pärnu and Virtsu. The coefficients of determination exceeding 0,5 are highlighted in bold.

	2003	2004	2005	2006	2007	2008	2009	2010
Pärnu		0,82	0,89	− 0.45	0,23	0,10	0,91	0,46
Virtsu		0,18	0,36	− 0.42	− 0.11	0,4	0,35	0,05
Tallinn	0,9	0,27	0,19	− 0.42	0,59	− 0.82	0,14	
Kunda	0,9	0,86	0,83	0,81	0,79	− 0.24	0,82	
Sillamäe	0,66	0,34	0,8	0,87	0,79	0,28	0,92	

Table 6
Correlations between mean annual CDOM/TSM concentration and mean annual flow rate of the nearest river in four different harbours.

	CDOM	TSM
	R (p value)	R (p value)
Sillamäe vs. Narva River	0.25 (0.52)	0.005 (0.99)
Pärnu vs. Pärnu River	0.59 (0.075)	− 0.49 (0.15)
Virtsu vs. Kasari River	0.073 (0.84)	0.052 (0.88)
Kunda vs. Kunda River	0.09 (0.81)	0.26 (0.47)

the correlation was not significant (*R* = 49, *p* = 0.15). Comparison of mean annual flow rate and CDOM values revealed a correlation for the Pärnu site. The increase in flow rate from Pärnu River increased mean annual CDOM (*R* = 0.59, *p* = 0.075).

4. Discussion

The mean TSM for July in harbours Pärnu, Tallinn, Sillamäe and Kunda calculated from MERIS images for the decade (2002–2011) were in coincidence with our previous study (Raag et al., 2014) where mean TSM for July was calculated from MERIS images for period of 2006–2011. The interannual variations in water quality parameters were observed at each study site and the drives for these variations are discussed in the following chapters.

4.1. Drivers of inter-annual TSM variations in harbours

4.1.1. Vessel traffic

Ship traffic is a known source of sediment resuspension as shown by previous studies. Rapaglia et al. (2015) demonstrated the effects of ship traffic on sediment concentration and transport in the Venice lagoon. Briciu-Burghina et al. (2014) showed that turbidity events in the Dublin port are largely related to vessel activity. However, these studies have focused on relatively short periods and on individual ships effecting turbidity. We compared vessel traffic data and annual TSM

concentrations for the harbours of Pärnu, Kunda and Tallinn over a 10-year period to identify vessel traffic effects on water quality parameters. Our analysis shows that in Tallinn Harbour, which presents intense levels of vessel traffic (Fig. 6), there is a significant relationship between the mean annual TSM and vessel traffic ($R = 0.66$, $p = 0.035$) (Fig. 9). Our results confirm that the increase in vessel traffic increases mean annual TSM concentrations in harbour areas and thus affects water quality in Tallinn Bay. No significant relationship ($R = 0.24$, $p = 0.50$ and $R = 0.8$, $p = 0.43$ correspondingly) between the annual TSM and ship traffic (Fig. 9) was found in the harbours of Pärnu and Kunda. Therefore, vessel traffic has no effect on TSM when the annual vessel visit level is < 1000 . It can be concluded from the analysis that in cases of intense vessel traffic (> 6000 visits per year), effects on harbour water quality are identifiable from mean annual TSM concentration data retrieved from remote sensing imagery while in case of low traffic rates (< 1000 vessel visits per year), the impact is not detectable.

4.1.2. Wind speed and direction

We found no relationship between the annual mean wind speed and annual mean TSM in any of the harbours, indicating that inter-annual TSM variability is not related to changes in wind speed. However, Table 5 indicates that there is correlation between monthly mean wind speed and monthly mean TSM concentrations for some years in each harbour (except Virtsu). In harbours of Kunda and Sillamäe locating in the Eastern Gulf of Finland the TSM concentration and wind speed correlated in most of the analysed years. This indicates that near these harbours the changes in wind speed are the main drivers of monthly mean TSM concentration changes during the analysed years. In Pärnu Harbour, the monthly mean wind speed and monthly mean TSM values show a strong correlation (up to 0.91) during 3 of the 7 analysed years. The strong correlation between monthly mean wind speed and monthly mean TSM concentrations is expected; as Pärnu Bay is shallow (max depth of 8 m) and even moderate winds cause resuspension. Inter-annual variations in TSM (Fig. 3) showed a sharp decrease in 2006 in Pärnu Harbour. The mean annual TSM level was low also in 2007 and then slightly increased again. This corresponds with wind data for 2006, 2007 and 2008, when the monthly mean TSM concentration was not correlated with wind speed (Table 6). This could be explained by the shift in wind direction that occurred during these years. Wind roses (distribution of wind speed and direction) at the Kihnu station were recorded over three periods: 2004–2005, 2006–2007 and 2008–2009 (Fig. 10). It is evident from Fig. 10 that dominant winds shifted from the southwest in 2004–2005 to the west in 2006–2007, and from 2008 to 2009 dominant winds were again from the southwest. The Pärnu Bay is well protected from westerlies compared to southwestern winds (Fig. 1), and this could explain the reverse correlation found between

the monthly mean TSM and monthly mean wind speed for 2006 and 2007.

4.1.3. River discharge

River discharge is known to influence coastal water quality (Horner-Devine et al., 2008; Mendes et al., 2014). Based on the analysis of MERIS TSM imagery collected over a 10-year period Loisel et al. (2014) have shown that seasonal flow rate fluctuations affect the TSM concentration in Vietnam's coastal sea. Shen et al. (2013) presented the effects of decreased river discharge and its seasonal fluctuations on suspended sediment concentrations in the Yangtze estuary from 2003 to 2010. Soosaar et al. (2016) showed that Daugava River discharge affects coastal TSM concentrations in the Gulf of Riga and Baltic Sea through MERIS daily image analyses. As noted in the Results section, we did not find a significant correlation between TSM concentrations and mean annual river flow rates. We assume that the effects of TSM are detectable during prominent discharge events (e.g., spring time snow-melt runoff) (e.g., Soosaar et al., 2016) but they cannot be identified from the mean annual TSM concentration data. Therefore, we can assume that the effects of river discharge on inter-annual variations in TSM concentration are not as significant as the effects of wind regime.

4.2. Drivers of inter-annual CDOM variations in harbours

The majority of coastal CDOM is related to river inflows (Coble et al., 2004). The impact of riverine inputs on coastal Baltic Sea is also confirmed by previous studies. Based on MERIS imagery analysis, Vaičiūtė et al. (2015) have shown that discharge from the Nemunas River is related to variations in CDOM concentrations in the Curonian Lagoon (Baltic Sea). We analysed mean annual inflow and CDOM coincidence levels in harbours located close to river mouths. We found a positive correlation (with $R = 0.59$ $p = 0.075$) between the annual mean river inflow rate from the Pärnu River and the mean annual CDOM concentration in Pärnu Harbour. Increased flow rates from the Pärnu River increase annual CDOM in Pärnu Harbour.

Virtsu Harbour is located approximately 30 km away from the Kasari River outflow and the distance between Sillamäe harbour and Narva river mouth is 25 km (Fig. 1). We found no correlation between river discharge and CDOM concentrations at these harbours. The harbours are positioned far enough from the river outlet, and the local hydrodynamic regime does not support riverine water transport to the harbour region. Therefore, water quality levels in the harbour area are not influenced by riverine water. We found no relationship between the Kunda River flow rate and CDOM in Kunda Harbour, even though Kunda Harbour is located roughly 1 km from the river mouth. This can be explained by the relatively low ($\sim 4.6 \text{ m}^3 \text{ s}^{-1}$) mean annual flow rates of the Kunda River.

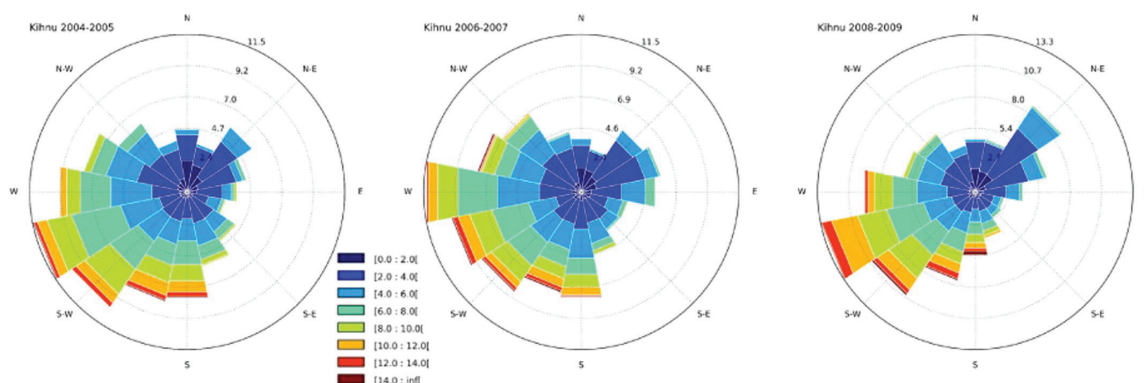


Fig. 10. Wind rose calculated from Kihnu station data.

5. Conclusions and future outlook

The MERIS database, heritage from ESA's ENVISAT mission has contributed significantly to coastal water monitoring in the Baltic Sea and worldwide. Current study is an addition to exploration of MERIS full resolution dataset. The primary aim of the study was to analyse the inter-annual variability of TSM and CDOM in harbours from MERIS FR data and explain the causes of the variations. Our study revealed the capability of MERIS full resolution data to determine average background of TSM and CDOM and their inter-annual variations in harbour areas that are in the scale of 1–3 km².

The range of average annual TSM in harbours located along the Estonian coastline (~1200 km) was from 1.93 mg L⁻¹ in Tallinn Harbour to 14.94 mg L⁻¹ in Pärnu harbour. We found a decline in the TSM concentrations in Pärnu Harbour over the examined decade (2002–2011). In other harbours, no significant ($p < 0.05$) TSM concentration trend was found.

The study also provided information on how the changes in hydro-meteorological conditions affect the inter-annual variability of TSM and CDOM. Changes in wind regimes (especially shifts in dominant wind directions) can decrease mean annual TSM concentrations by 30% (i.e., Pärnu Harbour located in a shallow bay).

Our study shows that mean annual values cannot be used to determine wind speed effects on mean annual TSM concentrations. However, we found a significant correlation ($R > 0.59$, $p < 0.05$) between monthly mean wind speed and monthly mean TSM concentrations in certain years in most of the harbours. Changes in monthly mean wind speed in harbours of Sillamäe and Kunda (located in the eastern Gulf of Finland) were in coincidence with variations in TSM concentrations in most of the years during the analysed decade. In Virtsu harbour the TSM and wind speed were not correlated ($R < 0.35$) in any of the years showing that in Moonsund area the wind speed variations do not reflect in changes of TSM concentration.

Annual changes in CDOM concentrations in harbours located close to a river mouth can be related to river discharge patterns. An increase in discharge in the Pärnu River from 30 to 60 m³ s⁻¹ increased the annual mean CDOM from 1 m⁻¹ to 2 m⁻¹.

Our study revealed that in harbours with intense levels of traffic (Tallinn Harbour), inter-annual variations of TSM were found to be related to vessel traffic. An increase in vessel visit levels from 4300 to 12,300 increased mean annual TSM concentrations from 1.3 mg L⁻¹ to 2.5 mg L⁻¹. In harbours where the annual number of vessel visits remained at < 1000, traffic did not affect variations in mean annual TSM concentrations.

The results of the present study specify the effects of marine traffic on water quality levels in harbours. The listed information on inter-annual TSM and CDOM variability in harbours along the Eastern Baltic coastal sea can be used to support future spatial planning and maintenance in harbour areas. For environmental management of harbour areas it is important to collect and analyse long term changes in coastal water quality and therefore the launch of Sentinel missions by ESA can contribute significantly to achievement of that goal. Especially the Sentinel-3 mission with primary objective to provide continuity of an ENVISAT type ocean measurement capability for Copernicus Services with a consistent quality, a very high level of availability (> 95%), high accuracy and reliability (Donlon et al., 2012). Sentinel-3 Ocean and Land Colour Instrument (OLCI) bands are optimised to measure ocean colour over open and coastal zones. S-3 OLCI instrument is based on the opto-mechanical and imaging design of ENVISAT MERIS but incorporates some significant improvements when compared to MERIS. Increased number of spectral bands and improvement signal to noise ratio. Also important for ocean colour data is mitigation of sun glint and improved global coverage.

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Appendix 5

Publication V

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Article

Mapping Flood Extent and Frequency from Sentinel-1 Imagery during the Extremely Warm Winter of 2020 in Boreal Floodplains and Forests

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Abstract: The current study presents a methodology for water mapping from Sentinel-1 (S1) data and a flood extent analysis of the three largest floodplains in Estonia. The automatic processing scheme of S1 data was set up for the mapping of open-water flooding (OWF) and flooding under vegetation (FUV). The extremely mild winter of 2019/2020 resulted in several large floods at floodplains that were detected from S1 imagery with a maximal OWF extent up to 5000 ha and maximal FUV extent up to 4500 ha. A significant correlation ($r^2 > 0.6$) between the OWF extent and the closest gauge data was obtained for inland riverbank floodplains. The outcome enabled us to define the water level at which the water exceeds the shoreline and flooding starts. However, for a coastal river delta floodplain, a lower correlation ($r^2 < 0.34$) with gauge data was obtained, and the excess of river coastline could not be related to a certain water level. At inland riverbank floodplains, the extent of FUV was three times larger compared to that of OWF. The correlation between the water level and FUV was < 0.51 , indicating that the river water level at these test sites can be used as a proxy for forest floods. Relating conventional gauge data to S1 time series data contributes to flood risk mitigation.

Keywords: Sentinel-1; flood; climate change



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1. Introduction

Near real-time and statistical information about flooded areas is essential for several public services, i.e., emergency, rescue, recovery, spatial planning, habitat monitoring, and adaption to climate change. Satellite remote sensing can provide timely and operational data as well as statistical spatial information about inundated areas covered with water. Two types of satellite imagery are available for monitoring surface flood dynamics: optical and synthetic aperture radar (SAR). Optical satellite remote sensing can only be applied in cloud-free situations. However, floods often occur during long-lasting periods of precipitation and persistent cloud cover. Therefore, SAR systems are usually a preferred tool for the monitoring of floods from space. A smooth open water surface is characterized by a low SAR backscatter, and this difference in backscatter response generally allows flood mapping [1]. Over the last decade, various methods for deriving the flood extent from SAR data have been proposed [2–18]. Based on summaries by Martinis et al. [18] and Liang and Liu [8], the most commonly applied methodology for flood mapping from a single image is histogram thresholding, which can be used in combination with different image processing approaches. Temporal change detection techniques [19,20] and coherence analysis [21] have also been used for open water mapping. However, temporal change detection approaches require two images and can therefore be limited by the temporal coverage of satellite imagery. To improve flood mapping accuracy, the advantages of ancillary data, such as the DEM (digital elevation model) derived HAND (height above the nearest drainage) index and the catchment derived DIST (distance from drainage) index as well as land use map, have been demonstrated in several studies [17,18,20,22]. Most of the proposed approaches

for flood mapping are semi-automatic. A fully automatic methodology that integrates split thresholding and fuzzy logic classification has been proposed and applied by Martinis et al. [18] for the processing of TerraSAR-X, and by Twele et al. [23] for the processing of Sentinel-1 (S1).

Recent studies by Grimaldi et al. [24] and Tsyganskaya et al. [25] have summarized the approaches of flood mapping under the forest canopy. The study by Grimaldi et al. [24] shows that the most commonly applied method for the detection of flooded areas under vegetation is the identification of increased backscatter values compared to other objects. The penetration depth of the SAR signal into vegetation is higher for longer wavelengths, so the use of the L-band has been recommended [26–28]. However, several studies [20,29,30] have demonstrated the capabilities of C-band and X-band data in the identification of flooded vegetation, especially in the case of sparse forests and leaf-off conditions. Co-polarized signals (HH or VV) are preferred over cross-polarized signals for mapping water under vegetation. Studies have indicated that the use of HH-polarization leads to more accurate results compared to VV-polarization [31,32]. Moreover, the use of polarimetric decomposition and/or interferometric SAR coherence has been utilized for the mapping of floods under vegetation [33]. However, the availability of full polarimetric data is often limited in terms of spatial extent and temporal coverage.

Estonia is known for its large seasonal riverside areas that are flooded over annually. The surface area of the Estonian floodplain grasslands with a high nature conservation value is estimated to be 16,000 hectares. According to the EU Habitats Directive, northern boreal alluvial meadows (habitat type code 6450) are grasslands situated on the banks of large rivers, in sections with slow flow, which are frozen in the winter and flooded in the spring–summer period. However, extremely warm winters in Estonia during the last five years have also caused large flooding during winter [34]. Extreme changes in inundation extent, depth, and duration define phenological patterns, animal migration routes, and human living spaces [35]. Therefore, it is important to monitor the temporal and spatial changes in flooded areas.

The boreal forest encompasses approximately 30% of the global forest area and provides critical services to local, regional, and global populations. Communities benefit from ecosystem services provided by forests for fishing, hunting, leisure activities, and economic opportunities [36]. Countries such as Canada, Finland, Sweden, and Russia extract wood from boreal regions for their forest industries [36]. Flooding causes disturbances in forest management, resulting in economic losses. The vulnerability of the forest ecosystem in a changing climate has been discussed in Gauthier et al. [36] and Hari and Kulmala [37]. Previous studies have expressed the importance of flood monitoring in areas with emerging vegetation for a comprehensive evaluation of the economic and environmental costs of floods [38–40]. Recent mild winters in Estonia have affected the forest industry. Forest management is impossible due to unfrozen soils and floods [41]. However, the spatial extent and duration of floods during the winter period in Estonia is still unknown.

At the European scale, two flood-monitoring services are provided. The (1) Copernicus Emergency Management Service (EMS) [42] provides a free-of-charge mapping service in cases of natural disasters, man-made emergencies, and humanitarian crises throughout the world. This service can be triggered by request in the case of an emergency. The (2) Copernicus Land Monitoring Service (CLMS) provides a pan-European, high-resolution product known as Water and Wetness. This product shows the occurrence of water and wet surfaces over the 2009–2018 period. Thematic maps were produced for the years 2015 and 2018. These layers are compiled from multi-temporal high-resolution optical and radar satellite imagery [43].

However, these services do not provide information about the inter-annual variability of water extent on the floodplains, nor information about the flooded forest areas. Therefore, the current study was initiated with the following aims:

- Set up an optimal automatic workflow for open-water and flooded forest mapping from S1 data.

- Apply the workflow for the mapping of flood duration and extent on three of the largest floodplains in Estonia during an extremely mild winter (1 November 2019–31 March 2020).
- Analyze the correlation between flood extent and the water level measured in the closest hydrological station. Define the water level that indicates the occurrence of flooding (river coastline excess) on floodplains.

2. Study Sites and Data

2.1. Study Sites

Floodplain grasslands can be found all over Estonia, and most of them lie on the larger rivers—Emajõgi, Põltsamaa, Pedja, Kasari, Halliste, Raudna, Piusa, Koiva, Mustjõgi, and Narva headwaters—but some also near lakes (Peipsi, etc.). We chose the three largest floodplain grasslands (Alam-Pedja, Soomaa, and Matsalu) as our study sites. Figure 1 shows study areas with the areas of environmental restrictions, maps of natural grasslands and forests (CLC 2018 from CLMS), and the official shoreline from the Estonian Topographic Database (ETD). Matsalu is a coastal test site located at the River Kasari delta. The defined region of interest used in the analysis of the current study was 1068 km² (Figure 1). The inland riverbank test sites of Alam-Pedja (located by the River Emajõgi) and Soomaa (located by the Halliste and Navesti rivers) have regions of interest of 546 km² and 255 km², respectively (Figure 1, Table 1).

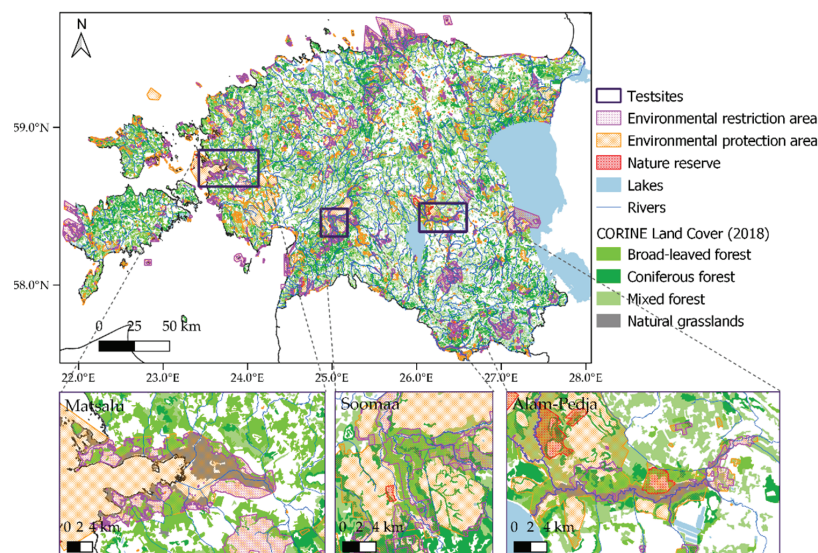


Figure 1. Location of the test sites.

Table 1. Share of natural grassland and forest types at study sites according to CLC 2018.

Test Site	Total Size (km ²)	Broad-Leaved Forest Area (%)	Coniferous Forest Area (%)	Mixed Forest Area (%)	Natural Grasslands Area (%)
Alam-Pedja	546	11.5	9.3	20.9	5.5
Soomaa	1068	2.0	4.4	3.8	7.8
Matsalu	255	17.2	11.1	11.3	0.8

Natural grasslands along rivers have a high nature conservation interest (Figure 1). The habitats of floodplain grassland vegetation are considerably more variable in com-

parison to boreo-nemoral grasslands—26 different plant communities have been noted as opposed to the 13 found in boreo-nemoral grasslands. Approximately 20–22, maximally 30, bird species are native to the floodplains in Estonia. The share of natural grassland differs between study sites—at Matsalu the share of natural grassland is 7.8% of the study area, while at Soomaa the natural grassland covers 0.8% of the total study area (Table 1).

The share of forest types according to CLC 2018 are shown in Table 1. The dominant forest type at Matsalu and Soomaa is the broad-leaf forest, while at Alam-Pedja the mixed forest type is dominant. The coniferous forest represents the smallest share of forest (Table 1).

2.2. Satellite Data

The S1 mission that carries the C-band SAR sensor provides routine data in two imaging modes: interferometric wide swath mode (IW) and extended wide swath mode (EW). The spatial resolution of the IW mode data is 5×20 m, and the spatial resolution of the EW mode data is 20×40 m [44]. The Sentinel-2 (S2) optical data are beneficial during cloud-free conditions and have a spatial resolution of 10×10 , 20×20 , and 60×60 m depending on the wavelength band [45]. The medium spatial resolution data and sufficient repeat cycle of S1 (12 days with one satellite and 6 days with two satellites) and S2 (10 days with one satellite and 5 days with two satellites) missions form a solid basis for statistical flood mapping applications and the operational flood monitoring service [46].

S1 SAR and cloud-free S2 multispectral imager (MSI) data were downloaded from the Copernicus Open Access Hub [47]. The dataset was divided into two parts: (1) algorithm development/validation and (2) algorithm application for statistical analysis. The overview of the data used for algorithm development is given in Table 2. The numbers of images included in the statistical analysis per month at each test site are given in Table 3. To eliminate the water lookalikes caused by thin ice cover, we excluded images that were acquired in the case of negative air temperature from our analysis.

Table 2. Numbers of S1 (IW mode and EW mode), S2, and UAV (unmanned aerial vehicle) images used for algorithm development and validation in open water flood (OWF) and flood under vegetation (FUV) conditions.

Purpose of Data	S1 IW	S1 EW	S2	UAV
Algorithm development (sensitivity)	1	1		
Algorithm development OWF (incidence angle backscattering dependence)	7	12		
Algorithm development FUV (incidence angle backscattering dependence)		3		
Validation	2	2	4	44

Table 3. Number of images included in analysis per month per test site. OWF represents the number of images from which open-water flood was mapped. FUV represents the number of images from which flood under vegetation was mapped.

Test Site	Nov 2019 OWF/FUV	Dec 2019 OWF/FUV	Jan 2020 OWF/FUV	Feb 2020 OWF/FUV	March 2020 OWF/FUV
Alam-Pedja	13/7	18/11	19/14	14/9	19/13
Soomaa	18/10	19/13	20/12	15/9	21/11
Matsalu	10/8	12/8	14/6	10/8	18/9

2.3. Auxiliary Data

Auxiliary datasets used in the study include different maps and hydro-meteorological information gathered during the study period.

Maps of wetlands, shorelines, inland waters, wooden areas, and buildings were downloaded from the Estonian Topographic Database (ETD) (provided by the Estonian

Land Board) [48]. Maps of areas with environmental restrictions were downloaded from the Estonian Environment Agency WFS service [49]. The digital elevation model (DEM) with a five-meter resolution was downloaded from the Estonian Land Board database [50]. CLC+ (2018) was downloaded from CLMS [43].

Air temperature and water level data measured at national hydro-meteorological stations were obtained from the Estonian Environment Agency [51].

Observations at the time of flooding and UAV flight were performed on 22 March 2019 at the Soomaa test site. In total 44 observations were used for algorithm development.

3. Methodology

3.1. Sentinel-1 Data Processing

We evaluated the sensitivity of S1 polarizations for land and water discrimination [52,53]. The overall backscatter differences resulting from the sensitivity analysis are summarized in Table 4. In the case of the IW imaging mode, the greatest difference between terrestrial and open water signals was obtained for VH polarization (10.5 dB). Data were acquired with an incidence angle of 39.5–47°. In the EW mode, the differences were the greatest for HV polarization (9.6 dB). The data were acquired with an incidence angle of 37.5–46°.

Table 4. Summary of sensitivity analysis for land and water discrimination for different S1 polarizations [52].

S1 Mode	Polarization	Water/Dry Land Difference (dB)	Flooded Forest/Unflooded Forest Difference (dB)	Range of Incidence Angle
IW	VH	10.6	0.17	39.5–47
IW	VV	10.2	1.32	39.5–47
EW	HH	7.7	4.5	37.5–46
EW	HV	9.6	0.6	37.5–46

We also evaluated the sensitivity of S1 for the discrimination of flooded forests from dry forest areas. The greatest differences were observed in the case of HH polarization (a difference of 4.5 dB). The data were acquired with an incidence angle of 37.5–46°.

Relying on the sensitivity analysis, the open water mapping algorithm was developed for IW VH and EW HV datasets, and water under vegetation was mapped from EW HH data in the current study.

Previous studies have shown the advantage of using multiple incidence angles for water mapping [54]. Therefore, we established an empirical relationship between the local incidence angle and surface water backscattering collected at our test sites. The dataset of open water backscattering from known waterbodies was collected from 7 IW and 12 EW mode images acquired at the time of flooding in October, November, December, and April in three consecutive years (2017–2019). The relationships between the local incidence angle (θ) and surface water backscattering (σ^0) for polarizations with the greatest sensitivity (Table 4 in the previous section) are shown in Figure 2a (original source of data [52]). An established relationship was used for the water mapping algorithm (Table 5) dependency. The algorithms for open water mapping from IW VH and EW HV polarizations are summarized in Table 5.

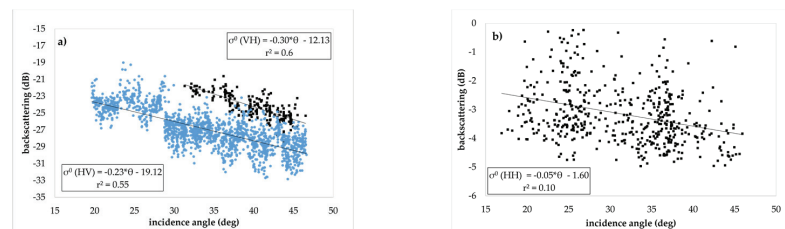


Figure 2. (a) Relationship between open-water backscattered signal (σ^0) and incidence angle (θ). IW mode data (VH) were acquired from 80 and 58 orbit overflights, and EW mode data (HV) were acquired from 51, 58, 87, 153, and 160 orbit overflights [52]. (b) Relationship between flooded forest backscattered signal (σ^0) and incidence angle (θ). EW mode data (HH) were acquired from 51, 58, 87, 153, and 160 orbit overflights.

Table 5. Water mapping threshold conditions for different polarizations, imaging modes, and flood types (FUV and OWF).

S1 Mode	Polarization	Threshold for Water Mapping	SD	No
IW	VH	Water $< -0.30 \times \theta - 12.13 + 2 \times \text{SD}$	1.43	1
EW	HV	Water $< -0.23 \times \theta - 19.12 + 2 \times \text{SD}$	2.26	2
EW	HH	Flooded forest $> -3.15 - 1.06$	1.06	3

A study by Lang et al. [55] showed the relationship between the incidence angle and backscatter of water under vegetation. The study demonstrated a decrease in backscatter by 2.45 dB at the incidence angle between 23.5° and 47°, in the case of Radarsat data. For the evaluation of the dependence of incidence angle on the backscattering in the case of a flooded forest, the data were collected at the time of flooding from images acquired on 08 November 2019, 13 November 2019, and 11 April 2018. However, analysis of our dataset did not confirm the relationship between the incidence angle and backscattered signal in a flooded forest (Figure 2b). Relying on our analysis, a threshold condition of $HH > -4.21\text{dB}$ was set for flooded forest mapping. The threshold was estimated on an averaged backscattered signal (σ^0) +1 standard deviation (SD) in flooded forest areas determined from visual observations.

The data processing scheme was set up in a cluster computing environment. The data processing setup is schematically shown in Figure 3. Pre-processing included the following steps: radar signal calibration, noise filtering, terrain correction, and the image processing technical processes of reading, cutting, and extracting data (Figure 3). Pre-processing was performed using the processors from SNAP (Sentinel Application Platform) software. Water mapping was performed according to Equations (1)–(3) presented in Table 5. The automatic water mapping processes were set up in a cluster computing environment using SHELL script to download the imagery from the Sentinel Open Data Hub and to run SNAP based GPT for water mapping. A combination of the DIST and HAND approaches was applied for the elimination of water lookalikes. The auxiliary data from the Estonian Land Board, namely, the DEM dataset with 5×5 m resolution and the official inland water body map (from ETD), were used to improve the mapping accuracy. In the first step of post-processing, the data were polygonised. In the case of inland water bodies, open water polygons (mapped from S1) that intersected with the inland waters map (ETD) with a buffer zone of 100 m were extracted for further analysis. At the coastal zone of the Baltic Sea, the open water polygons that intersected with a coastal area of up to a one meter elevation were extracted for further analysis. GDAL (Geospatial Data Abstraction Library) software processors were used for the post-processing of the data.

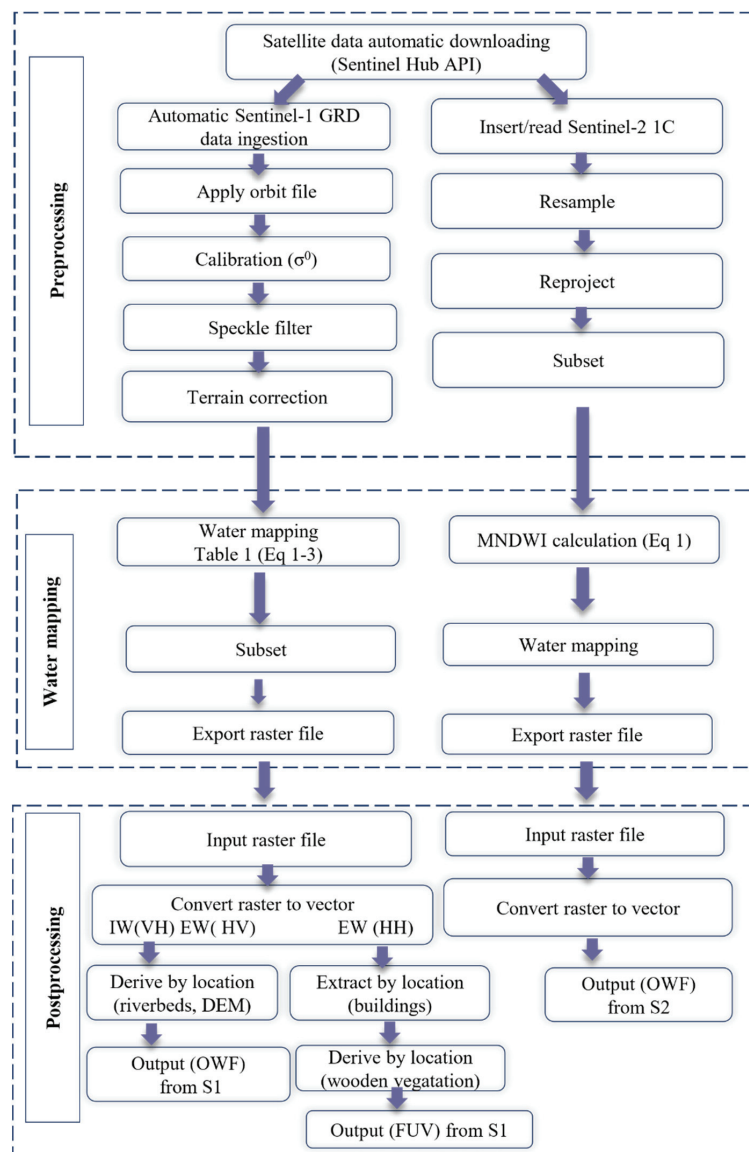


Figure 3. Data processing setup.

In the post-processing of the water mapped under vegetation, the noise (false-positives) from buildings was extracted by removing the polygons that intersected with the buildings map (from ETD). After removal of the areas with elevated backscattering caused by buildings, the water polygons related to the wooden area map (ETD) were extracted for future analysis.

3.2. Sentinel-2 Data Processing

S2 data were used as a validation dataset for an accuracy estimation of the water mapped from S1. S2 data processing is shown in the block scheme in Figure 3. The modified normalized difference water index (MNDWI) was calculated as follows:

$$\text{MNDWI} = (\text{Band 3} - \text{Band 11}) / (\text{Band 3} + \text{Band 11}) \quad (1)$$

where Band 3 is the top-of-atmosphere (TOA) reflectance of the green band of S2, and Band 11 is the TOA reflectance of the shortwave infrared band of S2. Band 3 and Band 11 have different spatial resolutions of 10 and 20 m, respectively. For the estimation of the MNDWI index, the spatial resolution of Band 11 was scaled to 10 m. In order to determine the water-covered areas from the MNDWI map, the $\text{MNDWI} > 0.6$ condition was applied. The condition was set by visually comparing the Sentinel-2 RGB images to the derived MNDWI map. The relatively high MNDWI threshold is caused by the low values of Band 11 (shortwave infrared) during wintertime. A threshold of 0.6 was sufficient to avoid a large number of false-positive detections.

3.3. Accuracy Evaluation

The accuracy of open-water flood mapping from S1 was evaluated against water mapped from S2 by estimating the overall accuracy and kappa hat coefficient. For accuracy assessment, the Semi-Automatic Classification Plugin in QGIS was used [56]. The kappa hat coefficient (κ_c) was estimated for the evaluation of classification accuracy between water mapped from S1 and S2 datasets as follows:

$$\kappa_c = \frac{p_a - p_e}{1 - p_e} \quad (2)$$

where p_a represents the overall percentage of agreements between S1 and S2 data in raster and p_e represents the percentage of chance agreement of S1 and S2 data.

The evaluation of accuracy in the case of water mapped under the vegetation is a complicated task, as water under vegetation cannot be directly mapped from the optical satellite images. The evaluation of water mapped under the vegetation was performed using drone photos and observations (44 observation points) collected at the Soomaa test site on 22 March 2019.

4. Results

4.1. Mapping Accuracy

The open water mapping accuracy from EW HV polarization data was evaluated against the MNDWI index estimated from S2 imagery at three test sites (Table 6, Figure 4). The accuracy of open water mapped from S1 EW HV polarization data at the Matsalu test site was 97.8% with a kappa hat coefficient of 0.94 (Figure 4a, Table 6). The accuracy and kappa hat coefficient of S1 IW VH data from the Alam-Pedja (96.70% and 0.84, respectively; Figure 4c) and Matsalu (95.90% and 0.86, respectively; Figure 4b) test sites were very high, while at the Soomaa test site, the corresponding numbers were lower, 93.60% and 0.62, respectively (Figure 4d).

Table 6. Validation results. Accuracy and κ_c values for different test sites and imaging modes.

Location	Date	Imaging Mode/Polarization	Accuracy (%)	κ_c
Matsalu	24 September 2019	IW/VH	95.90	0.86
Matsalu	3–4 April 2019	EW/HV	97.80	0.94
Alam-Pedja	5 April 2019	IW/VH	96.70	0.84
Soomaa	16 November 2017	IW/VH	93.60	0.62

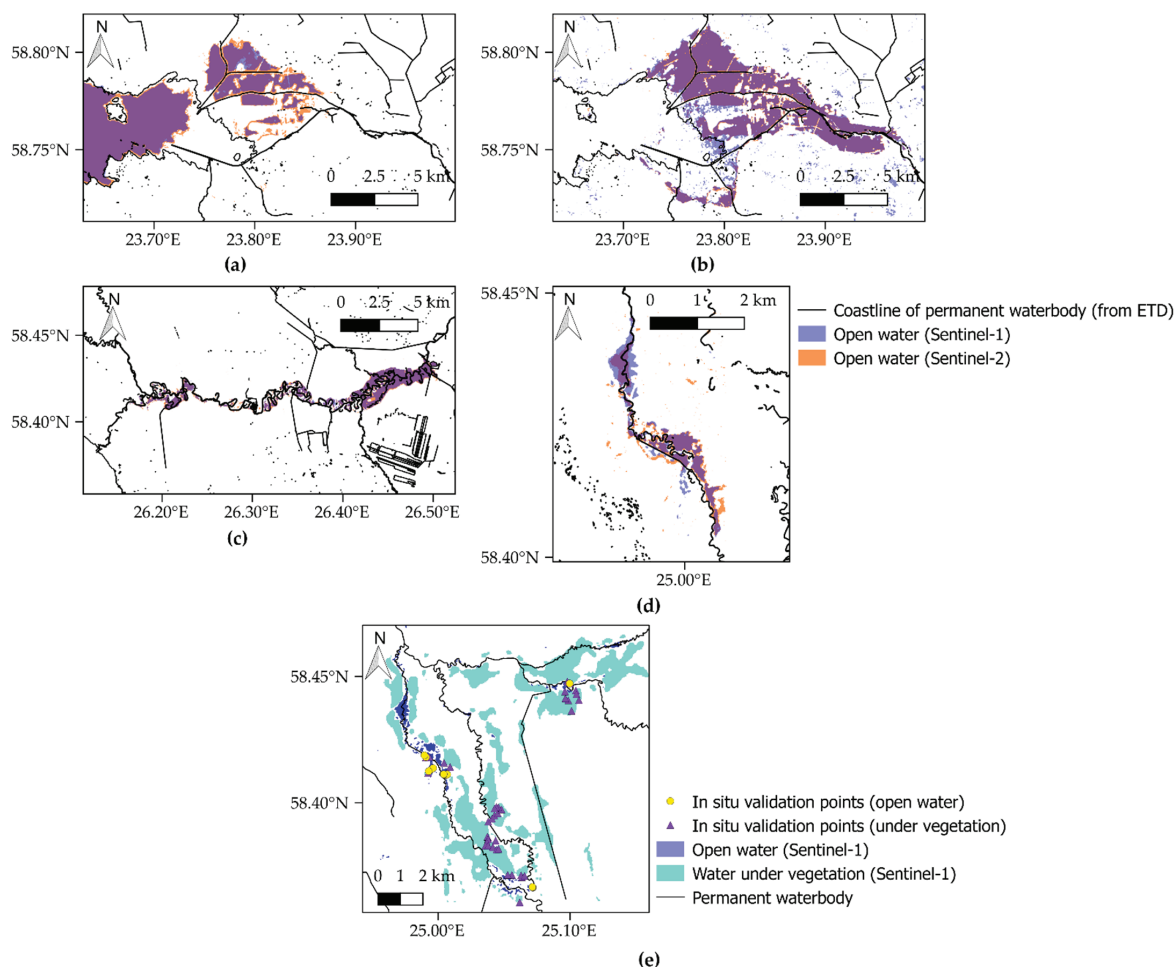


Figure 4. Validation results. (a) Open water mapped from S1 EW HV data vs. S2 MNDWI (4 April 2019), (b) Open water mapped from S1 IW VH data vs. S2 MNDWI (23 March 2019), (c) Open water mapped from S1 IW VH data vs. S2 MNDWI (5 April 2019), (d) Open water mapped from S1 IW VH data vs. S2 MNDWI (16 November 2017) and (e) Comparison of in situ validation points (22 March 2019) with open water mapped from S1 VH data (24 March 2019) and water mapped under vegetation from S1 EW HH data (23 March 2019).

The evaluation of the water mapped under vegetation was performed using drone photos and observations collected at the Soomaa test site on 22 March 2019. Figure 4e shows the water mapped from S1 images and observation points of the water. As seen in Figure 4e, the validation points coincide with mapped water under vegetation from the S1 EW mode HH data. However, it must be noted that the applied methodology for mapping FUV is less accurate (incidence angle normalization is not applicable) (Figure 2b). Still, we see that statistical analysis enables the identification of areas where water accumulates in forested areas.

4.2. Flood Extent and Frequency for Winter 2019/2020 in Estonian Floodplains

In Figure 5, open water and water under vegetation mapped from S1 data for winter 2019/2020 at our test sites are presented. The winter of 2019/2020 was extremely warm in Estonia. The monthly average temperatures from November 2019 to March 2020 were above zero (Figure 6). Climatological averages for December, January, February, and March

have been negative in Estonia in the past (Figure 6). Due to positive air temperatures in the 2019/2020 winter, the soils did not freeze, there was no permanent ice cover on inland waters, and the precipitation was mostly rain. Due to the environmental conditions of winter 2019/2020, open water could be mapped throughout the winter. The flooded area (in hectares—ha) was estimated as the extent of water-covered area outside the official shoreline within the region of interest shown in Figure 1.

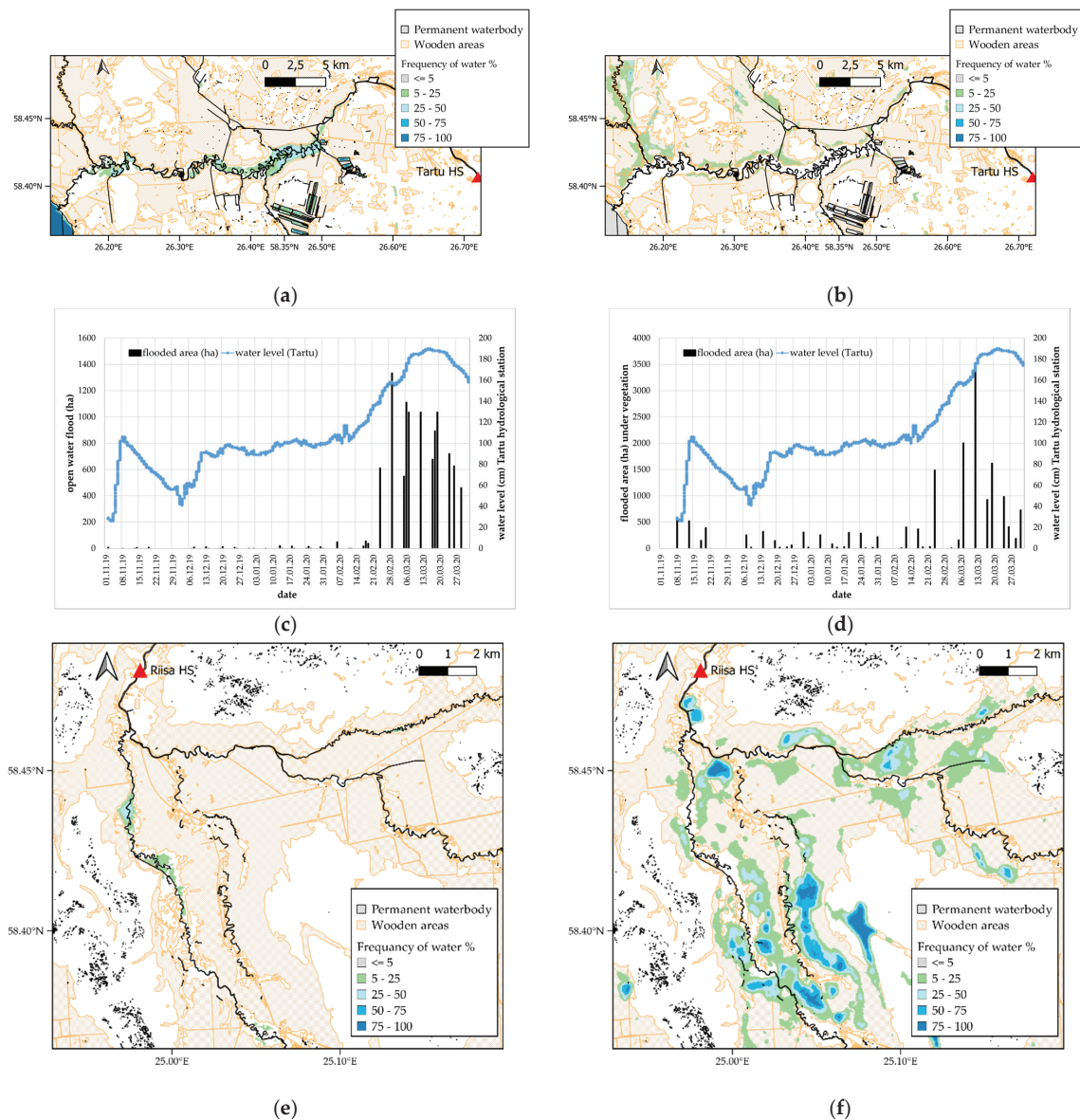


Figure 5. Cont.

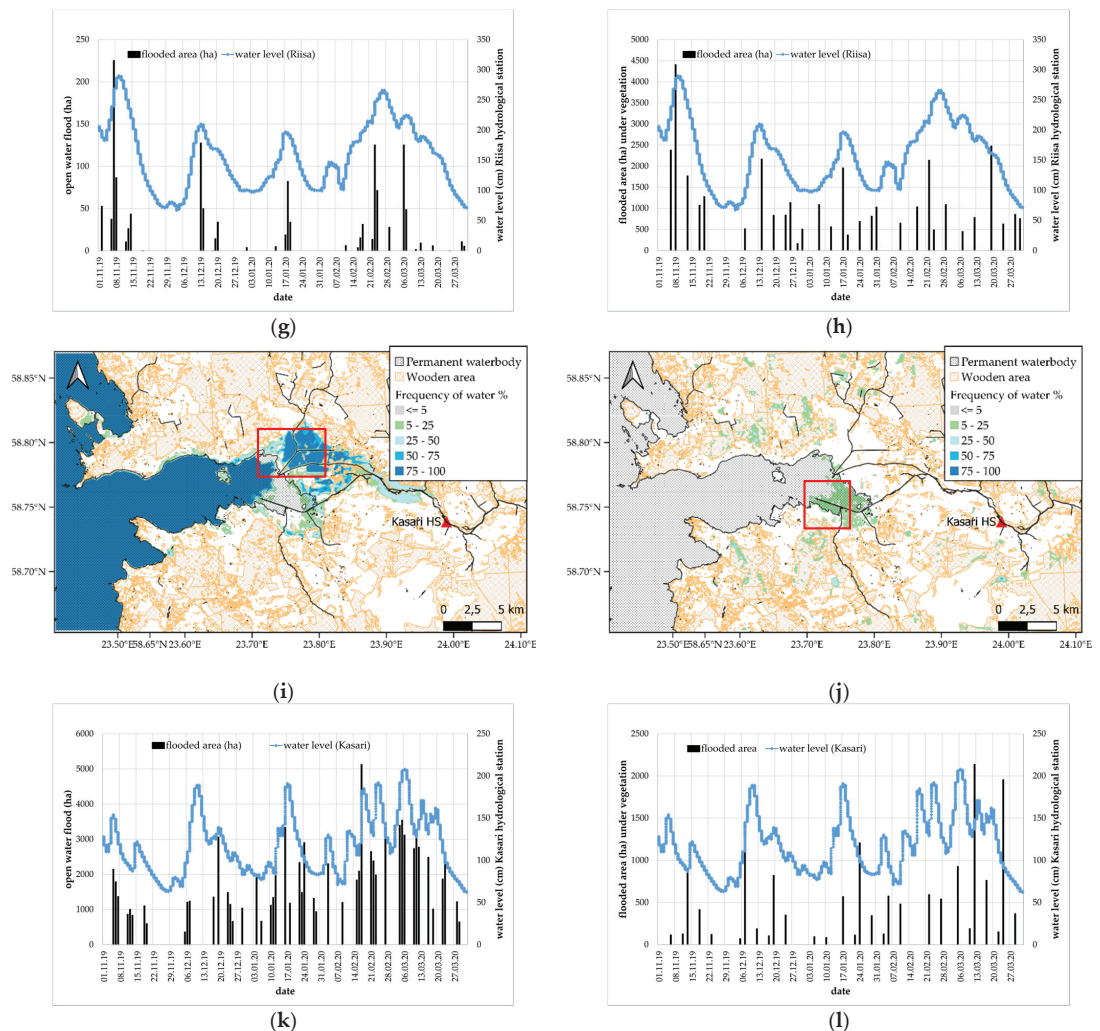


Figure 5. Floods mapped at test sites; (a) Open water frequency (%) at Alam-Pedja, (b) Frequency of water under vegetation (%) at Alam-Pedja, (c) Extent of open-water flood (ha) and water level (cm) at Alam-Pedja, (d) Extent of flood under vegetation (ha) and water level (cm) at Alam-Pedja, (e) Open water frequency (%) at Soomaa, (f) Frequency of water under vegetation (%) at Soomaa, (g) Extent of open-water flood (ha) and water level (cm) at Soomaa, (h) Extent of flood under vegetation (ha) and water level (cm) at Soomaa, (i) Open water frequency (%) at Matsalu, (j) Frequency of water under vegetation (%) at Matsalu, (k) Extent of open-water flood (ha) and water level (cm) at Matsalu, (l) Extent of flood under vegetation (ha) and water level (cm) at Matsalu.

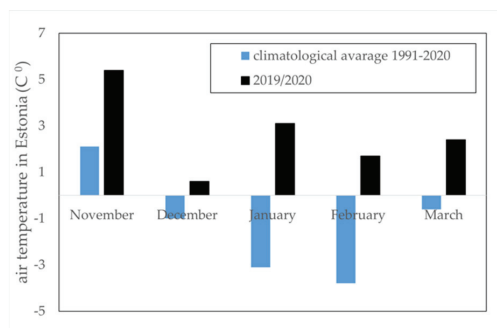


Figure 6. Meteorological data: monthly average air temperature (black) and corresponding climatological average (blue).

At the Alam-Pedja test site, open-water floods occurred near the Emajõgi river. The frequency of flood in pixel varied mainly between 5 and 25%; however, in some areas it reached over 50% (Figure 5a). Figure 5c also shows the water level measured at the Tartu hydrological station on the Emajõgi river and the estimated open-water flood extent. From mid-February, the water covered area repeatedly exceeds the shoreline, and the maximum open-water flood extent (>1000 ha) lasted from February 29 until 15 March 2020 (Figure 5c). In Figure 5, the flood frequency (Figure 5b) and extent (Figure 5d) under the vegetation at the Alam-Pedja test site are also shown. The extent of the flooded area under the vegetation was about three times larger than that of the open-water flood, reaching up to 3500 ha on 13 March 2020 (Figure 5d). However, the frequency of FUV was lower than that of the open-water flood, between 5 and 25%.

At the Soomaa floodplain, the largest flood extent was detected at the beginning of the study period on 7 November 2019, when the open-water flood reached up to 230 ha and the flooded area under the vegetation was 4400 ha (Figure 5g,h). Starting from mid-November, the open-water flood decreased, and the following flood events occurred in mid-December and mid-January. The last flood event lasted from mid-February until mid-March (Figure 5g). The maximal water level measured at the Riisa hydrological station corresponds well to the maximal open-water flood events (Figure 5g). The frequency of open-water flooding remained below 50% in Soomaa. The flood extent analysis revealed that floods detected under the vegetated area lasted through the winter. In the forested area at the Soomaa test site, the floods were absent only during the second half of November (Figure 5h). The flood frequency map presented in Figure 5f indicates the forested areas (dark blue denotes flood frequency >75%) where floods occurred throughout almost the whole duration of the winter.

At the Matsalu test site, large open-water floods outside the official shoreline (ETD) could be detected throughout almost the whole duration of the winter (Figure 5k). The maximum open-water flood extent was detected in March, reaching up to 3000 ha (Figure 5k). In Figure 5i, there is a highlighted area (red rectangle) where open-water floods were observed most frequently (on more than 70% of images). The Matsalu test site has fewer forested areas than the Alam-Pedja and Soomaa test sites. However, there are large areas covered with coastal reed at this test site. The largest floods under the vegetation at this test site are related to an area with coastal reeds (Figure 5j, red rectangle). At the Matsalu test site, the floods under the vegetated area were smaller at 1300 ha (Figure 5k), compared to the open area floods at 3000 ha (Figure 5l).

4.3. Causation Analysis between Flood Extent and Water Level Measured at Hydrological Stations

An analysis was performed with the aim of defining the critical water level at the closest hydrological station that indicates the start of a flooding event (shoreline excess), and to find site specific relationships between the measured water level and flood extent.

At the Alam-Pedja test site, a polynomial relationship between the flooded area extent and water level measured at the Tartu hydrological station (HS) was observed (Figure 7). The correlation (r^2) with water level was most significant (0.94) for the open-water flood extent estimated from IW VH data; the correlation (r^2) for EW HV was 0.85 (Figure 7). The r^2 between the flooded area extent under vegetation and the water level measured at the Tartu HS was 0.51 (Figure 7). Our analysis indicated that open-water floodings at the Alam-Pedja floodplain occur when the water level at the Tartu HS increases above 120 cm (Figure 7, red line). Additionally, there was a significant correlation (0.51) between the extent of the flooded area under vegetation and the water level measured at the Tartu HS. It was not possible to define the precise critical water level for the Tartu HS at which flooding under vegetation starts (Figure 7).

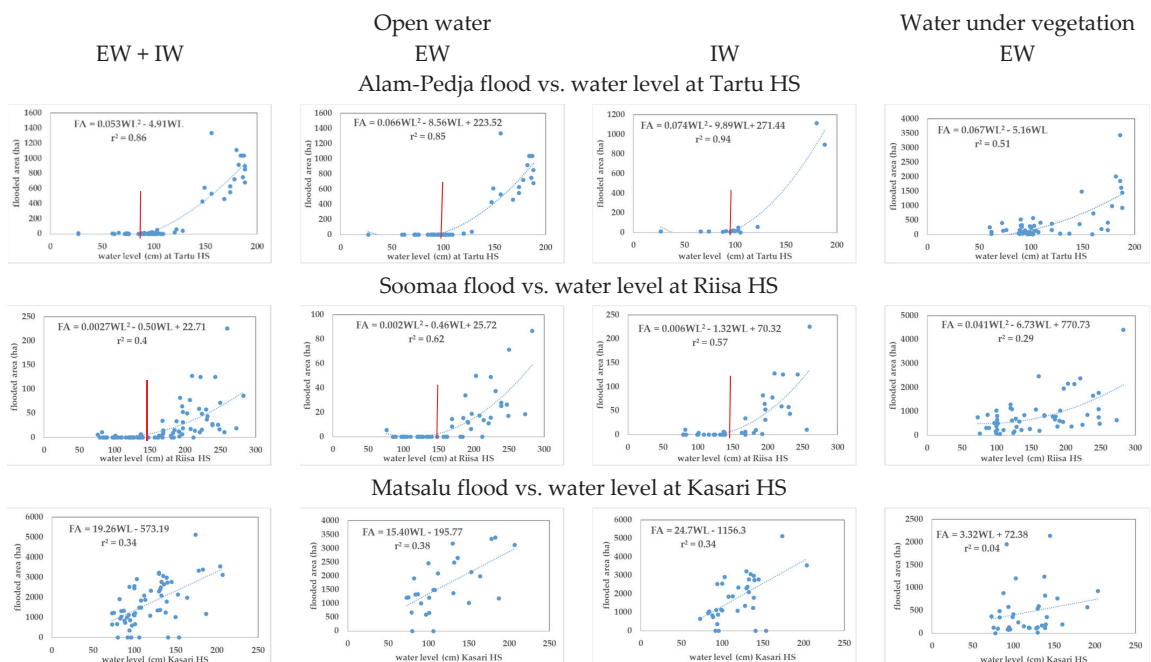


Figure 7. Correlation between flooded area and water level at the closest hydrological station. FA: flooded area extent; WL: water level. Red line denotes the critical water level at which coastline excess occurs and flooding starts.

The relationship between the water level at the Riisa HS and the flooded area extent at Soomaa was polynomial (Figure 7). The correlation coefficient (r^2) between the Soomaa open-water flood extent and the water level measured at the Riisa hydrological station was 0.62 for EW HV data and 0.57 for IW VH data (Figure 7). The correlation (r^2) between the water level measured at the Riisa hydrological station and the flooded area extent under vegetation was 0.29 (Figure 7). Our analysis showed that open-water floodings occur when the water level at the Riisa HS increases above 160 cm (Figure 7, red line).

While the relationship between the water level and the extent of the flooded area was polynomial at the Alam-Pedja and Soomaa test sites, the relationship was linear at the Matsalu test site. The r^2 between the open-water flood extent at the Matsalu site and the water level measured at the Kasari hydrological station was 0.34 for IW VH data and 0.38 for EW HV data (Figure 7). There was no correlation between the water under vegetation and the water level measured at the Kasari HS (Figure 7). At the Matsalu test site, floods occurred throughout the winter, and it was not possible to define a precise critical water level at the Kasari HS that could be related to the beginning of flooding.

5. Discussion

Previous studies have shown the advantages of incidence angle dependent thresholding in the case of TerraSAR-X and Envisat ASAR datasets [18,54]. Our operational setup for flood mapping from S1 data for Estonian floodplains integrates incident angle dependent water thresholding and post-processing using auxiliary information from the Estonian Topographic Database. Post-processing using information from the ETD enables the elimination of water lookalikes. We evaluated the open water mapping accuracy for IW mode VH polarization at our test sites. There was good agreement between the water mapped from IW VH data and the S2 MNDWI index, with an accuracy as high as 96.70% and a kappa hat of 0.86 (Table 6). The accuracy of flood mapping using S1 VH polarization has also been evaluated by Twele et al. [23], who obtained a kappa hat coefficient of 0.88 and an accuracy of 94%. While their operational methodology applied for flood mapping differs from that used in our study, the overall accuracy of the flood mapping is comparable. In the study conducted by Twele et al. [23], the split based thresholding for water mapping was used together with the HAND index in the post-processing step.

During the winter season, the default imaging mode of S1 over the Baltic Sea region is the EW regime. To delineate the information about flooded areas in Estonia, an algorithm for open water mapping for the EW regime was established and applied. The open water mapping accuracy from EW HV polarization data was 97.8%. By including the information from EW data, we could delineate the flood maps approximately using 55 images from each test site. Combining the information from IW and EW regimes, we analyzed 83 images from the Alam-Pedja test site, 93 from the Soomaa test site, and 64 from the Matsalu test site for open water mapping for the period of 1 November 2019–31 March 2020 (Figure 5). Thus, the proposed flood mapping method was tested on a large and diverse dataset. The method developed and proposed in the current study has potential for operational mapping of floods in Estonia and neighboring countries (e.g., Latvia).

The winter of 2019/2020 was extremely mild in Estonia, and there was no permanent ice on the rivers, nor was there snow cover. The monthly averaged air temperature was above 0 °C at all meteorological stations. Our analysis of flood duration and extent showed that in the winter of 2019/2020, floods were observed almost through the whole period of winter. However, the dynamics of the floods differed between the test sites. The maximum flooding observed at Alam-Pedja occurred in March, while at Soomaa and Matsalu several flood events were detected during the winter of 2019/2020. Analysis of the open-water flood extent and water level measured at the closest hydrological station confirmed the correlation between these variables. The correlation was more significant ($r^2 < 0.6$) for the inland riverside floodplains of Alam-Pedja and Soomaa. For the coastal floodplain at Matsalu, the correlation was 0.34, indicating that the river gauge data cannot be used as proxy for flood extent as the coastal flood was significantly influenced by marine processes (not only by riverine hydrology and precipitation). The analysis also revealed that at Alam-Pedja, floods occur when the water level rises above 120 cm at the Tartu HS. At the Soomaa test site, floods occur when the water level rises above 170 cm at the Riisa HS. At the Matsalu test site, open water outside the official coastline could be observed throughout the winter, and we could not define the precise water level at the Kasari HS that results in a flooding at the floodplain. The Matsalu floodplain is located at the outflow to the Baltic Sea; therefore, it is also influenced by the water level in the sea.

Defining the water level at the closest hydrological station from which the floods start (shoreline excess occurs) can provide information for risk mitigation. Hydraulic modelling is a common tool used in flood risk estimation [57]. However, for hydraulic and hydrological modelling, detailed information about riverbed topography, a digital elevation model of the landscape, and a flow rate are needed. These datasets are not always available; therefore, analysis of remote sensing information in combination with standard gauge data can give valuable information from a single source. S1 time series analysis with local gauge data has been used to determine the positional accuracy of riverside embankments [58]. A study conducted by Wood et al. [58] also pointed out the

possibility of determining the positional accuracy of embankments using only a sequence of S1 imagery and gauge data without using topographic data.

In the winter of 2019/2020, several floods in forested areas that harmed economic activities were also reported in the Estonian press [41]. However, the economic loss caused by wintertime flooding in Estonia is unknown. The current study indicated that at the inland riverside floodplains of Soomaa and Alam-Pedja, the flooded areas under vegetation reached up to 4500 ha and were about three times larger than open-water floods at these test sites. Voormasik et al. [30] analyzed the flood extent at Alam-Pedja from TerraSAR-X imagery and estimated the area of flooded forest to be about three times larger than the extent of the open-water flood. Studies indicate that an evaluation of the extent of flooded forest near inland riverbank floodplains is necessary for the estimation of the total flood extent and its economic consequences. Our analysis also revealed that in the case of the inland water floodplains of Alam-Pedja and Soomaa, flood under vegetation could be correlated with the water levels measured at the closest hydrological station.

6. Conclusions

The current paper presents an automatic water mapping method for S1 EW and IW modes by compiling local incident angle thresholding and the application of ancillary information from the Estonian Topographic Database in a post-processing scheme. The proposed method was used to analyze the flood duration and extent in Estonian floodplains during the extremely mild winter of 2019/2020. Our analysis revealed the areas that are most frequently inundated in Estonian floodplains. The observed flood maps allowed us to evaluate the connections between the extent of the flooded area and the water level measured at the closest hydrological station. The study enabled us to determine the water level at which floods occur at the floodplains and to provide valuable information for risk mitigation purposes (standard water level readings from automatic stations are available with a ten-minute interval). The analysis of the extent and frequency of wintertime floods can form the basis for various economic analyses, evaluations of revenue foregone in the forest industry due to mild winters, and evaluations of stress to northern boreal alluvial meadows. The analysis also contributes to the implementation of flood risk assessment and management directive in Estonia [59]. Moreover, the proposed method can be implemented for operational flood mapping in Estonia and neighboring countries.

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