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AVE ANSPER-TOOMSALU

Synergy of Earth Observation data to advance monitoring of optically complex waters

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Synergy of Earth Observation data to advance monitoring of optically complex waters

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Department of Remote Sensing, Tartu Observatory, Faculty of Science and Technology, University of Tartu, Estonia.

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TABLE OF CONTENTS

LIST OF ORIGINAL PUBLICATIONS 6

ABBREVIATIONS AND ACRONYMS 8

1. INTRODUCTION... 10
   1.1. Background 10
   1.2. Objectives of this work 16

2. MATERIALS AND METHODS 17
   2.1. Study areas 17
   2.2. *In situ* data 18
   2.3. Satellite data 19
   2.4. Methodology 21
      2.4.1. Validation of water-leaving reflectance (I, III) and in-water algorithms' products (IV) 21
      2.4.2. Testing and developing Chl-a algorithms (I, IV, V, VI) 23
      2.4.3. Estimating the ecological status of the lake based on Chl-a (I)... 23
      2.4.4. Combining optical and altimetry data (II) 23

3. RESULTS AND DISCUSSION 24
   3.1. Validation of AC processors and in-water algorithms applied to S2 MSI and S3 OLCI data over optically complex waters (I, III, IV) .. 24
      3.1.1. Validation of satellite-derived water-leaving reflectance 24
      3.1.2. Validation of satellite-derived water quality parameters 26
   3.2. Developing and testing Chl-a algorithms over optically complex waters (I, IV, V, VI).. 28
   3.3. Developing applications using satellite data for supplementing estimation of the ecological status of lakes under the EU WFD (I).... 32
   3.4. Correcting optical water quality parameters in respectively to water level and creating synergy between optical and altimetry data for improved assessment of the ecological status under WFD (II)........... 34

CONCLUSIONS 38

REFERENCES... 40

SUMMARY IN ESTONIAN 52

ACKNOWLEDGMENTS.. 55

PUBLICATIONS 57

CURRICULUM VITAE 248

ELULOOKIRJELDUS.. 251

LIST OF ORIGINAL PUBLICATIONS

The study is based on the following publications, which are referred in the text by the Roman numerals. The full publications are included at the end of the thesis:

I **Ansper, A**., Alikas, K. (2019). Retrieval of chlorophyll a from Sentinel-2 MSI data for the European Union Water Framework Directive reporting purposes. *Remote Sensing* 11 (64). https://doi.org/10.3390/rs11010064.

II **Ansper-Toomsalu, A**., Alikas, K., Nielsen, K., Tuvikene, L., Kangro, K. (2021). Synergy between satellite altimetry and optical water quality data towards improved estimation of lakes ecological status. *Remote Sensing* 13 (770). https://doi.org/10.3390/rs13040770.

III Alikas, K., Ansko, I., Vabson, V., **Ansper, A**., Kangro, K., Uudeberg, K., Ligi, M. (2020). Consistency of radiometric satellite data over lakes and coastal waters with local field measurements. *Remote Sensing* 12 (616). https://doi.org/10.3390/rs12040616.

IV **Ansper-Toomsalu, A**.*, Uusõue, M.*, Kangro, K., Hieronymi, M., Alikas, K. (submitted to *Frontiers in Remote Sensing* on April 2024). Suitability of different in-water algorithms for eutrophic and absorbing waters applied on Sentinel-2 MSI and Sentinel-3 OLCI data. (* These authors contributed equally to this work and share first authorship).

V Uudeberg, K., Ansko, I., Põru, G., **Ansper, A.**, Reinart, A. (2019). Using optical water types to monitor changes in optically complex inland and coastal waters. *Remote Sensing* 11 (2297). https://doi.org/10.3390/rs11192297.

VI 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 (931). https://doi.org/10.3390/rs12060931.

AUTHOR'S CONTRIBUTION

The study is based on the publications, which are the result of collaboration with all authors' contributions. The Author's contribution to individual articles is as follows:

I Participation in the fieldwork to collect *in situ* data. Downloading, processing and analysing Sentinel-2 MultiSpectral Instrument (S2 MSI) data, finding chlorophyll-a algorithms from the literature, applying them to various datasets and validating with *in situ* data, writing and editing the manuscript. Conceptualization together with Krista Alikas.

II Downloading, processing and analysing Sentinel-3 Ocean and Land Colour Instrument (S3 OLCI) data, comparing S3 Synthetic Aperture Radar Altimeter data and optical water quality products with *in situ* data, combining altimetry and optical data to expand water level correction methodology on satellite data, deriving corrected ecological status classes according to European Union Water Framework Directive, writing and editing manuscript. Conceptualization together with Krista Alikas.

III Participation in the fieldwork to collect *in situ* data. Downloading and processing S3 OLCI data and writing a part of the methodology about data processing in the manuscript.

IV Downloading and processing S2 MSI and S3 OLCI data, analysing the accuracy of satellite-derived products in respective to the vicinity of land and consistency between S2 MSI and S3 OLCI data, creating all figures in the manuscript. Writing parts of an abstract, introduction, satellite data processing, results, discussion and conclusions about effects associated with the vicinity of land and consistency between S2 MSI and S3 OLCI data, editing the manuscript. Conceptualization together with Mirjam Uusõue and Krista Alikas.

V Participation in the fieldwork to collect *in situ* data. Downloading and processing S2 MSI data, writing about S2 MSI data processing in the methodology section of the manuscript.

VI Participation in the fieldwork to collect *in situ* data, finding chlorophyll-a algorithms suitable for different optical water types from the literature.

ABBREVIATIONS AND ACRONYMS

ρ_w	Water-leaving reflectance (*dimensionless*)
A4O	Atmospheric correction for diverse optical water types
AC	Atmospheric correction
AltNN	Alternative Neural Network
APE	Absolute percentage error (%)
AXIC-Aqua	Atmospheric Correction Intercomparison eXercise
C2RCC	Case2Regional Coast Colour
CCI	Climate Change Initiative
CDOM	Coloured dissolved organic matter (m^{-1})
CHIME	Copernicus Hyperspectral Imaging Mission for the Environment
Chl-a	Chlorophyll-a concentration (mg/m^3)
ENVISAT	Environmental Satellite
EO	Earth Observation
EOMORES	Earth Observation-based Services for Monitoring and Reporting of Ecological Status
ESA	European Space Agency
EU	European Union
FBM	Phytoplankton biomass (g/m^3)
FRM	Fiducial reference measurements
FRM4SOC	FRM for Satellite Ocean Colour
GLaSS	Global Lakes Sentinel Services
GLORIA	The GLObal Reflectance community dataset
HELCOM	Baltic Marine Environment Protection Commission
IOPs	Inherent optical properties
L1	Level-1
L2	Level-2
MERIS	Medium Resolution Imaging Spectrometer
MCI	Maximum Chlorophyll Index
MODIS	Moderate Resolution Imaging Spectroradiometer
MSI	MultiSpectral Instrument
NASA PACE	The National Aeronautics and Space Administration's Plankton, Aerosol, Climate, ocean Ecosystem satellite mission
NIR	Near-infrared spectral range
NN	Neural network
OAS	Optically active substances
OLCI	Ocean and Land Colour Instrument
OWT	Optical water types
QA4EO	Quality Assurance framework for Earth Observation
Polymer	POLYnomial-based approach established for the atmospheric correction of MERIS data
PRISMA	PRecursore IperSpettrale della Missione Applicativa

RMSE	Root mean square error (%)
S2	Sentinel-2
S3	Sentinel-3
S6-MF	Sentinel-6 Michael Freilich
SACSO	Spectral matching Atmospheric Correction for Sentinel Ocean colour measurements
SDD	Secchi disc depth (m)
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SIRAL	Synthetic Aperture Radar/Interferometric Radar Altimeter
SRAL	Synthetic Aperture Radar Altimeter
TSM	Total suspended matter (mg/L)
VIIRS	Visible Infrared Imaging Radiometer Suite
WFD	Water Framework Directive

1. INTRODUCTION

1.1. Background

Lakes and coastal areas are vital parts of the water ecosystem, being the regulators for climate and carbon cycles, providing a living environment for water inhabitants and guaranteeing thereby biodiversity, ensuring drinking water for living organisms, and offering ecosystem services for humans (Tranvik et al. 2009; Biggs et al. 2017). It is essential to secure a sustainable water environment through consistent monitoring and management to evaluate the influence of anthropogenic, such as agricultural and industrial pollution, and natural factors, such as diurnal and seasonal changes (Wang et al. 2007; Nõges et al. 2007; Khatri and Tyagi 2015; Koff et al. 2016). Therefore, implementing accurate, effective, and cost-efficient techniques for consistent monitoring is a priority.

Traditional *in situ* monitoring (collecting water samples and analysing them in the laboratory) is time- and money-consuming, being limited over spatial and temporal scales (Adjovu et al. 2013; Yang et al. 2022). Since the launch of the first ocean colour satellite, Coastal Zone Colour Scanner onboard Nimbus-7 in 1978 for estimating phytoplankton pigment concentration in the oceans (Gordon et al. 1980), many multispectral ocean colour satellite sensors have been developed (*e.g.* Sea-viewing Wide Field-of-view Sensor (SeaWiFS), Moderate Resolution Imaging Spectroradiometer (MODIS), Medium Resolution Imaging Spectrometer (MERIS), Visible Infrared Imaging Radiometer Suite (VIIRS), Ocean and Land Colour Imager (OLCI)) to monitor water environments regularly from a local to global scale (Groom et al. 2019). Besides, the era of hyperspectral satellites (PRecursore IperSpettrale della Missione Applicativa (PRISMA) launched in 2019, The National Aeronautics and Space Administration's Plankton, Aerosol, Climate, ocean Ecosystem (NASA PACE) launched in 2024 and European Space Agency's (ESA) Copernicus Hyperspectral Imaging Mission for the Environment (CHIME) planned to be launched in 2028) has been gaining interest in recent years (Niroumand-Jadidi et al. 2020; Gauto et al. 2022; Nieke et al. 2023). Hyperspectral sensors' data will complement multispectral data by filling the gaps in the spectrum, which lead to the development of new algorithms and application concepts to observe aquatic ecosystems in more detail, for example to identify phytoplankton community composition (Dierssen et al. 2023).

European Union's (EU) Earth Observation (EO) programme, named Copernicus, provides complete, free, and open data available to anyone through the set of Sentinel satellite data. MultiSpectral Instrument (MSI) sensor onboard the Sentinel-2 (S2) satellite (S2A launched in 2015, S2B in 2017, S2C planned to be launched in 2024, S2D in 2028) has been designed for land applications to monitor land-cover/land-use change and vegetation. However, spatial resolution of 10–60 m is also suitable for monitoring small lakes and coastal areas (Toming et al. 2016; Dörnhöfer et al. 2016; Bresciani et al. 2018a; Grendaitė and Stonevičius 2018; Salama et al. 2022). OLCI is one of the four sensors onboard the

Sentinel-3 (S3) satellite (S3A launched in 2016, S3B in 2018, S3C is planned to launch in 2026, S3D in 2028), which has been designed for ocean and land colour monitoring being the continuation of MERIS sensor on board Environmental Satellite (ENVISAT) satellite (operational 2002–2012). It has suitable spectral resolution (21 bands from 400–1020 nm, band-width 9–21 nm) for developing algorithms to estimate water quality. However, the spatial resolution of 300 m is not suitable for monitoring small and complex spatial structure lakes and coastal bays (Pirasteh et al. 2020; Soomets et al. 2020). The second of the four sensors onboard S3 satellite is Synthetic Aperture Radar Altimeter (SRAL), which is designed for monitoring ocean topography and provides water level data over lakes and coastal areas. Spatial resolution in the along-track is 300 m, and across-track is 1.64 km with 27 days repeat cycle with S3A and S3B (Nielsen et al. 2020; Liibusk et al. 2020).

Monitoring lakes and coastal waters using satellite data gives advantages over traditional *in situ* monitoring regarding spatial and temporal resolution. However, it is also challenging because of the complexity of the substances in the water (Odermatt et al. 2012; Woźniak and Meler 2020), the vicinity of the land (Candiani et al. 2007) and the influence of the atmosphere (Warren et al. 2019). Optically active substances (OAS) such as chlorophyll-a (Chl-a), total suspended matter (TSM), and coloured dissolved organic matter (CDOM) are influencing underwater light field and relate to the water quality at the same time. Chl-a is the main pigment in the phytoplankton and is a proxy of its biomass. Phytoplankton blooms are natural processes in the water environment caused by eutrophication, which also decreases water quality (Anderson et al. 2002). However, cyano-bacteria blooms can be toxic and harmful to living organisms' health and local ecosystems (World Health Organization 2003). Chl-a is detectable using satellite data because it has a unique absorption peak in the blue (440–500 nm) and in the red (650–680 nm) part of the spectrum (Kirk 2011). TSM is linked to sediments in the water environment, such as suspended particulate organic and inorganic matter, which scatter the light depending on the size, shape, and the origin of the particle. TSM decreases the light available for primary production (Doxaran et al. 2002). It increases the reflectance over all wavelengths, whereas the maximum reflectance peak moves to longer wavelengths (Lodhi et al. 1997). Secchi disk depth (SDD) is a measure of water transparency, which relates to the amount of OAS in the water (Preisendorfer 1986). CDOM is a component of dissolved organic matter, which reduces the amount of light going back to the sensor especially in the blue part (350–450 nm) of the spectrum and decreases in longer wavelengths. Due to overlapping absorption features, it causes the increase of uncertainties in the shorter wavelengths to discriminate between CDOM and Chl-a (Bricaud et al. 1981; Aurin et al. 2018), but in highly absorbing waters can have an impact on the reflectance over the entire visible wavelengths (Kutser et al. 2016).

Morel and Prieur (1977) divided waterbodies into two classes, such as Case-1 and Case-2 waters. In Case-1 waters, optical properties are mainly determined by phytoplankton and related CDOM and detritus degradation products. Case-2 waters are all the other waters, where optical properties are also determined by the mineral particles and CDOM, which are not covarying with phytoplankton. Typically, Case-2 waters are coastal areas and lakes. These waters are often eutrophic and absorbing CDOM-dominant waters, which are challenging to monitor with remote sensing techniques. The vicinity of the land, different amounts of OAS, river runoffs, and resuspension of sediments from the shallow bottom make lakes and coastal areas highly variable (Moore et al. 2014). Also, spatial and seasonal changes are more pronounced. Therefore, developing algorithms for deriving water quality parameters for Case-2 waters is very challenging. Band ratio algorithms have been widely used for Case-2 waters focusing on green, red and near-infrared (NIR) part of the spectrum (Gilerson et al. 2010; Matthews 2011; Yacobi et al. 2011). Besides band ratio algorithms, the development of machine learning approaches has shown potential as a more advanced techniques to derive OAS (Blix et al. 2019; Sun et al. 2021; Niroumand-Jadidi and Bovolo 2022; Chusnah et al. 2023). However, these algorithms are often validated in specific areas (Sent et al. 2021; Sòria-Perpinyà et al. 2021; Seleem et al. 2022) and are suitable where optical conditions are in the same range as in the algorithm training dataset. For more accurate algorithms development for dynamic Case-2 waters, different methods have been used for classifying waters (Wernand et al. 2013; Woerd and Wernand 2015; Spyrakos et al. 2018). One solution is to classify waters into optical water types (OWTs), which are related to specific reflectance spectrum and OAS in the water (Moore et al. 2014; Eleveld et al. 2017; Jackson et al. 2017; Spyrakos et al. 2018). However, any algorithm development needs a high quality and wide range of training data. Testing the algorithms needs a wide range of good conditions' (*e.g.* clear sky) match-up data between satellite and *in situ* radiometric measurements; thereby algorithms development and testing are more often regionally limited (Syariz et al. 2020; Hadjal et al. 2023). Removing the influence associated with the vicinity of the land is also a challenging task, where land pixels have higher reflectance compared to water surface (Li et al. 2017; Alikas et al. 2020; Paulino et al. 2022). The influence of the vicinity of the land depends on the atmosphere composition, type of land cover, sensor characteristics and viewing geometry, shape, size and the OWTs of the waterbody (Bulgarelli et al. 2014; Bulgarelli and Zibordi 2018).

Atmosphere contributes approximately 80–90% of the radiance from the water reaching to the sensor (Gordon 1978). For retrieving signal from the water surface called water-leaving reflectance (ρ_w), the atmospheric correction (AC) procedure is essential for removing the influence of the atmosphere. Various schemes for AC exist. S3 OLCI has a standard ρ_w product (L2) for Case-1 waters, which are not optimal for Case-2 waters. However, S3 OLCI has standard water quality products for Case-2 waters. With the launch of Landsat and S2 MSI satellites, there is a need and possibility to develop applications for lakes despite the spectral resolution is not optimal for fine-scale studies. Besides S3 OLCI standard L2 ρ_w product, many alternative AC processors have been developed to remove the influence of the atmosphere from the signal reaching the sensor (Steinmetz et al. 2011; Sterckx et al. 2011; Franz et al. 2015; Brockmann et al. 2016; Hieronymi et al. 2016; Vanhellemont and Ruddick 2016). These AC processors differ by their processing scheme, suitability to the sensor, aerosol model, glint correction, cloud masking, Rayleigh correction and considering effects coming from the land (Pahlevan et al. 2021). Several studies have found, that OWT-based classification would be beneficial in validating AC processors (Pahlevan et al. 2021; Hieronymi et al. 2023). S3 mission requirements (Drinkwater and Rebhan 2007) have foreseen 5% accuracy for ρ_w over all bands. This sets high limits to *in situ* data during the validation, because *in situ* data accuracy should be higher. Uncertainties allow us to know the level of confidence in satellite data (Tran et al. 2023), which is becoming more focused era lately (Zheng and DiGiacomo 2017; Mayr et al. 2021; Werther and Burggraaff 2023). However, *in situ* measurements also have uncertainties, which should be quantified, and minimized, if possible, to provide high-quality reference data for satellite data validation. It is crucial that the uncertainties in the *in situ* data are smaller compared to the expected uncertainties in the EO data. Therefore, for more accurate validation, the quantification of uncertainties has been studied in water remote sensing community in recent years (Vabson et al. 2019; Białek et al. 2020; Tilstone et al. 2020). The fiducial reference measurements (FRM) (Goryl et al. 2023) purpose is to follow Quality Assurance framework for Earth Observation (QA4EO) requirements to implement guidelines for ground-based radiometric measurements. During the FRM projects, guidelines for vegetation, air quality, surface temperature and ocean colour have been developed. FRM for Satellite Ocean Colour (FRM4SOC) Phase-1 aim was to ensure that ground-based measurements for ocean colour monitoring are traceable to SI standards to support validating satellite data with high-quality reference data (Banks et al. 2020). FRM4SOC Phase-2 followed to continue Phase-1 with an aim to ensure the adoption of FRM principles across the ocean colour community. Estimating uncertainties for both, for *in situ* measured and for satellite-derived ρ_w is important, because ρ_w is the base for deriving water quality parameters and developing satellite-based applications. Therefore, there is a need to quantify the uncertainties and avoid error propagations through the processing chain to minimize uncertainties in the final products.

Natural factors, such as daily changes, seasonality and atmospheric circulation are influencing water quality parameters (Nõges et al. 2007). It is more pronounced in shallow lakes, where water levels can have large variations. Therefore, Tuvikene et al. (2011) have suggested to apply water level correction on water quality parameters to improve estimation of the ecological status in lakes. A combination of optical sensors has been used for estimating water quality parameters (Moses et al. 2009; Zeng and Binding 2021) and a combination of altimetry sensors has been used for estimating water level (Berry et al. 2005; Qin et al. 2023). However, estimating the ecological status of water using satellite data is parameter-specific and no external factors are often considered (Bresciani et al. 2011; Attila et al. 2018). Altimetry data have shown potential deriving water levels in lakes with a low root-mean-error < 0.2 m (Nielsen et al. 2015; An et al. 2022; Xu et al. 2024). Nielsen et al. (2020) found that the size of the lake is not causing larger errors, than the surrounding around the lake (topography, shape of the lake, *etc.*). However, there is a lack of studies combining altimetry data with optical data to improve the ecological status assessment. The combination of different types of data has raised interests in recent years. During different projects (Climate Change Initiative, Copernicus Land Monitoring Service, *etc.*), optical data, altimetry data, *etc.*, have been gathered globally from lakes to extend spatio-temporal scale in lake monitoring and develop global water quality algorithms (Crétaux et al. 2020; Warren et al. 2021). This gives opportunity to use the synergy of data for more advanced monitoring of inland waters and develop new applications.

The EU Water Framework Directive (2000/60/EC) (WFD) states to implement water management in EU member states to achieve at least Good ecological status in lakes by 2027 or maintain it if it already exists (European Commission 2000). The ecological status is divided into five classes from Very Good to Very Bad, where the category Good indicates very light bias due to human activity from reference conditions (Ministry of Environment 2009). Water protection and sustainable management are ensured through consistent monitoring and requirements by WFD. To estimate the ecological status of water, biological (*e.g.* phytoplankton), physicochemical (*e.g.* transparency) and hydromorphological (*e.g.* depth variations) parameters with certain thresholds should be considered. EO-based applications have been successfully developed for supplementing monitoring under WFD to estimate specific water quality parameters, such as Chl-a, FBM, SDD regionally (Alikas et al. 2015; Arle et al. 2016; Sent et al. 2021). However, all the parameters for estimating the ecological status are not possible to derive from satellite data, therefore EO data only complements *in situ* data in WFD assessment.

Chl-a is one of the key parameters for estimating the ecological status (WFD 2000) and has been monitored since the beginning of the water remote sensing era. Blue-green band ratio algorithms are not suitable for Case-2 waters, because of the scattering and absorption by TSM and CDOM. Band ratio algorithms using multiple bands in red-NIR part of the spectrum have been developed based on the Chl-a absorption peak around at 670 nm and reflectance peak at around 700 nm (Gitelson 1992; Gilerson et al. 2010). Besides band ratio algorithms, semi- and quasi-analytical (Lee et al. 2002; Rotta et al. 2021), index-based (Gower et al.1999; Gower et al. 2005; Mishra and Mishra 2012) and machine-learning-based algorithms (Cao et al. 2020; Pahlevan et al. 2020; Woo Kim et al. 2022) have been developed. For better accuracy in specific region, waterbody or OWTs, tuned algorithms with special coefficients is necessary step (Kolluru et al. 2023).

During the project named Water scenarios For Copernicus Exploitation (Water-ForCE), the Roadmap was created to analyse current Copernicus water-related services available for monitoring and to give recommendations for the future to provide better integration in these services (Kutser et al. 2024). It suggests to consider water as an identifiable market sector and to make water services functional for users. It also suggests to integrate EO data to national monitoring programme. The White Paper was created during the Earth Observation-based Services for Monitoring and Reporting of Ecological Status (EOMORES) project to demonstrate satellite data usability supporting the monitoring obligations under WFD (Papathanasopoulou et al. 2019). It concludes that there is a need for more quality-controlled data, a need for improved technical expertise in agencies and authorities, a need for an integrated system among EU member states for using satellite data and a need to map satellite-derived metrics suitable for estimating the ecological status. Besides monitoring lakes and coastal areas by WFD, for example, the Marine Strategy Framework Directive (2008/56/EC) (MSFD) is obligated to control and protect the marine environment and the Bathing Directive (2006/7/EC) is obligated to monitor cyanobacteria blooms in European waters. Using EO data under these directives has shown potential complementing *in situ* measurements (Chen et al. 2007; Cristina et al. 2015; Karsten et al. 2022; Rahn et al. 2023). Finnish Environmental Institute has developed applications to support WFD and MSFD reporting obligations using EO data as a complementary source of information. These applications are based on Sentinel and Landsat data, and they have developed open and freely available water quality products service over Finnish lakes and the Baltic Sea named TARRKA (syke.fi/TARKKA/en).

Remote sensing offers advantages on spatial and temporal scales. However, it is challenging and needs consistent development and research for more precise products, especially in shallow, small and complex eutrophic and CDOM-dominated lakes. Gordon et al. (1983) and Gordon (1987) estimated, that 5% uncertainty in the blue part of the spectrum can lead to 35% uncertainty in the derived Chl-a estimation in oligotrophic waters. This means that we need reliable satellite data for developing algorithms and applications. Lakes are not homogeneous waterbodies; they change daily, seasonally, and spatially. Therefore, one global algorithm is not applicable, and more advanced techniques are needed. Satellite-based applications have shown potential for implementing EU WFD; however for more precise assessment, external factors should be considered. Combining different types of data such as *in situ*, optical and altimetry, would demonstrate new advanced EO techniques for the future and the possibility of applying these to current and new satellite data.

1.2. Objectives of this work

The main objective of this work is to estimate the suitability of various EO processing schemes over different water types and conditions and to develop satellite-based applications using synergy between different types of data in optically complex waters. The specific objectives of this work are:

1. To analyse the accuracy and the suitability of ρ_w (**I**, **III**) and water quality products (**IV**) derived from S2 MSI and S3 OLCI data with *in situ* measurements over optically complex lakes;
2. To test current and to develop new Chl-a algorithms for optically complex waters applied to S2 MSI and S3 OLCI (**I**, **IV**, **V**,**VI**);
3. To develop applications using *in situ* and satellite data to support the estimation of the ecological status of lakes according to Chl-a under the European Union Water Framework Directive (**I**);
4. To advance satellite-based methods to increase the accuracy of the water ecological status assessment by combining *in situ*, optical and altimetry data (**II**).

2. MATERIALS AND METHODS

2.1. Study areas

Study areas were situated in Europe, where most of the used data were gathered from Estonian lakes and the coastal areas (Figure 1). Variation of water quality parameters in study areas is shown in Table 1.

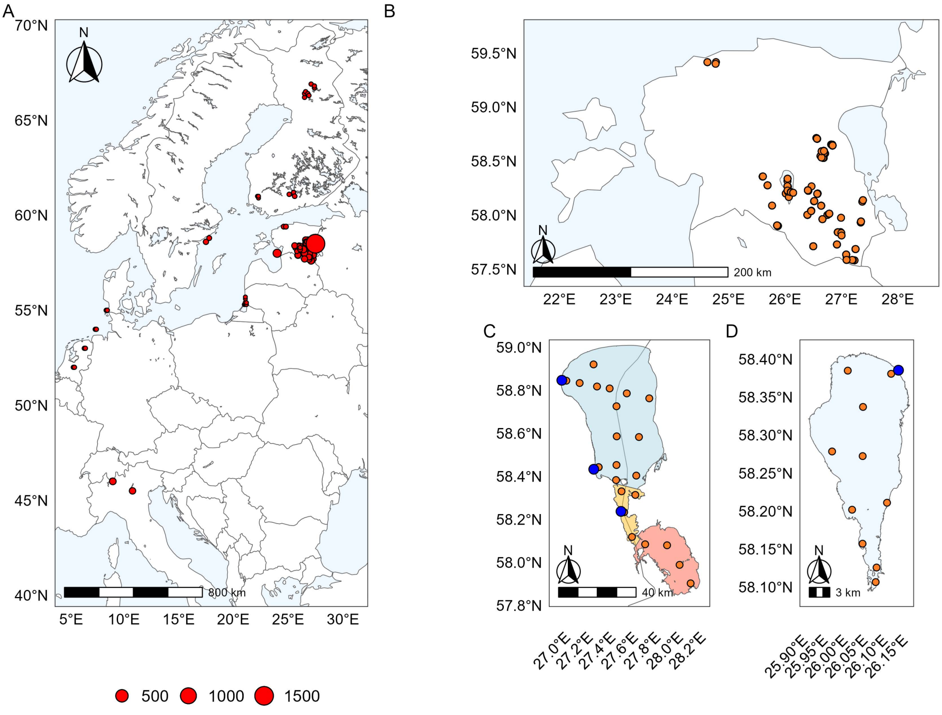

Figure 1. Locations of used data in Europe (A), Estonian small lakes (B), Lake Peipsi (C) and Võrtsjärv (D). The size of the red dots shows amount of data used. Orange dots indicate water quality data and blue dots indicate water level stations. Lake Peipsi is divided into three parts: Peipsi *sensu stricto* (blue), Lämmijärv (yellow) and Pihkva (pink).

Lake Peipsi (Figure 1A) is a shallow transboundary lake with a water surface area of 3555 km^2 and an average depth of 7.1 m. Lake Peipsi is divided into three parts where the northern part is mesotrophic Peipsi *sensu stricto* (*s.s.*) with a water surface area of 2611 km² and an average depth of 7 m (Figure 1C blue part). The southern part is the hypereutrophic lake Pihkva (Figure 1C pink part) with a water surface area of 708 km² and an average depth of 3 m, and in the middle is the eutrophic lake Lämmijärv (Figure 1C yellow part) with a water surface area of 236 km² and an average depth of 2.5 m.

Võrtsjärv (Figure 1D) is a shallow eutrophic lake with a water surface area of 270 km^2 and an average depth of 2.8 m. Estonian small lakes (Figure 1B) and the Baltic Sea varied from low quantities of water quality parameters (*e.g.* with Secchi depth of 7 m) to waters with high Chl-a (106 mg/m^3) and $a_{CDOM(443)}$ (47 m^{-1}) (*e.g.* with Secchi depth of 0.1 m). The depth varied from 1–38 m. Lakes in the GLaSS dataset varied from oligotrophic Maggiore in Italy (average Chl-a 1.6 mg/m^3) to hypereutrophic Betuwe area in the Netherlands (Chl-a up to 150 mg/m^3).

A detailed description of Lake Peipsi (**I–VI)**, Võrtsjärv (**I–VI)**, Estonian small lakes and coastal areas (**I**, **IV–VI)**, Baltic Sea (**III**, **IV**), Finnish lakes (**VI**) and GLaSS dataset lakes (**I**) are in each publication separately.

Table 1. Minimum and maximum values of water quality parameters in all study sites, Lake Peipsi, Võrtsjärv, Estonian small lakes and the Baltic Sea. The median is shown in the brackets.

	All data	Lake Peipsi	Võrtsjärv	Estonian small lakes	Baltic Sea
Chl-a (mg/m^3)	0.2–215 (15)	2–215 (20.2)	1.8–83 (31.9)	0.8–106 (10.3)	1.2–27 (6.5)
TSM (m/L)	0.1–143 (6)	0.01–36 (8)	0.1–49 (15.4)	0.6–143 (4)	0.7–21 (8.8)
$a_{CDOM(443)}$ (m^{-1})	0.04–47 (2)	1–17 (2.3)	1–13 (2.3)	0.5–47 (1.7)	0.4–8 (0.9)
SDD (m)	0.1–11 (1.4)	0.4–3 (1.3)	0.3–3 (0.6)	0.1–7 (1.8)	0.7–7 (1.2)

2.2. In situ data

Four types of *in situ* data were used in this study. A detailed description of *in situ* data is in each publication separately.

1) Water samples were collected, and SDD was measured by the workgroups of Tartu Observatory of the University of Tartu and Estonian national monitoring from Estonian small lakes (**I**, **IV–VI**), Lake Peipsi (**I–VI**), Võrtsjärv (**I–VI**), the Baltic Sea (**I**, **III–VI**) and Finnish lakes (**VI**). Water samples were analysed in Tartu Observatory of the University of Tartu or the Centre of Limnology laboratories to derive Chl-a, TSM and FBM concentration and absorption parameters. Scattering parameters were measured with the volume scattering function meter described in detail publication **IV**. Water samples were collected from May to October from 2015–2022. Water samples and SDD measurements were used 1) to test and develop Chl-a algorithms (**I**, **VI**), 2) to estimate the ecological status of lakes (**I**, **II**), and 3) to validate satellite-derived water quality parameters with *in situ* measurements (**IV**).

2) Radiometric measurements were performed by the Tartu Observatory of the University of Tartu workgroup simultaneously while collecting water samples, and additional ancillary data (wave height, wind speed, sun elevation, *etc.*) were recorded (**III**, **V**, **VI**). Radiometric measurements were performed with Ramses TriOS 1) to validate satellite-derived ρ_w with *in situ* measured ρ_w (**I**, **III**), and 2) to develop OWT classification methodology (**V**, **VI**).

3) Water levels were gathered by Estonian national monitoring from Rannu-Jõesuu station in Võrtsjärv (Figure 1D) and from Mehikoorma, Mustvee, Praaga stations in Lake Peipsi (Figure 1C). Water levels in Rannu-Jõesuu station were available from 1927, Mustvee and Praaga from 1921 and Mehikoorma from 1949–2019. *In situ* water levels were averaged daily to compare with satellite-derived water level data (**II**).

4) *In situ* radiometric measurements and water quality parameters (Chl-a, TSM, SDD, $a_{CDOM(443)}$) were gathered during the project named Global Lakes Sentinel Services (GLaSS, project number 313256) in 2013–2016. S2 MSI spectral response function was applied to *in situ* radiometric measurements. Data were gathered from Estonia, the Netherlands, Finland and Italy to test and develop Chl-a algorithms (**I**).

2.3. Satellite data

Non-Time Critical level-1 (L1) or level-2 (L2) optical data (Table 2) were used in this study described in Table 2. AC processors were applied to L1 data described in Table 3. S2 MSI and S3 OLCI data were used 1) to validate satellite-derived ρ_w with *in situ* measured ρ_w (**I**, **III)**, 2) to validate satellite-derived water quality parameters with *in situ* measured water quality parameters (**IV**), and 3) to process satellite data for Chl-a algorithm development, for the estimation of ecological status and OWT classification (**I**, **II**, **V**, **VI**). A detailed description of satellite data is in each publication separately.

Table 2. Description of downloaded satellite data.

Satellite and sensor	Processing level	Database	Time range	Pixel resolution	Processing baseline
S2 MSI A/B	L1	Copernicus Access Datahub https://scihub.copernicus.eu/	2015–2022	Resampled to 10 m or 60 m	02.04–04.00
S3 OLCI A/B	L1, L2	Coda https://coda.eumetsat.int, Codarep https://codarep.eumetsat.int, Datastore https://data.eumetsat.int, EstHUB https://ehcalvalus.maaamet.ee	2016–2022	Full resolution 300 m	Collection 002 and 003

Table 3. Description of AC processors applied to L1 satellite data.

AC processor	Version	Publication	Reference
Acolite	v20170718.0*	**V**	Vanhellemont and Ruddick 2016, 2018
	v20180925.0*	**I**	
	v20221114.0***	**IV**	
Case-2 Regional CoastColour (C2RCC)	v0.15*	**I, V**	Brockmann et al. 2016
	v1.0**	**III, VI**	
	v1.15**	**VI**	
	v2.1***	**IV**	
POLYnomial based algorithm applied to MERIS (Polymer)	v1.1*	**I, V**	Steinmetz et al. 2011
	v4.10***	**II**	
		III	
	v4.16**	**IV**	
Sentinel-2 standard L2 (Sen2Cor)	v2.1.2*	**I, V**	Main-Knorn et al. 2017
Atmospheric Correction for Optical Water Type (A4O)	v1.0**	**IV**	Hieronymi, et al. 2017
Alternative Neural Net (altNN)	v1**	**III, V**	Brockmann et al. 2016

* applied to S2 MSI, ** applied to S3 OLCI, *** applied to S2 MSI and S3 OLCI

Altimetry data from 2016–2019 were used to derive water level from satellite data and were compared with *in situ* measured water level from Võrtsjärv and Lake Peipsi:

- S3 SRAL A/B Non Time Critical L2 Enhanced data were used for monitoring Lake Peipsi. S3 SRAL B data were used for monitoring Võrtsjärv from 2018. It has a repeat period of 27 days in a specific track.
- Cryosat SIRAL ESA L1B baseline D data were used for monitoring Lake Peipsi and Võrtsjärv. It has repeat period of 369 days in a specific track.

2.4. Methodology

2.4.1. Validation of water-leaving reflectance (I, III) and in-water algorithms' products (IV)

Satellite-derived ρ_w and water quality products were analysed with *in situ* measurements. *In situ* radiometric measurements were calculated to S2 MSI or S3 OLCI bands using spectral response function. Match-ups between satellite overpass and *in situ* measurements were selected by one day (**III**, **IV**, **V**) or up to three days (**I**) difference. Uncertainty budgets were calculated to *in situ* radiometric data to analyse the level of uncertainties and remove data with higher uncertainties (**III**). The impact of the changing environmental conditions on the uncertainty budget was analysed based on the recorded variable conditions (*e.g.* wave height, wind speed, sun elevation) during fieldwork to find optimal conditions to perform radiometric measurements.

AC processors were applied to S2 MSI (**I**, **IV**) and S3 OLCI L1 (**III**, **IV**) data. Additionally, S3 OLCI L2 standard ρ_w and water quality products were used (**III**, **IV**). Processor-based flagging was used to exclude invalid pixels (*e.g.* clouds, glint, out-of-scope, land). *In situ* point measurements were compared with satellite-derived 1×1 (**III–IV**) or 3×3 (**I, III, IV**) pixel areas. Outliers of 3×3 pixel areas were eliminated by following the recommendation for S3 OLCI product validation (EUMETSAT 2021). Distance from each *in situ* measurement location was calculated from the closest point of the land to estimate effects associated with the vicinity of the land (**III**, **IV**).

To validate in-water algorithms, satellite-derived water quality parameters were compared with *in situ* measured parameters shown in Table 4. A detailed description of each in-water algorithm is in the publication **IV**.

Statistical analysis was performed (coefficient of determination (R^2), root-mean-square-error (RMSE), dispersion, bias, and absolute percentage error (APE), number of match-ups (N)) to analyse the difference between satellite-derived and *in situ* measured ρ_w and water quality parameters.

Table 4. Outputs derived from AC processors, corresponding names, and explanation of *in situ* parameters. Blue colour indicates absorption products and grey colour scattering products.

In-water algorithm output	*In situ* parameter	Explanation of *in situ* parameter
Conc_chl (C2RCC), CHL_NN (L2), IOP_CHL (A4O), CHL_ONNS (A4O), chl_re_gons(740) (Acolite), chl_re_moses3b(740) (Acolite), chl_re_mishra (Acolite), chl_re_bramich (Acolite), logchl (Polymer)	Chl-a	Chl-a concentration
conc_tsm (C2RCC), TSM_NN (L2), SPM_nechad2016 (Acolite), TSM_ONNS (A4O)	TSM	TSM concentration
iop_apig (C2RCC), a_{pig} (L2), a_p_440_ONNS (A4O)	a_{pig}	absorption coefficient of phytoplankton pigments at 443 nm
iop_adet (C2RCC)	a_{NAP}	absorption coefficient of detritus at 443 nm
iop_agelb (C2RCC), CDOM_ONNS (A4O)	a_{CDOM}	absorption coefficient of CDOM at 443 nm
a_m_440_ONNS (A4O)	a_{NAP}	absorption coefficient of CDOM at 440 nm
iop_adg (C2RCC), ADG443_NN (A4O), a_g_440_ONNS (A4O)	a_{dg}	absorption by detritus + CDOM absorption at 443 nm
a_dg_412_ONNS (A4O)	a_{dg}	absorption by detritus + CDOM absorption at 412 nm
iop_atot (C2RCC), a_{tot} (L2), a_tot_440_ONNS (A4O)	a_{tot}	phytoplankton + detritus + CDOM absorption at 443
iop_bpart (C2RCC)	b_{part}	scattering coefficient of particles at 443 nm
iop_btot (C2RCC), b_tot_440_ONNS (A4O)	b_{tot}	total particle scattering at 443 nm
b_p_440_ONNS (A4O)	b_{part}/SPOM	scattering coefficient of phytoplankton particles at 440 nm
b_m_440_ONNS (A4O)	b_{part}/SPIM	scattering coefficient of detritus at 440 nm
b_bp_510_ONNS (A4O)	bb_{part} at 510 nm	total backscattering coefficient of all particles at 510 nm

2.4.2. Testing and developing Chl-a algorithms (I, IV, V, VI)

During testing and developing Chl-a algorithms, three different approaches were investigated:

1) Chl-a algorithms were found in the literature and were tested on the GLaSS dataset. Conversion factors were found to calculate satellite-derived Chl-a using empirical algorithms (**I**);
2) Chl-a was derived from different AC processors' in-water algorithms and compared with *in situ* measured Chl-a (**IV**);
3) *In situ* radiometric measurements were classified into OWTs based on the ρ_w (**V**). Based on the statistical analysis, the most suitable Chl-a algorithms were selected based on the OWT (**VI**). OWT-based Chl-a algorithms were applied to satellite data.

2.4.3. Estimating the ecological status of the lake based on Chl-a (I)

Chl-a was calculated using three approaches: 1) Maximum Chlorophyll Index (MCI) algorithm was applied to S2 MSI L1 data, 2) 28 empirical Chl-a algorithms were tested on the GLaSS *in situ* measured radiometric data calculated to S2 MSI bands and, 3) S2 MSI data were processed by C2RCC, and then Chl-a algorithms were applied. Time series were derived to evaluate consistency between satellite-derived and *in situ* measured Chl-a. The ecological status of lakes was estimated by using satellite-derived and *in situ* measurements of Chl-a. The thresholds and the relevant monitoring period for estimating the ecological status classes of lakes were defined by the Ministry of Environment (2009).

2.4.4. Combining optical and altimetry data (II)

Water quality parameters were derived from S3 OLCI data. Chl-a and FBM were calculated using regionally tuned algorithms based on the MCI applied to L1 data. Secchi disk depth was calculated using the diffuse attenuation coefficient of down-welling irradiance ($Kd_{(490)}$) (Alikas and Kratzer 2017) applied to ρ_w data derived by Polymer. Water levels were derived from S3 SRAL and Cryosat-2 SIRAL data, which were calculated using the altitude of the satellite, geoid height, and the distance from the satellite to the water surface (**II**, Eq 9 and Eq 10). Long-term monthly mean water levels were calculated based on the *in situ* measured water levels in Lake Peipsi and Võrtsjärv. Statistical analysis on monthly basis between water quality parameters and water level was performed using satellite data. Deviations of water level were calculated based on regression equations between long-term monthly mean water level and sampling day water level. The deviation was added to derive corrected water quality parameter. The ecological status of lakes was estimated based on Chl-a, FBM and SDD calculated before and after applying water level correction. A description of the methodology developed for *in situ* data can be found Tuvikene et al. (2011).

3. RESULTS AND DISCUSSION

3.1. Validation of AC processors and in-water algorithms applied to S2 MSI and S3 OLCI data over optically complex waters (I, III, IV)

3.1.1. Validation of satellite-derived water-leaving reflectance

Thirteen match-ups between the S2 MSI overpass and *in situ* radiometric measurements were found covering the period of 2015–2017 over nine different waterbodies in Estonia (**I**). Statistical analysis was performed between AC-processors derived ρ_w and *in situ* measured ρ_w shown in **I**, Table 4. Water-leaving reflectance derived from AC processors (Table 3) showed higher inaccuracies and fewer match-ups in small CDOM-dominated lakes. C2RCC was able to derive ρ_w in CDOM-dominated waters with the highest amount of match-ups (N = 13). However, ρ_w in all bands was underestimated compared to *in situ* measured ρ_w. C2RCC had the highest accuracy compared to other AC processors at the main Chl-a algorithm development bands at 560 nm, 665 nm, and 705 nm ($R^2 > 0.7$, dispersion < 58%, RMSE < 0.005, bias > –58%). Water-leaving reflectance at band 665 nm was estimated relatively accurately with the bias of –46% and dispersion of 51%, but all ρ_w at band 705 nm was underestimated (bias –58%) (**I**, Figure 3). As the band 705 nm was underestimated, therefore Chl-a peak was not estimated correctly, which limits to derive high order products (*e.g.* Chl-a and ecological status). Polymer was also comparable with C2RCC at the main Chl-a algorithm development bands at 560 nm, 665 nm, and 705 nm (dispersion < 41%, RMSE < 0.004, bias greater than –0.32%). However, Polymer flagged out most of the match-ups (N = 7) in small and CDOM-dominated waterbodies with a lower coefficient of determination ($R^2 < 0.7$). Acolite and Sen2Cor showed lower accuracy ($R^2 < 0.6$, dispersion > 60%, RMSE > 0.008) and overestimated the blue part of the spectrum (bias > 80%). Acolite also overestimated the NIR part of the spectrum, (bias > 700%), which could be due to the vicinity of the land. Based on the statistics, C2RCC was the most favourable AC processor due to its ability to work in CDOM-dominated waters for S2 MSI data.

Forty-nine match-ups between S3 OLCI and *in situ* radiometric measurements were found covering the period of 2016–2018 over Lake Peipsi, Võrtsjärv and Estonian coastal areas (**III**). Ancillary data (wave height, sun elevation, cloudiness, *etc.*) were recorded at each *in situ* sampling station. *In situ* measured ρ_w were calculated on S3 OLCI bands. *In situ* measured ρ_w showed the highest uncertainties from 400 nm to 560 nm and increased again from 753.75 nm (**III**, Figure 1). Median uncertainty was less than 10% for bands 490–708.75 nm, where the band 560 nm had the lowest (3.9%) median uncertainty. Half of the measurements for bands 510–708.75 nm were obtained with < 5% uncertainties. Based on the uncertainty budget, higher uncertainties also appeared in conditions, when the solar elevation angle was lower than 30 degrees, wave height higher than

0.4 m and wind speed higher than 5 m/s (**III**). Based on the uncertainties in the *in situ* measured ρ_w, 5% uncertainty criterion was applied to improve the accuracy of the *in situ* data for satellite validation. If at least one band in the ρ_w spectrum had uncertainty < 5%, then the spectrum remained, otherwise ρ_w spectrum was eliminated. Based on this criterion, about 55% of match-ups were filtered out.

Validating satellite-derived ρ_w and *in situ* measured ρ_w, the highest errors occurred in the first five kilometres from the shore (**III**, Figure 9). The ρ_w retrievals of S3 OLCI L2 were the most affected from the distance of the shore, then C2RCC and altNN, and Polymer was least affected. Statistical analysis was performed between AC processors-derived ρ_w and *in situ* measured ρ_w shown in **III**, Table 3. Polymer had the highest accuracy compared to other AC processors (dispersion < 74% in all bands), whereas blue bands (400–560 nm) had also lower errors (dispersion < 50%) compared to other AC processors. Bands 560–665 nm had the lowest errors among all AC processors (dispersion 30–70%), whereas C2RCC and altNN had the highest errors (dispersion up to 70%). C2RCC and altNN often showed ρ_w peak at 620 nm instead of 560 nm in eutrophic lakes and flagged out the most of the match-ups in CDOM-dominated waters. S3 OLCI L2 gave systematic negative values in the blue bands (bias more than –50%), but was comparable with other AC processors from band 560 nm to 708.75 nm (dispersion 40–70%).

The base of the AC processors' validation is high-quality *in situ* data, which is important for vicarious calibration, algorithm and applications development. The study found that *in situ* measured ρ_w uncertainties were higher in the blue, red and NIR part of the ρ_w spectrum. Uncertainties increased when the measurements were performed in not optimal environmental conditions. Using the data with the known uncertainties allowed to estimate the suitability of various AC processors over different OWTs and analyse the adjacency effect impact.

A comparison of AC processors, which were applied to S2 MSI and S3 OLCI, showed the highest errors in the blue part and the lowest errors in the green part of the ρ_w spectrum. Errors in the blue part of the ρ_w spectrum (bands < 560 nm) also cause difficulties in deriving CDOM absorption from satellite data (Chen et al. 2022). High errors in the blue bands correspond with other studies (Mograne et al. 2019; Pahlevan et al. 2021; Vanhellemont and Ruddick 2021). Green and red bands were the most accurate for both S2 MSI and S3 OLCI, which are also the main bands for developing Chl-a algorithms (Gitelson et al. 2008; Moses et al. 2009b; Gitelson et al. 2009; Odermatt et al. 2012).

C2RCC applied to S2 MSI data, was able to derive a similar ρ_w spectrum to *in situ* measured ρ_w in CDOM-dominated waters. However, errors were higher in ρ_w spectrum when C2RCC was applied to S3 OLCI data. It often failed to derive correct Chl-a features in reflectance peak (**I**, **III**). Polymer-derived ρ_w had the highest accuracy when applied to S3 OLCI data (**III**), however it flagged-out the most of the data when applied to S2 MSI (**I**). Warren et al. (2019) found that C2RCC was more accurate at deriving ρ_w in all bands, whereas Polymer had the highest accuracy at 560 nm, which is one of the main bands in water quality algorithms. This corresponded to **I**, where Polymer had high accuracy at the 560 nm band (dispersion 20%, RMSE = 0.004, bias –0.1%). Mograne et al. (2019) also states that, efficiency is also important when comparing AC processors, where Polymer was the fastest. S3 OLCI L2 often strongly underestimated ρ_w values up to 560 nm, but in longer wavelengths were comparable with other processors. S3 OLCI L2 ρ_w product is designed for oceanic waters, which could cause negative values in Case-2 waters. However, development for an improved AC processor is ongoing for a better ρ_w product for Case-2 waters (Steinmetz and Constant 2021; Mazeran 2023).

3.1.2. Validation of satellite-derived water quality parameters

Thirty-three in-water algorithms were validated with *in situ* measured OAS and their IOPs (Table 4). Match-ups between S2 MSI and S3 OLCI overpass covered the period of 2016–2022 over Estonian lakes and the Baltic Sea coastal areas (**IV**). In-water algorithm retrievals, from both 1×1 and 3×3 pixel area were compared against *in situ* data, which showed, 3×3 pixel area tended to give more accurate results (lower dispersion and bias, higher coefficient of determination). Therefore, statistical analysis was performed (**IV**, Table 3–5) and further discussion is based on 3×3 pixel area between satellite-derived and *in situ* measured water quality parameters.

S3 OLCI derived TSM products were overestimated compared to *in situ* measurements (bias > 88%) (**IV**, Table 3). Among all TSM algorithms applied to S3 OLCI data, TSM_NN (S3 OLCI L2) had the highest accuracy ($R^2 = 0.69$, dispersion and bias ~88%). S2 MSI derived TSM products were slightly underestimated compared to *in situ* measurements (**IV**, Table 3). Conc_tsm (C2RCC) applied to S2 MSI data, had the highest accuracy compared to other algorithms ($R^2 = 0.74$, dispersion 24%, close to 1:1 line, bias –12%). Applying CDOM absorption algorithms on S2 MSI and S3 OLCI data, all in-water algorithms had poor performance ($R^2 < 0.1$, dispersion > 59%, bias less than –29%) (**IV**, Table 4).

Comparing absorption products (Table 4) derived from S3 OLCI data processed by C2RCC, results were not very accurate compared to *in situ* measurements (**IV**, Table 4). $a_{CDOM(443)}$ was strongly underestimating *in situ* measured values with high scatter (bias –91%, dispersion 91%). Iop_adet$_{(443)}$ was substantially overestimated (bias 85%, dispersion 85%) and iop_adg$_{(443)}$ underestimated (bias –51%). Iop_apig$_{(443)}$ was overestimated at lower values (< 1 m^{-1}) and underestimated at higher values (> 1 m^{-1}) (dispersion 42%). Therefore, the use of iop_apig$_{(443)}$ product as an input for Chl-a estimation is proned to errors, especially over eutrophic waters. However, iop_atot$_{(443)}$, which is the sum of all absorption parameters, was derived the most accurately with a slight underestimation and low scatter (bias –39%, dispersion 43%). There is a lack of studies investigating and validating different absorption parameters separately and summarizing them. C2RCC IOP products have been validated in sea (Toming et al. 2017; Kyryliuk and Kratzer 2019), but limited in lakes.

Satellite-derived scattering products (Table 4) also showed low accuracy derived from S2 MSI or S3 OLCI data (dispersion 25–377%, bias –21–377%)

compared to *in situ* measurements (**IV**, Table 5). The coefficient of determination was high in some cases (b_tot_440_ONNS (A4O), $R^2 > 0.9$), but a number of match-ups between satellite and *in situ* data were low for all products ($N < 18$) and satellite-derived scattering products were under- or overestimated.

Based on the validation studies, different AC processors and in-water algorithms were suitable either on S2 MSI and S3 OLCI. They also indicated the sensitivity to different amounts of OAS in the water *e.g.* to different OWTs. AC processors have been developed based on different processing schemes, where C2RCC, altNN and A4O are based on the NN method (Brockmann et al. 2016; Hieronymi et al. 2016), Polymer is based on the spectral matching method (Steinmetz et al. 2011) and Acolite is using dark fitting method (Vanhellemont and Ruddick 2016). C2RCC and altNN are developed for optically complex Case-2 waters and coastal areas, Polymer designed especially for eliminating sun glint, A4O for estimating OAS based on OWTs and Acolite designed for turbid waters such as lakes and coastal areas.

For the analysis of errors associated with the vicinity of the land, satellite-derived and *in situ* measured Chl-a of each match-up point were split into two groups (< 5 km and > 5 km). S2 MSI Chl-a retrievals had higher errors close to shore (< 5 km) (on average percentage error of 315%) than S3 OLCI (on average percentage error of 150%) (**IV**, Figure 9). Average percentage errors were lower off the shore (> 5 km) for both sensors' products for S2 MSI 35% and S3 OLCI 80%. Polymer Chl-a in-water algorithm had the lowest errors close to the shore (< 100%) and off the shore (< 50%) for S2 MSI and S3 OLCI. The highest difference between both distance groups had Acolite in-water algorithms (on average 360%) for S2 MSI and A4O (on average 310%) for S3 OLCI.

Polymer was least influenced by the vicinity of the land, however, it does not include adjacency effect correction in the processing scheme (Steinmetz et al. 2011) (**III**, **IV**). It is important to analyse errors caused by the vicinity of the land, because errors increased close to shore (< 5 km) for S2 MSI (315%) and S3 OLCI (150%) and were < 100% off the shore. Bulgarelli and Zibordi (2018a) have compared S2 MSI and S3 OLCI data to estimate effects associated with the vicinity of the land, which showed land effects from the shore for the S3 OLCI ~36 km and S2 MSI ~20 km. They also investigated the land effect's relation to water types and found that oligotrophic waters are slightly more influenced, especially the blue part of the spectra. To correct the influence of the vicinity of the land on satellite data, there are ongoing efforts to improve optical satellite remote sensing for small inland waters (De Keukelaere et al. 2018; Vanhellemont 2023).

To estimate consistency between S3 OLCI and S2 MSI (resampled to 300 m) in-water algorithms, 3×3 pixel area were studied. Twelve in-water algorithms were matching for S3 OLCI and S2 MSI (**IV**, Figure 10). Acolite Chl-a in-water algorithms had a high coefficient of determination between S3 OLCI and S2 MSI data ($R^2 > 0.8$). The highest consistency showed chl_re_cons (Acolite) algorithm (close to 1:1 line, $R^2 > 0.96$), but Chl-a derived from S2 MSI algorithm was overestimated in cases when Chl-a were less than 20 mg/m^3. Chl_re_bramich (Acolite) and chl_re_mishra (Acolite) also had high coefficient of determination

($R^2 > 0.8$), but Chl-a higher than 20 mg/m^3 were underestimated by S2 MSI more than S3 OLCI. It means that by applying the same algorithm on S2 MSI and S3 OLCI data, time series will differ for specific Chl-a ranges. Other in-water algorithms did not show very high consistency. Chl-a derived from chl_re_gons (Acolite), were compared with *in situ* measured Chl-a. Chl-a were overestimated by in-water algorithms applied to S2 MSI, more than S3 OLCI. The discrepancy between satellite-derived and *in situ* measured Chl-a was higher close to shore (< 2 km) (difference approximately –20 mg/m^3). There are not many studies for comparing consistency between S2 MSI and S3 OLCI in-water algorithms, but several studies have shown integration between these satellites for more frequent data (Sòria-Perpinyà et al. 2021; Salama et al. 2022). Combining different sensors' data is essential in the case of estimating water quality parameters globally over various sizes of lakes to evaluate changes over a broad period.

3.2. Developing and testing Chl-a algorithms over optically complex waters (I, IV, V, VI)

For testing the suitability of various Chl-a algorithms over optically complex waters, 28 empirical Chl-a algorithms were applied on the GLaSS dataset (*in situ* radiometric data calculated to S2 MSI bands), which represent various waters from oligotrophic to hypereutrophic (**I**, Table 5). Based on the coefficient of determination, empirical algorithms had a high correlation with *in situ* measured Chl-a for different types of waterbodies, were selected (**I**, Table 6). The Two-Band NIR-Red model algorithm $\frac{R_{705}}{R_{665}}$ had high accuracy in CDOM-low waters ($a_{CDOM(443)} < 4.1\ m^{-1}$), with a coefficient of determination $R^2 = 0.97$. The Three-Band NIR-Red model algorithms had a high accuracy in a high Chl-a waters (Chl-a up to 150 mg/m^3), where the band ratio $\left(\frac{1}{R_{665}} - \frac{1}{R_{705}}\right) \times R_{740}$or R_{783} had a coefficient of determination $R^2 > 0.92$. The Four-Band NIR-Red model algorithms showed high accuracy in high TSM waters (TSM > 10 mg/L), where the band ratio $\left(\frac{1}{R_{705}} - \frac{1}{R_{665}}\right) \div \left(\frac{1}{R_{705}} + \frac{1}{R_{665}}\right)$ had a coefficient of determination $R^2 > 0.9$. MCI algorithm applied to L1 data estimated *in situ* measured Chl-a dynamics well in case of Chl-a > 15 mg/m^3, however the coefficient of determination was low $R^2 < 0.3$. Based on the results, different Chl-a empirical band ratio algorithms were OWT dependent, varying with different amounts of OAS in the water. Therefore, further investigation is needed for better assessment of different waters.

S3 OLCI L2 (CHL_NN) and alternative processing schemes were applied to S3 OLCI data to derive Chl-a (**IV**). Statistical analysis were performed between satellite-derived and *in situ* measured Chl-a (**IV**, Figure 2, Table 2). Acolite has four, A4O has two and C2RCC and Polymer have one Chl-a product as an output (Table 4). Chl-a were the most accurately derived by chl_re_gons (Acolite) in-water algorithm ($R^2 = 0.7$, data aligned close to 1:1 line, dispersion 23%, bias 10%). However, the dispersion increased when Chl-a was higher than 40 mg/m^3. Chl_re_mishra (Acolite) also showed good accuracy ($R^2 = 0.58$, close to 1:1 line), but the scatter was higher in the case of Chl-a higher than 20 mg/m^3. Chl_re_bramich (Acolite), chl_re_moses3b (Acolite) and CHL_IOP_ONNS (A4O) showed a systematic overestimation (bias > 45%). Conc_chl (C2RCC) and CHL_NN (L2) systematically underestimated Chl-a especially from Chl-a more than 20 mg/m^3 (bias –35%).

Chl-a in-water algorithms were applied to S2 MSI data (**IV**). Acolite has six Chl-a in-water algorithms, C2RCC and Polymer have one (Table 4). All Chl-a algorithms' retrievals had low relationship between satellite-derived and *in situ* measured Chl-a ($R^2 < 0.37$) with a high scatter in low values (**IV**, Figure 3). Chl-a derived from chl_re_gons740 (Acolite) was the most accurate compared to *in situ* measured Chl-a ($R^2 = 0.37$). Low concentrations (Chl-a < 10 mg/m^3) were overestimated, but accuracy was better in the case of Chl-a > 25 mg/m^3. Chl-a derived from conc_chl (C2RCC) and logchl (Polymer) tended to underestimate *in situ* measured Chl-a. Acolite Chl-a in-water algorithms gave the most accurate results compared to other algorithms for both S2 MSI and S3 OLCI, whereas chl_re_gons and chl_re_gons740 (Acolite) had the highest accuracy for S3 OLCI and chl_re_gons740 for S2 MSI.

As Chl-a algorithms showed OWT dependence – sensitivity to different Chl-a but at the same time to other OAS (TSM, CDOM) in the water, OWT guided approach was tested. Classification of *in situ* radiometric ρ_w into five OWT classes (Clear, Moderate, Turbid, Very Turbid, Brown) was performed (Figure 2) (**V**, **VI**). Each OWT class had its specific spectrum features:

- Clear has maximum ρ_w at wavelengths 540–580 nm, with a low amount of OAS and high SDD;
- Moderate has maximum ρ_w at wavelengths 540–580 nm with a sharper slope of ρ_w than Clear and increased amount of OAS and absorption;
- Turbid has maximum ρ_w at wavelengths in the green part of the spectrum (500–700 nm), the highest among all OWT with dominant TSM;
- Very Turbid has maximum ρ_w at wavelengths 685–715 nm with dominant Chl-a;
- Brown has maximum ρ_w at wavelengths in the red part of the spectrum with very low ρ_w values.

In situ radiometric ρ_w were calculated on S2 MSI and S3 OLCI bands. OWT classes calculated on *in situ* measured ρ_w were matching 95% between OWT classes calculated on S2 MSI and S3 OLCI bands.

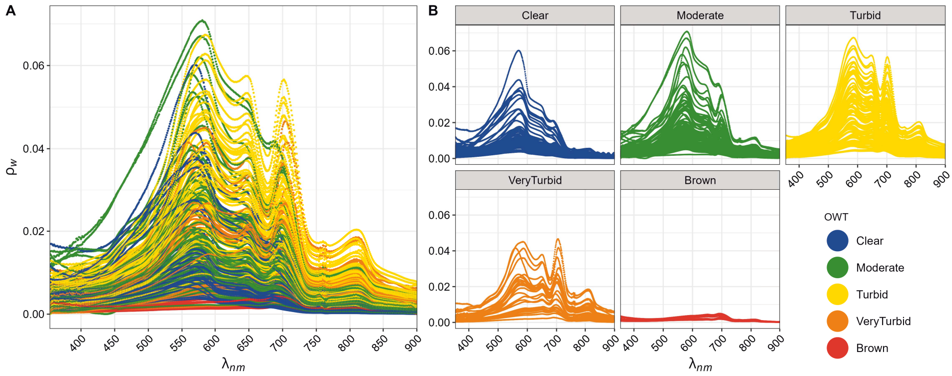

Figure 2. Variation of OWTs based on *in situ* measured radiometric ρ_w. (A). Each OWT ρ_w spectra separately (B).

The most suitable Chl-a algorithm was found for each OWT based on the ranking system described in the publication **VI**. 60 algorithms were tested for deriving Chl-a for five OWTs (**IV**, Table 2).

- For Clear OWT, different algorithms were the most accurate for S2 MSI and S3 OLCI. The best performance showed Gitelson (1992) algorithm using ρ_w peak at near 700 nm for S3 OLCI and MCI algorithm for S2 MSI (Gower et al. 2008);
- For Moderate OWT, Red-NIR algorithm was the most accurate for both S2 MSI and S3 OLCI;
- For Turbid, different algorithms were the most accurate for S2 MSI and S3 OLCI. The best performance showed Gitelson et al. (2009) Three-Band algorithm for S3 OLCI and Zimba and Gitelson (2006) Four-Band algorithm for S2 MSI;
- For Very Turbid OWT, also different algorithms were the most accurate for S2 MSI and S3 OLCI. However, the same Red-NIR algorithm, which was the most suitable for S2 MSI Moderate OWT, was the most suitable for Very Turbid for S2 MSI. Normalized Difference Chlorophyll Index (Mishra and Mishra 2012) had the best performance for S3 OLCI;
- For Brown OWT, NIR-Red algorithm showed best performance for both S2 MSI and S3 OLCI, however this algorithm explained only about 40% of the variance observed in the *in situ* measured Chl-a.

For deriving Chl-a using the most applicable algorithms based on OWT and compared with *in situ* measured Chl-a, coefficient of determination showed a high correlation for S2 MSI ($R^2 = 0.85$) and S3 OLCI ($R^2 = 0.86$).

S2 MSI has nine bands in the visible and NIR part of the spectrum, whereas S3 OLCI has 21 bands, which makes estimating the Chl-a absorption peak at 680 nm easier with band location at 681 nm from S3 OLCI. Also, band-widths are narrower for S3 OLCI and it gives more frequent data than S2 MSI. Less available S2 MSI data is also impacted by the flagging and the OWTs, where majority of the pixels could flagged out. With the launch of the new S2 satellites, the time coverage and the constant improvement of AC processors and bio-optical models will improve.

Estimating Chl-a in lakes using S2 MSI data have been studied in recent years because of the suitable spatial resolution (Grendaitė and Stonevičius 2018; Bramich et al. 2021; Tóth et al. 2021). Optically complex waters have a wide range of OAS, therefore one standard algorithm often fails in these conditions (Darecki et al. 2003; Palmer et al. 2015) or is meant for specific region or OWTs (Le et al. 2009; Lins et al. 2017). However, the amount of OAS could vary even inside the waterbody, also daily, seasonally and annually (Simis et al. 2017). Also, studies developing and validating Chl-a algorithms over Baltic Sea region have been done (Arst and Kutser 1994; Kutser 2004; Reinart and Kutser 2006; Toming et al. 2016, 2017; Ligi et al. 2017; Soomets et al. 2020b). Alikas et al. (2023) compared six different methods to derive Chl-a from optically complex lakes and found that these different methods complemented each other, but were not transferable to each other due to the change in environmental conditions, methodology and seasonality. Remote sensing spatial resolution, will help to monitor the entire waterbody and classify every pixel, but it requires sophisticated algorithms in order to quantitatively derive precise ranges of Chl-a.

Figure 3 shows OWT variance spatially and seasonally in Lake Peipsi in 2023. It shows that the OWTs vary from Clear in the northern part of Lake Peipsi to Brown in the southern part of Lake Peipsi in the beginning of spring. In the end of the summer, OWTs vary from Moderate in the northern part of Lake Peipsi to Very Turbid in the southern part of Lake Peipsi. Such classification helps to retrieve more accurate results by applying specific water quality algorithms suitable for certain OWT. Empirical band ratio algorithms using red and NIR part of the spectrum were the most suitable for high amounts of OAS in the water, representing such Turbid, Very Turbid and Brown. Still, the basis of the Chl-a algorithm development is accurately derived ρ_w with low errors. Alikas et al. 2010 and Toming et al. 2016 have shown the suitability of using MCI on L1 data to derive Chl-a. It could be a good alternative to avoid errors caused by AC processors. However, it is not working in low Chl-a waters (< 15 mg/m^3) and it is not applicable for all waters, but should considered as one solution. Similarly to ocean colour radiometric data, there is ongoing effort for estimating uncertainties deriving Chl-a (Canuti et al. 2022). Inter-comparison exercises have been done between satellite-derived and *in situ* measured Chl-a for more accurate Chl-a estimation. To validate Chl-a derived from satellite data, 25% accuracy has been considered acceptable (Canuti et al. 2022).

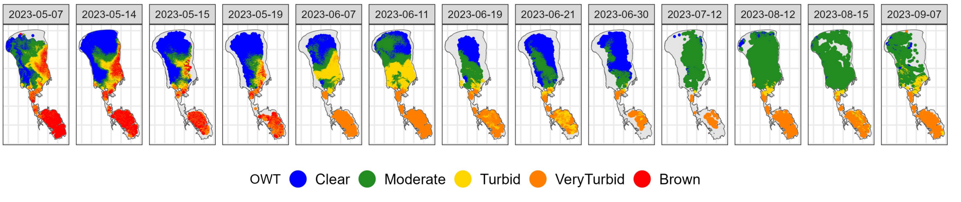

Figure 3. Seasonal changes of OWT applied to S3 OLCI processed by Polymer in Lake Peipsi in 2023.

3.3. Developing applications using satellite data for supplementing estimation of the ecological status of lakes under the EU WFD (I)

Using satellite data for developing applications, to support estimation of the ecological status under EU WFD is beneficial. EO data potential as a complementary source of information for estimating the ecological status of waterbody based on Chl-a was explored. S2 MSI data were investigated because of the suitability for small lakes. Different approaches were investigated for deriving Chl-a from S2 MSI data 1) empirical band ratio algorithms and MCI applied to C2RCC processed data, 2) neural network product conc_chl (C2RCC) and, 3) MCI applied to L1 data (**I**, Table 6). Investigated lakes represent optically complex waterbodies with different sizes and OWTs (Figure 4). The ecological status classes are defined by the Chl-a in specific lakes over respective period of time (Ministry of Environment 2009).

Lake Verevi was the smallest (water surface area ~12 ha) investigated lake, with low SDD (average 1.65 m), where *in situ* measured Chl-a ranged from 15–31 mg/m^3 and $a_{CDOM(443)}$ from 6–9 m^{-1} (Figure 4A). MCI algorithm applied to L1 data gave the most similar Chl-a dynamics compared to *in situ* measured Chl-a, estimating the ecological status similarly Moderate as based on *in situ* measured Chl-a. MCI applied to C2RCC processed data classified the ecological status of Verevi as Good and conc_chl (C2RCC) as Very Good. However, it was not accurate, because the values of Chl-a were too low and Chl-a seasonal dynamics was not visible in Verevi, which was possibly caused by the incorrect ρ_w derived from C2RCC (Figure 4B).

Lakes with larger surface area showed more accurate C2RCC-derived ρ_w spectrum (Figure 4D, F, H) and empirical band ratio algorithms and conc_chl (C2RCC) estimated Chl-a more accurately. Ermistu (water surface ~450 ha) has higher SDD (average 1.8 m), and lower Chl-a (5–8 mg/m^3) with lower $a_{CDOM\,(443)}$ 4–7 m^{-1}. Chl-a derived from Four–Band NIR–Red model $\mathrm{Chl-a} = 43.2 \times \left(\frac{1}{R_{665}} - \frac{1}{R_{705}}\right) \div \left(\frac{1}{R_{740}} - \frac{1}{R_{705}}\right) + 10.2$ showed the most similar dynamics to *in situ* measured Chl-a (Figure 4C). Conc_chl (C2RCC) was also comparable with other empirical algorithms, but the range of minimum and maximum values was higher and made it less stable for estimating Chl-a. It could be due to the underestimated ρ_w values at 705 nm (**I**, Figure 4). The ecological status in lake Ermistu was estimated as Very Good by both *in situ* measurements (average *in situ* Chl-a 6.0 mg/m^3, N = 4) and by satellite-derived Chl-a (average 5.7 mg/m^3, N = 10).

Lake Ähijärv (water surface ~180 ha, SDD 1.8 m) has Chl-a 9–26 mg/m^3 and $a_{CDOM\,(443)}$ 2.7–3.5 m^{-1} (Figure 4E). Chl-a derived from Three-Band NIR-Red model $\mathrm{Chl-a} = 24385.4 \times \left(R_{705} - \frac{R_{665}+R_{740}}{2}\right) + 7.7$ gave the most similar dynamics to *in situ* measured Chl-a, however Chl-a measurements were not collected and recorded when Chl-a was ~20 mg/m^3 in July. MCI algorithm applied to L1 data showed also similar dynamics to *in situ* measured Chl-a, whereas conc_chl (C2RCC) gave too high or too low Ch-a. Again, it could be due to the underestimated ρ_w values at 705 nm. The ecological status in Ähijärv was estimated as Moderate by *in situ* measurements (average *in situ* Chl-a 18.0 mg/m^3, N = 4) as well as satellite-derived Chl-a (average empirical algorithm 14.7 mg/m^3, N = 9) and by MCI applied to L1 (23.6 mg/m^3, N = 9).

Lake Peipsi station 2 (~7 km from the shore) SDD was low < 1 m with Chl-a between 10–21 mg/m^3. Chl-a derived from Three-Band NIR-Red model $\mathrm{Chl-a} = 260.5 \times \left(\left(\frac{1}{R_{665}} - \frac{1}{R_{705}}\right) \times R_{740}\right) + 27.8$ applied to C2RCC processed data and conc_chl (C2RCC) showed similar dynamics to *in situ* measured Chl-a (Figure 4G). In the beginning of the summer, when Chl-a was lower (< 20 mg/m^3), Chl-a was underestimated by MCI applied on L1 data, which is typical for MCI algorithm. Higher Chl-a in the end of the summer had better agreement with *in situ* Chl-a. Chl-a derived from satellite data showed seasonal dynamics, when Chl-a decreases in July and August. As Chl-a *in situ* measurements are very sparse (once in a month), therefore seasonal dynamics were not captured, which is possible with satellite data. Therefore, the ecological status in Lake Peipsi station 2, was classified as Moderate by *in situ* measurements (average *in situ* Chl-a 16.8 mg/m^3, N = 4), Good and Moderate by satellite-derived Chl-a (average 7.4 and 16.7 mg/m^3, N = 13).

Satellite-derived Chl-a showed similar dynamics to *in situ* measured Chl-a in case of correct ρ_w values. Therefore, it is important to develop or use AC processors, which are working in challenging conditions. Especially, when the vicinity of the land influences water pixels and different amounts of OAS are in the water (especially CDOM-dominated), otherwise all algorithms will fail. Errors of ρ_w were higher in smaller lakes, like Verevi and lower in lakes, where water surface area were larger. Applying MCI algorithm on L1 data would be one solution to derive Chl-a in more productive waters to eliminate failures caused by AC processors. The NN method (conc_chl) should have a benefit over empirical band ratio algorithms, because of the consideration of other OAS in the water. Nevertheless, it derived low or high Chl-a values caused by the C2RCC-derived ρ_w spectrum, which underestimated ρ_w values at 705 nm. Three-Band NIR-Red or Four-Band NIR-Red models were able to work seasonally in different conditions, when ρ_w was derived correctly. The inclusion of both *in situ* and EO data could improve the ecological status assessment in terms of data availability. It would show better the trends in the lakes and would allow the user to give more weight either on *in situ* or EO data or use the synergy of both.

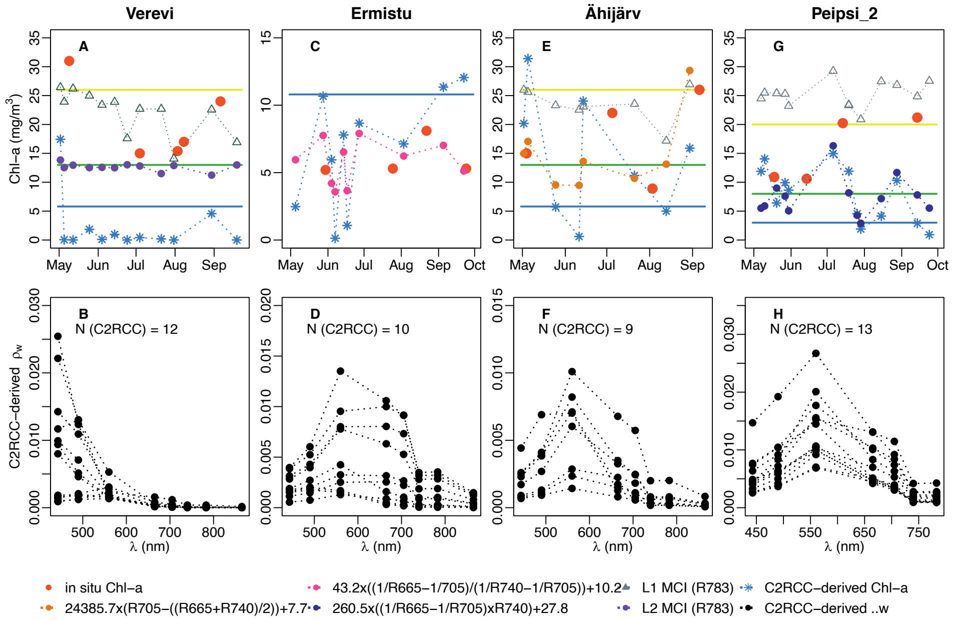

Figure 4. Estimation of Chl-a seasonal dynamics in Verevi (2017) (A), Ermistu (2017) (C), Ähijärv (2017) (E) and Peipsi station 2 (2016) (G) with C2RCC-derived ρ_w values on each lake (B, D, F, H). Colour bars represent the thresholds of the ecological classes, where the blue line indicates Very Good, the green line Good and the yellow line Moderate class (**I**).

3.4. Correcting optical water quality parameters in respectively to water level and creating synergy between optical and altimetry data for improved assessment of the ecological status under WFD (II)

Optical and altimetry data were used to monitor Lake Peipsi and Võrtsjärv from the period of 2016–2019. *In situ* measured water levels were derived from four stations (Figure 1) and were compared with water level derived from altimetry S3 SRAL and Cryosat-2 SIRAL data. Satellite-derived water level showed high accuracy compared to *in situ* measured water level, with a bias of < 0.4 m, RMSE < 0.1 m and $R^2 > 0.98$ (Figure 5). Chl-a derived from satellite data had a coefficient of determination $R^2 = 0.7$, FBM had $R^2 = 0.6$, and SDD had $R^2 = 0.4$ with *in situ* measurements. The methodology developed by Tuvikene et al. (2011) for *in situ* data was applied to satellite data. Significant relationships (p-value < 0.05) were found between long-term monthly mean water level and water quality parameters. Significant relationships occurred more in Võrtsjärv and Lämmijärv, than Lake Peipsi *s.s.* and Pihkva. When the water level was higher than the long-term monthly mean water level and when statistically significant relationships between water quality parameters and water levels occurred, the value of the water quality parameter (Chl-a, FBM, SDD) was higher after the correction. If the water level was lower, then the value of the water quality parameter was lower after the correction. This directly changed water quality parameters' mean value of the month, as well as minimum and maximum values, which directly affected the ecological status of water. Greater changes in water level compared to long-term monthly mean water level, changed the ecological status class from one to another. Smaller changes in water level compared to long-term monthly mean water level, changed the mean values of water quality parameters, but not the ecological status class of the water.

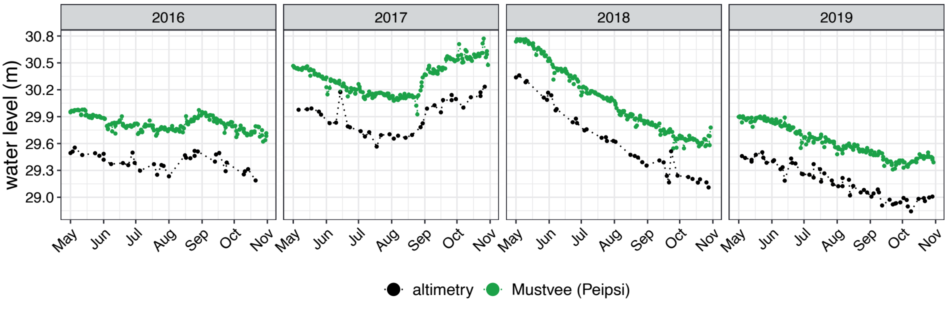

Figure 5. *In situ* measured (green) and satellite-derived (black) water level in Lake Peipsi Mustvee station from 2016–2019 (**II**).

According to the Ministry of Environment (2009) the ecological status of Võrtsjärv based on the Chl-a, the monitoring period from July to August is considered. In estimating the ecological status based on SDD, the monitoring period from May to November is considered. However, FBM is not considered as an important parameter in Võrtsjärv. Correcting water quality parameters according to water level (Figure 6), corrected Chl-a values increased monthly mean values of Chl-a (Figure 6B) and decreased SDD (Figure 6D) over the monitoring period in 2016, because sampling day water level was higher than long-term monthly mean water level. Monthly mean values of Chl-a decreased and SDD increased in 2017–2019, because the sampling day water level was lower than the long-term monthly mean water level.

These changes in water quality parameters affected the ecological status based on Chl-a, which improved in 2017 and 2018 from Moderate to Good and 2019 from Bad to Moderate. The ecological status remained the same after correcting Chl-a in 2016, however the mean value of the Chl-a over the monitoring period increased. The ecological status according to SDD improved from Good to Very Good in 2018 and 2019.

In Lake Peipsi, there were less statistically significant relationships between water quality parameters and water level. In Peipsi *s.s.*, only FBM had astatistically significant relationship with the water level in June and September. However, it did not change the ecological status class in Peipsi *s.s.* More statistical relationships occurred in Lämmijärv, which is shallower than Peipsi *s.s.* The ecological status class changed only in 2019 according to SDD from Moderate to Good. Other water quality parameters' monthly mean values did not affect the estimation of the ecological status.

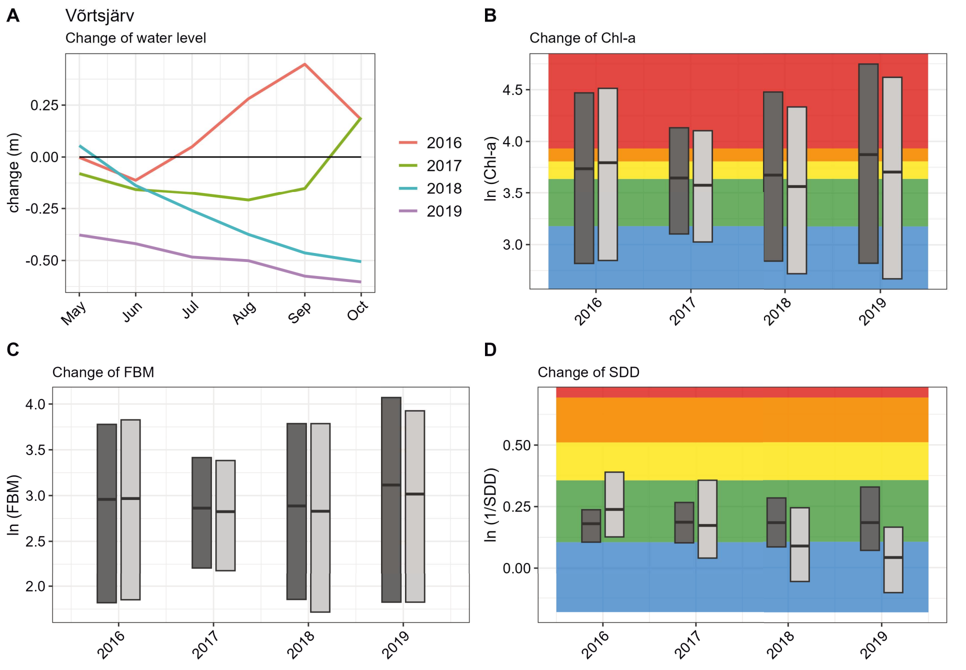

Figure 6. Water level change from long-term monthly mean water level during the study period in Võrtsjärv (A). Value 0 indicates the long-term monthly mean water level. Mean, maximum and minimum values of EO-derived water quality parameters are represented on the graphs (B, C, D), where dark gray indicates values before and light grey indicates values after applying water level correction. Colours represent the thresholds of ecological classes, where blue indicates Very Good, green Good, yellow Moderate, orange Bad and red Very Bad ecological status class according to EU WFD (**II**).

The water level is influenced by different factors, such as seasonal temperature variability, precipitation, evaporation, snow and ice melting (Górniak and Piekarski 2002; Mooij et al. 2005; Jeppesen at al. 2014; Torabi et al. 2015), which in turn affects the ecological status of the waterbody, especially in shallow lakes (Tuvikene et al. 2011). As *in situ* stations for measuring water levels are expensive to maintain and some lakes do not have any stations (Avisse et al. 2017; Jiang et al. 2017; Sheffield et al. 2018), the use of altimetry data has been increased (Göttl et al. 2016; Nielsen et al. 2017; Sun et al. 2021; Ma et al. 2024). The combination of different altimetry sensors data, will give frequent estimation of water level dynamics and its change (Song et al. 2015; Wu et al. 2017; Li et al. 2020). Recent studies have shown potential using altimetry data on lakes using S3 SRAL altimetry sensor' data (Liibusk et al. 2020; Nielsen et al. 2020; Sun et al. 2021). Water levels have been monitored without gaps since 1992 by the altimeter French–US Topex Poseidon. Water quality has been monitored continuously from 1997 with SeaWiFS, whereas Landsat satellites provided data even from 1972, and the current Sentinel mission will provide data at least 15 years from now. With continuous satellite missions, we will have long time series, which help us monitor lake ecosystems more precisely and estimate future predictions.

According to the WFD, assessment of the ecological status is based on specific waterbody and parameter. The monitoring period for Chl-a is only two months in Võrtsjärv, therefore higher amount of data will show more dynamics and a better overview of the changes in the lake (Figure 7B), which is possible with the combination of different optical sensors (Baup et al. 2014; Ebaid and Aziz 2017; Bresciani et al. 2019; Asfaw et al. 2020). Separating anthropogenic factors from natural variability is very important research direction for better assessment under WFD. Combining optical and altimetry data, will give the possibility to estimate the influence of water level on the lake, which is more pronounced in shallow lakes.

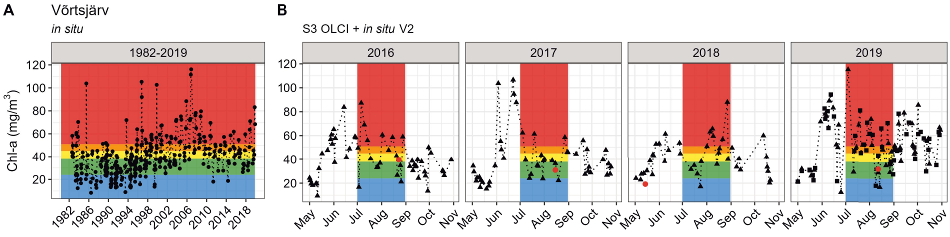

Figure 7. Long-term time series of *in situ* measured Chl-a in Võrtsjärv station 2 (A), and Chl-a derived from S3 OLCI 2016–2019 (B). Dots indicate *in situ* measured values and triangles S3 OLCI A and B values. Colour bars represent the thresholds of ecological classes, where blue indicates Very Good, green Good, yellow Moderate, orange Bad and red Very Bad class (**II**).

Estimating the ecological status of waterbody will help to understand the actions what current management needs for a sustainable future (Wang et al. 2012). To use satellite data as a complementary source to the assessment of the ecological status according to feasible parameters, we need to first validate every product in the EO data processing chain to decrease uncertainties in the final product. However, it is challenging in optically complex waters, especially in eutrophic and absorbing waters, where the vicinity of the land also plays a role. EO data processing must be lake and parameter-specific – currently there is no specific processor or algorithm suitable for deriving all optical water quality parameters in these challenging conditions. Also, identical approaches applied to different satellite sensors tend to give consistent outputs only for certain range of values and conditions. This needs to be considered when deriving time series from remote sensing data to analyse the changes and trends in the waterbodies. OWT-based classification helps to classify waterbodies spatially and find specific Chl-a algorithms. Combining EO data with *in situ* data, allows us to have a wider dataset to study the ecosystem and improve the assessment of the ecological status of waters.

CONCLUSIONS

The study concludes:

- Despite of the growing constellations of Copernicus Sentinel satellites, there is no standard product for ρ_w for Sentinel-2 MSI and Sentinel-3 OLCI for optically complex waters. Many alternative solutions exist. As the ρ_w is the core product for higher order products (*e.g.* Chl-a), it must be derived, and the accuracy should be quantified. Suitable atmospheric correction processors for optically complex waters were investigated to estimate their accuracy in order to avoid biased results in higher order products.
- All atmospheric correction processors had low accuracy in deriving ρ_w in the blue and NIR part of the spectrum. Accuracy was the highest at bands from 560 nm to 740 nm, where all atmospheric correction processors showed comparable results. Their performance depended, in particular, on the sensor, optical water type and the vicinity of the land. In general, C2RCC and Polymer showed the best performance compared to other tested atmospheric correction processors. For S2 MSI, C2RCC was able to work in CDOM-dominated waters, however it systematically underestimated reflectance peak at 705 nm and therefore Chl-a absorption features at 665 nm was difficult to estimate. For S3 OLCI, the reflectance peak at 620 nm was derived instead at 560 nm. Polymer applied on S2 MSI data flagged out most of the pixels in CDOM-dominated waters and applied on S3 OLCI had low accuracy at 865 nm. However, the pixels were less influenced by the vicinity of the land compared to all other tested atmospheric correction processors. Depending on the in-water algorithm (*e.g.* empirical, neural network), specific atmospheric correction processor must be chosen to ensure the high accuracy for the final product.
- Quantifying uncertainties in *in situ* data is essential for using high-quality reference data for satellite data validation. Uncertainties of *in situ* radiometric measurements were higher in the blue, red and NIR part, and were lower in the green part of the ρ_w spectrum. For the bands 490–708.75 nm, the median uncertainty was less than 10% and was the lowest for the band 560 nm (3.9%). Radiometric measurements were highly dependent on the measurement conditions, where wave height > 0.4 m, wind speed > 5 m/s and solar elevation angle < 30 degrees, resulted in ρ_w with elevated uncertainty.
- The study covered a wide range of OAS (Chl-a 0.16–215 mg/m^3, TSM 0.1–134 mg/L, $a_{CDOM(443)}$ 0.004–47 m^{-1}) based on the *in situ* measurements. Water in lakes and coastal areas can change spatially and seasonally, therefore one certain algorithm was not able to work in this kind of conditions. Accuracy of the algorithms were sensor and OAS dependent. Satellite-derived TSM was overestimated (S3 OLCI bias > 88 %) or underestimated (S2 MSI bias > –12%) compared to *in situ* measurements. Satellite-derived CDOM absorption had very low accuracy ($R^2 < 0.1$, dispersion > 59%, bias less than –29%). Comparing each absorption parameter (C2RCC) separately, there was low accuracy

(over-or underestimation). However, total absorption as the sum of all absorption parameters showed the most accurate results with a slight underestimation and low scatter (bias –39%, dispersion 43%). The quantification of each absorption parameter separately increased the error.

- As Chl-a is the key indicator for primary production and water quality, and also essential parameter for many directives (*e.g.* European Union Water Framework Directive), therefore Chl-a algorithms were further investigated. Satellite-derived Chl-a derived from S3 OLCI had high accuracy using chl_re_gons (Acolite) in-water algorithm ($R^2 = 0.70$, data aligned close to 1:1 line, dispersion 23%, bias 10%). Chl-a algorithms applied to S2 MSI data showed suitability on different water types and had lower accuracy compared to S3 OLCI. Two-Band NIR-Red model algorithms were the most suitable ($R^2 = 0.97$) in CDOM-low waters. Three-Band NIR-Red model algorithms were the most suitable ($R^2 > 0.92$) in high Chl-a waters, Four-Band NIR-Red model algorithms were the most suitable ($R^2 > 0.9$) in TSM-high waters. Absorption coefficient of phytoplankton pigment at 443 nm can be used as an input for deriving Chl-a. However, it was overestimated by S2 MSI (bias ~ 30%, dispersion ~ 40%) and higher concentrations were underestimated by S3 OLCI, which decrease the accuracy of Chl-a estimation. For reducing algorithm uncertainties caused by atmospheric correction processors and their dependence on the optical water types, Maximum Chlorophyll Index algorithm applied to L1 data showed similar Chl-a dynamics to *in situ* measurements over eutrophic waters. The inclusion of both *in situ* and satellite derived Chl-a estimates improved the ecological status assessment in terms of data availability, and would allow the user to give more weight either on *in situ* or EO data or use the synergy of both.
- Improving the assessment of the ecological status based on the European Union Water Framework Directive, natural factors should be also considered. One of the natural factors is water level change, which was derived from altimetry data showing good precision compared to *in situ* measurements (bias < 0.4 m, RMSE < 0.1 m and $R^2 > 0.98$). Combining water level derived from altimetry data and water quality parameters derived from optical data, the satellite-based methodology was tested to account for water level change respective to long-term monthly mean water level. In the case of very low water level compared to long-term monthly mean water level in Võrtsjärv in 2017–2019, the ecological status class based on Chl-a improved in 2017 and 2018 from Moderate to Good and 2019 from Bad to Moderate. Water level was slightly higher in 2016, however the ecological status did not change. A combination of *in situ*, altimetry and optical data will improve the estimation of the ecological status class.

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SUMMARY IN ESTONIAN

Sünergia loomine kaugseire abil täiustamaks optiliselt keeruliste vete seiret

Järved ja rannikualad on oluline osa vee ökosüsteemidest reguleerides kliimat ja süsinikuringet, pakkudes elukeskkonda veeorganismidele seejuures tagades bioloogilise mitmekesisuse, pakkudes joogivett ning olulisi ökosüsteemiteenuseid. Järvedele ja rannikualadele aga avaldavad mõju nii inimtekkelised kui looduslikud tegurid. Looduslikud tegurid nagu näiteks sesoonsus ja veetaseme muutus avaldab mõju veekvaliteedi hindamiseks kasutatavatele parameetritele nagu näiteks klorofüll-a, fütoplanktoni biomass ja vee läbipaistvus. Seetõttu on oluline jälgida veekogu seisundit pidevalt, et olulistele muutustele koheselt reageerida. Selleks on Euroopa Liidu liikmesriigid kohustatud hindama veekogude ökoloogilist seisundit veepoliitika raamdirektiivi alusel, et tagada jätkusuutlik veekeskkond ka tulevikus.

Copernicuse programmi Sentineli seeria Sentinel-3 Ocean and Land Colour Instrument (OLCI) on arendatud veekvaliteedi hindamiseks, kuid tema ruumiline lahutus 300 m pole piisav väikeste järvede seireks. Sentinel-2 MultiSpectral Instrument (MSI) sensoril on 10–60 meetrine ruumiline lahutus, kuid kanalite asukohad nähtava kiirguse lainealas ja kanalite laius on mõeldud eelkõige taimkatte uurimiseks. Sentinel-3 OLCI standard veeproduktid pole sobivad Case-2 vetele. Optiliselt keerulised veed sisaldavad optiliselt aktiivseid aineid nagu klorofüll-a (pigment fütoplanktonis), heljum (liivaosakeste setted) ja kollane aine (lahustunud orgaaniline aine). Neil on iseloomulik spekter, kuid kui kõik ained on vees erineval hulgal, siis ühe universaalse algoritmi leidmine on keeruline. Veed, kus kollane aine (CDOM) on dominante aine vees, on eriti keerulised, sest enamus valgusest neeldub. Optiliselt keerukad järved pole samuti ka homogeensed veekeskkonnad, mistõttu võib optiliselt aktiivsete ainete hulk muutuda nii veekogu siseselt kui ka sesoonselt.

Selleks, et arendada välja satelliitandmetel põhinevaid rakendusi, on oluline osa satelliitandmete täpsusel ja usaldusväärsusel. Sellest tulenevalt on doktoritöö peamiseks eesmärgiks arendada välja satelliitandmetel põhinevaid rakendusi optiliselt keerukatele vetele. Selle eesmärgi täitmiseks püsitati töös neli konkreetsemat eesmärki 1) valideerida atmosfäärikorrektsiooni protsessoreid ja veekvaliteedi parameetrite algoritme Sentinel-2 MSI ja Sentinel-3 OLCI andmetel; 2) testida olemasolevaid ja arendada välja uusi klorofüll-a algoritme; 3) arendada välja *in situ* ja satelliitandmetel põhinevaid rakendusi veekogude ökoloogilise klassi hindamiseks klorofüll-a alusel Euroopa Liidu veepoliitika raamdirektiivi jaoks 4) kombineerida *in situ*, optilisi ja altimeetria andmeid, et luua erinevate andmete vahel sünergia täiustamaks kaugseire andmetel põhinevaid meetoteid, et suurendada täpsust ökoloogilise klassi hindamisel.

Sentinel-3 OLCI standard töötlustasemega andmetes oli vee peegeldustegur spektri sinises osas alahinnatud ning negatiivne. Seetõttu võrreldi töös alternatiivseid atmosfäärikorrektsiooni protsessoreid. Sentinel-2 MSI ja Sentinel-3 OLCI andmetelt vee peegeldusteguri hindamiseks andsid täpseid tulemusi erinevad protsessorid, vastavalt C2RCC ja Polymer. C2RCC rakendatuna Sentinel-2 MSI andmetele andis kõige rohkem tulemusi ka CDOMi-rohketes vetes ning Polymer rakendatuna Sentinel-3 OLCI andmetele suutis anda täpseid tulemusi ka kalda-äärsetel aladel. Samuti hinnates veekvaliteedi parameetreid Sentinel-2 MSI ja Sentinel-3 OLCI andmetelt võrreldes veeproovidest saadud andmetega kasutades erinevaid algoritme, algoritmide täpsused olid pigem sensori ja parameetri põhised. Näiteks, C2RCC TSM algoritm rakendatuna Sentinel-2 MSI andmetele hindas TSM kontsentratsiooni suhteliselt täpselt (hälve –12%), kuid tugevalt üle-hindas rakendatuna S3 OLCI andmetele (hälve ~90%). CDOMi hindamiseks ei andnud ükski algoritm head tulemust (R^2 ~0.1).

Oluline osa satelliitandmete valideerimisel on ka kohapeal mõõdetud radio-meetrilistel andmetel ja nende mõõtemääramatustel. Töö käigus hinnati, millistel tingimustel on kohapeal mõõdetud veepeegeldusteguri mõõtemääramatused kõige suuremad. Keskkonnatingimustest tulenev mõõtemääramatus võib olla väga kõrge. Oludes, kus päikese kõrguse nurk on < 30 kraadi, laine kõrgus > 0.4 m ja tuule kiirus > 5 m/s, olid mõõtemääramatused kõige suuremad. Mõõtemääramatused olid kõrgemad kanalitel sinises ja punases ja lähi-infrapunases lainealas ning väikseimad kanalitel rohelises lainealas. Satelliitandmete puhul oli vead suure-mad kalda-äärsetel aladel (< 5 km). Rohkem oli kalda-äärsetest aladest mõjutatud Sentinel-2 MSI andmed (viga 315%) ja vähem Sentinel-3 OLCI andmed-(viga 150%). Kõige vähem kalda-äärsetest aladest oli mõjutatud Polymeriga töödeldud andmed (viga < 100%).

Ökoloogilise klassi hindamiseks klorofüll-a sisalduse alusel testiti olemas-olevaid ja loodi uusi klorofüll-a hindamise algoritme Sentinel-2 MSI andmetele. Satelliitandmetelt tuletatud klorofüll-a näitas sarnast dünaamikat kui veeproo-videst mõõdetud klorofüll-a sisaldus ning ökoloogilise klassi hinnang oli sama. Kui veepeegeldustegur oli ebakorrektne, siis algoritmid ei saanud ka korrektset klorofüll-a tulemust ning ökoloogiline klass erines ka veeproovidest saadud klorofüll-a alusel. See esines olukordades, kus uuritav veekogu oli väikese vee-peegli pindalaga (< 12 hektarit). Erinevad klorofüll-a algoritmid töötasid hästi erinvate veetüüpide puhul. Kuna ühtset algoritmi oli keeruline leida väga suure optiliselt aktiivsete ainete muutlikkuse tõttu vees, siis peegeldustegur klassi-fitseeriti erinevateks optilisteks veetüüpideks. Iga veetüübi jaoks leiti kõige sobi-vam klorofüll-a algoritm, mis erines vastavalt sensorile ja veetüübile. Kuna optiliselt aktiivsete ainete hulk veekogu siseselt on muutlik, siis veetüüpideks jagamine võimaldab täpsemalt hinnata veekvaliteedi parameetreid ruumiliselt.

Veekvaliteedi parameetritelt looduslike mõjude eemaldamiseks, kombineeriti töös Sentinel-3 OLCI optilistele andmetele arvutatud veekvaliteedi parameetrid ja Sentinel-3 SRAL ja Cryosat-2 SIRAL altimeetria andmetele arvutatud veetase. Satelliitandmetelt saadud veetase näitas head kokkulangevust kohapealmõõdetud veetasemega (hälve < 0.4 m ja R^2 > 0.98). Veekvaliteedi parameetrite ja vee-taseme vahel leiti statistiliselt olulised seosed, mis olid märgatavamad Võrtsjärves. Kui veetase oli kõrgem kui pikaajaline kuukeskmine veetase, siis veekvaliteedi parameetri väärtus muutus kõrgemaks, kui aga oli madalam, siis parameetri väärtus muutus väiksemaks. Sellest tulenevalt muutus ka veekogu ökoloogiline seisund. Näiteks 2017–2019 oli Võrtsjärves oli veetase madalam kui pikaajaline keskmine kuu veetase (rohkem kui 0.5 m), siis ökoloogiline klass muutus 2017 ja 2018 „Keskmisest“ „Heaks“ ja 2019 „Halvast“ „Keskmiseks. Veetase oli keskmisest kõrgem 2016. aastal, kuid ökoloogiline klass sellest ei muutunud. Kasutades kohapeal mõõdetud ja satelliitandmeid on võimalik täiustada ökoloogilise klassi hindamist.

Käesoleva tööga leiti, et erinevad atmosfäärikorrektsiooni protsessorid ja veekvaliteedi parameetri hindamise algoritmid sobivad erinevate omadustega vetele. Veetüübi põhine lähenemine aitab leida sobivamad klorofüll-a algoritmid optiliselt keerulistele vetele. Oluline osa on mõõtemääramatuste hindamisel ja nende vähendamisel, sest vead võivad lõpptulemuses minna väga suureks. Kombineerides *in situ*, optilisi ja altimeetria andmeid, on võimalik hinnata optiliselt keerukate vete ökoloogilist seisundit täpsemalt, mis annab võimaluse kasutada satelliitandmete eeliseid ruumilisel ja ajalisel skaalal.

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