

KRISTA ALIKAS

From research to applications:  
monitoring optically complex waters  
with MERIS/ENVISAT data





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Press

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## LIST OF ORIGINAL PUBLICATIONS

This thesis consists of an overview and six publications, which are referred to in the text by their Roman numerals. The full texts of the publications are reprinted with the kind permission from the publishers, and included at the end of the thesis.

- I** **K. Alikas**, A. Reinart, “Validation of the MERIS products on large European lakes: Peipsi, Vänern and Vättern,” *Hydrobiologia*, vol. 599, pp. 161–168, 2008.
- II** **K. Alikas**, K. Kangro, A. Reinart, “Detecting cyanobacterial blooms in large North European lakes using the Maximum Chlorophyll Index,” *Oceanologia*, vol. 52, pp. 237–257, 2010.
- III** **K. Alikas**, S. Kratzer, A. Reinart, T. Kauer, B. Paavel, “Robust remote sensing algorithms to derive the diffuse attenuation coefficient for lakes and coastal waters,” *Limnology and Oceanography: Methods*, vol. 13, pp. 402–415, 2015.
- IV** **K. Alikas**, K. Kangro, R. Randoja, P. Philipson, E. Asuküll, J. Pisek, A. Reinart, “Satellite based products for monitoring optically complex inland waters in support of EU Water Framework Directive,” *International Journal of Remote Sensing*, vol. 36, pp. 4446–4468, 2015.
- V** T. Kutser, **K. Alikas**, D. Kothawala, S. Köhler, “Impact of iron associated to organic matter on remote sensing estimates of lake carbon content,” *Remote Sensing of Environment*, vol. 156, pp. 109–116, 2015.
- VI** **K. Alikas**, S. Kratzer, “Improved retrieval of Secchi depth for optically-complex waters using remote sensing data,” submitted to *Ecological Indicators*.

## AUTHOR’S CONTRIBUTION

Several co-authors contributed to the articles this thesis is based on. The author’s contribution in presented publications is indicated by their Roman numbers below:

- I** processing and analyses of satellite data, analysis of the measurement results, validation of MERIS data against *in situ* data
- II** study design, processing and analysis of satellite data, validation of MERIS data against *in situ* data, lead author in writing the paper
- III** study design, processing and analysis of satellite data, validation of MERIS data against *in situ* data, lead author in writing the paper
- IV** study design, processing and analysis of satellite data, validation of MERIS data against *in situ* data, lead author in writing the paper
- V** processing and analysis of satellite data, validation of MERIS data against *in situ* data
- VI** study design, processing and analysis of satellite data, validation of MERIS data against *in situ* data, lead author in writing the paper

## ABBREVIATIONS AND ACRONYMS

$a(\lambda)$	absorption coefficient ( $\text{m}^{-1}$ )
$b(\lambda)$	scattering coefficient ( $\text{m}^{-1}$ )
$c(\lambda)$	beam attenuation coefficient ( $\text{m}^{-1}$ )
$\lambda$	wavelength (nm)
AC	atmospheric correction
AOPs	apparent optical properties
CDOM	coloured dissolved organic matter ( $\text{m}^{-1}$ )
CHL	chlorophyll- <i>a</i> concentration ( $\text{mg m}^{-3}$ )
CZCS	Coastal Zone Color Scanner
CY	cyanobacterial biomass ( $\text{g m}^{-3}$ )
EO	Earth Observation
ESA	European Space Agency
FR	full resolution
HELCOM	Convention on the Protection of the Marine Environment of the Baltic Sea Area
ICOL	Improved Contrast between Ocean and Land
IOPs	inherent optical properties
$K_d(\lambda)$	diffuse attenuation coefficient for downwelling irradiance ( $\text{m}^{-1}$ )
$L_{\text{TOA}}$	top of atmosphere radiance ( $\text{W m}^{-2} \text{sr}^{-1}$ )
MCI	Maximum Chlorophyll Index
MEGS	MERIS Ground Segment prototype processor
MERIS	Medium Resolution Imaging Spectrometer
MNB	mean normalized bias (%)
MODIS	Moderate Resolution Imaging Spectrometer
MSFD	Marine Strategy Framework Directive
MSI	Multispectral Imager
NASA	National Aeronautics and Space Administration
NIR	near infrared spectral range
NN	neural network
OC	ocean colour
OLCI	Ocean and Land Colour Imager
OLI	Operational Land Imager
OSPAR	Convention for the protection of the marine environment of the North-East Atlantic
PAR	photosynthetically active radiation
PC	phycocyanin
R	irradiance reflectance
RMSE	root mean square error
RRMSE	relative root mean square error (%)
RR	reduced resolution
$R_{rs}$	remote sensing reflectance ( $\text{sr}^{-1}$ )
S2	Sentinel-2

S3	Sentinel-3
SeaWiFS	Sea-Viewing Wide Field-of-View Sensor
SWIR	shortwave infrared
TBM	total phytoplankton biomass ( $\text{g m}^{-3}$ )
TOA	top of the atmosphere
TSM	total suspended matter ( $\text{g m}^{-3}$ )
VIIRS	Visible Infrared Imaging Radiometer Suite
WFD	Water Framework Directive
$Z_{SD}$	Secchi depth (m)



# 1. INTRODUCTION

## 1.1. Background

Inland and coastal waters contribute to various ecosystem services by providing resources for human use, important and diverse habitat for aquatic life by high levels of biodiversity, and support services that depend on the status of the local ecosystem. The assessment of the present and the future state of these ecosystems is important on regional to global scales. This would enable large-scale studies of the health of the environment, maintenance of biodiversity, climate change studies as well as for nutrient and carbon cycles. Tranvik *et al.* [1] showed that inland waters contribute significantly to the global carbon cycle. Due to the anthropogenic activities and due to future climate change their contribution is shifting depending on the number of lakes and aquatic impoundments which depends on the nature of the geographic zone. The response of aquatic ecosystems to climate change is mainly influenced by regional conditions, characteristics of the catchment, and water mixing regimes [2]. Since lakes and coastal ecosystems are influenced by biological and ecological effects as well as by anthropogenic pressure, it is a challenge to distinguish between natural and anthropogenic drivers of environmental changes as ecosystems respond to their combined pressure [3]. Therefore similar environmental effects can have different impact in different water bodies. While the more radical approach is to take advantage of extreme or episodic climate “events” to study the response of the ecosystem to these events [4], the more conventional approach is to establish monitoring networks from local to global scale. It would enable to collect data to provide long-term monitoring data to allow differentiate between signals and effects [5]. Monitoring and understanding of physical, chemical, biological status of inland and coastal waters is one focus of monitoring agencies and the public. It is the subject of several directives *e.g.* European Water Framework Directive [6], European Marine Strategy Framework Directive [7], Bathing Water Directive [8] and regional conventions *e.g.* HELCOM [9], OSPAR [10]. There is a consensus in the community to monitor and preserve the status, or if needed, to take actions to improve the ecological status of our coastal and inland waters. The list of indicators required to be measured to assign the ecological status is rather large, and quite a few of them can be derived from Earth observation (EO) data. The latter provides a unique opportunity due to its improved spatial and temporal coverage, consistency and global coverage. It allows acquisition of data at scales relevant to effective transboundary water management and provides comparability among various water bodies. Although *in situ* data is essential for algorithm development, calibration and validation, the conventional monitoring approaches are time consuming, and thus costly and limited in spatial and temporal scale. Therefore, satellite derived products have the potential to provide a valid complementary

source of information at regional to global scales in order to improve the monitoring and management of aquatic ecosystems.

Environmental monitoring from space started in 1972 with the launch of the Earth Resources Technology Satellite (ERTS-1 which was renamed Landsat-1) by NASA. First ocean colour (OC) satellite sensor was the Coastal Zone Color Scanner (CZCS) aboard Nimbus-7 launched in 1978 which was a “proof of concept” experiment to determine if EO data would enable to identify and quantify suspended or dissolved material in ocean waters through the scattering atmosphere [11]. The spectral, radiometric and spatial resolution were optimized for measurements over water. The successful CZCS mission was followed by the launch of SeaWiFS in 1997 as a start of a new generation of satellite sensors delivering daily observations of ocean colour data [12]. The OC missions have been continued by the data of MODIS (Aqua, Terra), MERIS (ENVISAT), HICO and currently by VIIRS (Suomi NPP), OLI (Landsat 8), MSI (S2), OLCI (S3) which contribute to the continuity of EO allowing the current and long term studies for monitoring ocean, coastal and inland waters [13].

The first EO instrument designed to monitor oceans as well as coastal areas was Medium Resolution Imaging Spectrometer (MERIS) launched in 2002 by the European Space Agency (ESA) onboard the polar orbiting ENVISAT satellite [14]. MERIS had high spectral and radiometric resolution and a dual (300 m, 1200 m) spatial resolution. The sensor had 15 spectral bands in the visible and infrared part of the spectrum. The bands in the infrared allowed aerosol characterization for atmospheric correction (AC) which is a crucial part in OC remote sensing procedures since about 90% of the TOA (Top of the Atmosphere) signal recorded by the sensor originates from the atmosphere [15]. The nine bands in the visible allowed both the retrieval of marine parameters as well as the separate quantification of different optically active substances: chlorophyll a (CHL) as a proxy for phytoplankton, mineral particles (TSM), coloured dissolved organic matter (CDOM) over optically complex waters [16]. Although the training ranges of MERIS standard bio-optical model are limited, efforts have been made via developing processors with different sets of bio-optical data for monitoring optically complex waters [17].

When the optical properties of the water are dominated by phytoplankton and their covariant by-products and also by the absorption and scattering due to water molecules, it is commonly referred to as optical Case-1 water [18]. In Case-2 waters, the optical properties are determined by molecular water, phytoplankton and two additional components – mineral particles and dissolved organic matter. These components represent a group of substances (different groups of phytoplankton, mineral particles of various types and sizes, and diverse dissolved substance) rather than a single substance, resulting in a variability in their optical signature. The concentration and the specific inherent optical properties can exhibit wide and independent variation [19]. Their inherent optical properties (IOPs) can be similar over the entire spectrum (*e.g.* the absorption spectra of CDOM and detrital particles) or over a part of the spec-

trum (*e.g.* the decrease of the absorption coefficients of phytoplankton and dissolved organic matter from about 440 nm to about 550 nm) [20]. Therefore over these complex cases, sensors with high spectral and radiometric resolution are required. Their data can lead to universally applicable approaches to derive accurate EO products over optically complex waters [21, 22], which has not been yet accomplished.

The first bio-optical model was published by Gordon *et al.* [23] in 1975 for Case-1 waters. It related the apparent optical properties (AOPs) to the IOPs allowing to derive CHL. For Case-2 waters, the first model that related the apparent and inherent optical properties was introduced by Bukata *et al.* [24, 25] in 1981. It was based on inland water bio-optical properties [26] which allowed to distinguish between concentrations of CHL, TSM and dissolved organic carbon from a single spectrum. Since then significant progress has been made by better characterization of the radiative transfer process and development of approaches to retrieve physical and biogeochemical parameters in optically complex waters [27]. In addition to simple empirical approaches [28] the more analytically-based inversion models are being developed and applied [21], also the list of parameters and ecological indicators available to derive from EO data has been expanding [29, 30].

Odermatt *et al.* [31] reviewed the water constituent retrieval algorithms for Case-2 waters using EO data. It was concluded that specific solutions to various types of optically complex waters exist although only few approaches have the suitable validity range for covering all optical water types under Case-2. The accuracy of the derived products is dependent on the selected AC procedure. The results indicated that for CHL retrieval the use of the blue-green ratio is applicable to oligotrophic waters, red-NIR ratios to more productive ( $\text{CHL} > 10 \text{ mg m}^{-3}$ ) waters with the need of spectral inversion techniques to cover all other conditions. TSM retrieval was estimated to be most robust where wavelengths from 550 nm with a shift to longer wavelengths with increasing TSM are used [32]. The results from CDOM retrieval showed highest uncertainties. This is due to the combined effects of strong and overlapping absorption by CDOM and CHL in the shorter wavelengths, and also by the inaccuracies in the reflectance in the blue part of the spectrum [33]. Inaccuracies due to invalid AC are largest in the shorter wavelengths [34] mainly due to an erroneous estimation of the water signal in the NIR region (due to possibly higher sediment loads or more abundant phytoplankton), which may result in negative remote sensing reflectance ( $R_{rs}$ ) in case of optically complex waters [35]. For these cases it is recommended to use the spectral shape of the  $R_{rs}$  *i.e.* the band ratios [34] to retrieve the optical properties of water. Also the determination of the contribution from absorbing aerosols is still a challenge [36], especially over a spatially and temporally changing atmosphere such as over coastal and inland waters. The methods to better characterize aerosols for atmospheric correction [37, 38, 39] and to increase the accuracy of the  $R_{rs}$  over blue bands (*i.e.* accounting for  $\text{NO}_2$  absorption [40]) are being constantly improved. Additionally, the combination of NIR and SWIR bands

[41] and also the SWIR based AC approaches [42] have shown better suitability for the optically complex waters than solely NIR based ones. Methods to correct for adjacency effects [43, 44] are also under development.

In addition to development and validation of retrieved standard level 2 products (both atmospherically-corrected reflectance and water quality products), there is a continuous effort to develop algorithms for additional parameters *e.g.* estimating transparency in order to assess light availability for underwater ecosystems. Transparency has been estimated via the diffuse attenuation coefficient ( $K_d(490)$ ) or via Secchi depth ( $Z_{SD}$ ) by empirical and analytical approaches from EO applications. Austin and Petzold [45] first developed an empirical band ratio algorithm, which used the blue-to-green ratio of water-leaving radiances  $L_w(443)/L_w(550)$  to derive  $K_d(490)$ . Their approach has been widely used with modifications in the exact band ratios. While the blue-to-green  $R_{rs}$  ratio [46] tends to give accurate results over Case-1 waters [47], a shift towards longer wavelengths is required over Case-2 waters and the ratios  $R_{rs}(490)/R_{rs}(620)$  [48],  $R_{rs}(490)/R_{rs}(670)$  [49] have been used with higher accuracy. Independently from optical water type (Case-1 or Case-2),  $K_d(\lambda)$  can be derived as a function of IOPs and respective light conditions by the means of radiative transfer models [50, 51, 52]. The validation results indicate the suitability of this approach for Case-1 and Case-2 [53, 54] waters. A knowledge of  $K_d$  allows to derive many indicators regarding light availability: (1) euphotic depth – in a homogeneously mixed water, *i.e.* the depth of 1% light level down to which there is enough light for photosynthesis, and defined as  $4.6/K_d$  [52] and (2)  $Z_{90}$  – penetration depth of light in water as the depth above which 90% of the diffusely reflected irradiance originates, and defined as  $1/K_d$  [55]. Additionally, by mean of the empirical regression,  $K_d$  has been used to estimate the Secchi depth ( $Z_{SD}$ ) from EO data [56, 48]. Tyler [57] showed that in theory, the sum of the total diffuse attenuation coefficients,  $K_d(\lambda)$ , and the beam attenuation coefficient  $c(\lambda)$  are inversely related to  $Z_{SD}$ . This approach has been tuned to regional conditions by empirical relationships between the  $Z_{SD}$  and  $K_d(\lambda)+c(\lambda)$  over coastal [57, 58, 59] and inland waters [60, 61]. Doron *et al.* [62] applied Tyler’s model [57] to EO data where instead of predefined empirical regressions, the satellite-derived  $c(\lambda)$  and  $K_d(\lambda)$  were complemented with  $R_{rs}(490)$  in order to represent the wavelength where light penetrates deepest.

EO data has many potential advantages over conventional monitoring approaches. It allows high-frequency monitoring with high spatial coverage which, allows to derive satellite-based products over the whole water body and provide environmental monitoring capabilities in less developed and inaccessible regions. The cost-efficiency and the synoptic capabilities of the EO have been recognized [63]. The use of EO data has advanced the knowledge of the trends and drivers of water quality. EO applications range from early warning of phytoplankton bloom [64] until systematically acquired data for global climate studies [65]. EO data available for ocean colour monitoring (MODIS, SeaWiFS, MERIS, OLCI) is stored in a centralized information systems, which are freely and easily accessible, allowing fast dissemination and data sharing. Compiling

and merging of historical records from various sensors can be established, which requires methods to overcome from the gaps and differences among data of various satellite sensors. While the list of parameters is relatively limited compared to *in situ* monitoring capabilities (although progressively advancing), the published algorithms can be very diverse and water type specific for mapping a certain parameter. Therefore optical properties of water must be considered prior the selection of the suitable algorithm. In case of clear and shallow water bodies, bottom effects have to be taken into consideration and in case of small lakes and close to the shoreline, the adjacency effect must be corrected for. Additionally, passive optical remote sensing is highly affected by cloud cover (both optically thick and thin clouds) and also cloud shadows.

Due to the advanced characteristics (spatial resolution at 300 m, 15 narrow bands in VIS-NIR region) compared to other OC sensors, MERIS has been widely used for monitoring inland waters and coastal areas. The data allows to derive a wide set of water quality parameters *e.g.* besides CHL, CDOM, TSM and transparency, also phycocyanin absorption [66], aquatic vegetation [67] etc. The knowledge gained during the MERIS mission from 2002–2012 can be now transferred to the Sentinel satellites since MERIS was a prototype for the Ocean Land Colour Instrument (OLCI) instrument on Sentinel-3 [68]. The first Sentinel-3 satellite was launched on February 16, 2016 (Sentinel-3A) which will be accompanied by S3B in 2017 to provide uniform quality data with large coverage and high-revisit time for environmental monitoring and assessment at least until 2029. This corresponds to the needs of EU global monitoring for environment and security program Copernicus (former GMES) which relies on a constellation of dedicated European space missions, the Sentinels. Copernicus system aims to provide services to European policy makers and individuals by means of EO and *in situ* data for systematic monitoring and forecasting of the Earth at regional to global scale [69].

## 1.2. Objectives of this work

The general aim of this thesis is to validate MERIS products and to develop new application fields based on MERIS data over optically complex inland and coastal waters.

The objectives were:

- To validate the existing algorithms for water quality products over inland and coastal waters in the northern latitudes where we can expect high amounts of dissolved organic substances and chlorophyll *a* present in the water which is not in accordance with the training ranges of standard ocean colour processors (Publication I, V).
- Improve the performance of the chlorophyll *a* algorithm for MERIS products over Estonian lakes Peipsi and Võrtsjärv. Chlorophyll *a* is a key indicator for the ecological status of aquatic ecosystems and simultaneously an important

parameter in bio-optical models for deriving water quality. Furthermore, to develop and tune the algorithms to site-specific conditions (Publication **II**).

- Improve the detection and the monitoring capabilities of potentially toxic cyanobacterial blooms (Publication **II**).
- Develop algorithms for water transparency which is not currently a MERIS standard water quality product. The colour of the water and the transparency give first guess for water clarity and the amounts of optically active substances in water column which in turn determine the underwater light field (Publication **III, VI**).
- Estimate the applications and possibilities of complimenting regular monitoring data with satellite derived products for improving the estimation of the ecological status of lakes for EU Water Framework Directive reporting purposes (Publication **IV**).

## 2. MATERIAL AND METHODS

### 2.1. MERIS/ENVISAT sensor and data products

The ENVISAT satellite was launched on 1 March 2002. It carried ten instruments to gather EO information about vegetation, water, ice and atmosphere. The ENVISAT mission ended on 8 April 2012, due to an unexpected loss of contact with the satellite [70]. The data gathered during 10-year mission made a significant contribution to environmental studies from regional to global scale.

The primary mission of MERIS sensor on-board ENVISAT was the measurement of sea colour in the oceans and in coastal areas [71] by retrieving the signal at sea level from the TOA radiance over the visible (VIS) and near-infrared (NIR) spectral domain [72]. The sensor measured the solar radiation reflected by Earth in 15 spectral bands at a ground spatial resolution of 300 m (full resolution data, FR). The FR data is aggregated to a nominal resolution of 1200 m which is more suitable for large scale and open ocean studies.

Due to the low radiance levels and their associated high signal-to-noise ratios in case of remote sensing above water, MERIS has both high radiometric as well as spectral resolution. The signal at the sea surface was expressed in term of reflectance, which accuracy is determined by the quality of TOA acquisition (*i.e.* sensor calibration) and the AC procedure (*i.e.* estimation and removal of atmospheric path contribution). The MERIS level 1b (L1b) product corresponds to geo-located and calibrated TOA radiance ( $L_{TOA}$ ). During the standard processing of MERIS level 2 (L2) products, each pixel is identified either as cloud, water or land which determines the consecutive processing chain. After the AC step (decoupling the atmospheric and marine signal) the reflectance spectrum at the sea-surface is retrieved which subsequently serves as an input into the bio-optical model [72] to calculate the inherent optical properties (*i.e.* scattering and absorption properties). The AC and the bio-optical procedures are both based on a neural network (NN) approach. During the different stages of processing the raw data to a level 2 product, flags are raised which are used for 1) surface type information (class flags); 2) additional scientific information relevant to interpretation (science flags); 3) product confidence information (confidence flags). To correct for the land adjacency effect L1b images can be pre-processed with ICOL processor (Improved Contrast between Land and Ocean) [73].

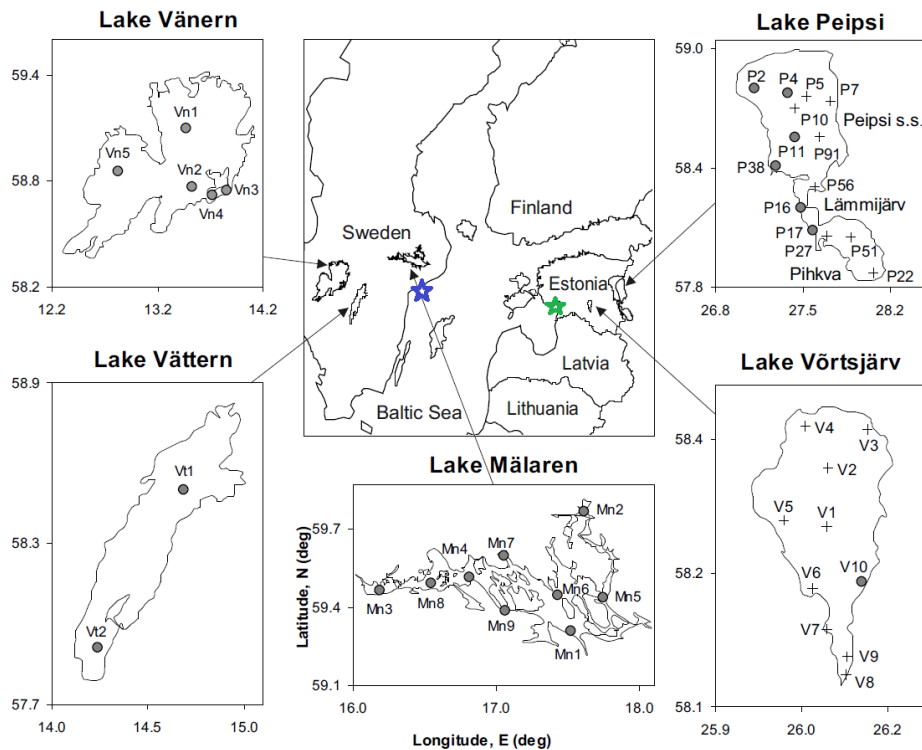
The bio-optical model used for the MERIS Case-2 algorithm [74] consists of three optical components: 1)  $a_{dg}$  – dissolved organic matter, which is defined as absorption by all substances in water which pass a filter with pore size 0.2  $\mu\text{m}$  and additionally the absorption by bleached particles; 2)  $b_p$  – the total suspended matter scattering and; 3)  $a_{ph}$  – the phytoplankton pigment absorption. These IOP coefficients are given at the wavelength 442 nm which are then converted into concentration of TSM (MEGS total\_susp product) and CHL (MEGS algal\_2 product) by using conversion factors based on coastal waters datasets measured in North Sea [75]. Since the algorithms used in the MERIS standard processing are not optimal for all optical water types, a series of Case-2 water processors

have been developed with modified AC and various bio-optical models – the Case II Regional (C2R), BOREAL and EUTROPHIC processors [76]. Similarly to the standard, MERIS Ground Segment prototype processor (MEGS), they are all based on the NN approach. While the AC is the same for the C2R and EUTROPHIC, there are small differences in case of BOREAL processor [77]. The bio-optical models of these processors differ in terms of the sets of IOPs that were used to train the NNs [78].

In this thesis MERIS L1b and L2 images from period 2002–2011 have been used to derive water quality products. Image processing has been done with BEAM and ODESA software. The exact processing chain applied on MERIS data has been described in each publication (I–VI).

## 2.2. Study areas

The study areas presented in this thesis are all situated in northern Europe, and include five large lakes in Sweden and Estonia and two coastal sites in the Baltic Sea (Figure 2.1). From the remote sensing perspective, all study areas belong to optically complex *i.e.* Case-2 water type. Morphometric data and the bio-optical properties of each area are shown in Table 2.1.



**Figure 2.1.** The location of the study areas. Five large northern European lakes and two coastal sites (blue star is Himmerfjärden Bay, green star in Pärnu Bay) in the Baltic Sea. The filled circles represent the regular monitoring stations in the lakes.



Lake Vättern is deep, oligotrophic and constitutes a single, rather narrow basin (width < 31 km). Lake Vänern is moderately nutrient rich and phytoplankton total biomass is characteristic for oligotrophic lakes, but cyanobacterial blooms can occur in smaller bays. The lake is separated into two main basins by a shallow archipelago area. Lake Mälaren is mesotrophic with relatively clear water in the eastern part (Görvåln Bay,  $Z_{SD} = 2.8 \pm 0.6$  m, Mn5 in Figure 2.1), whereas the western part is more turbid (Galten,  $Z_{SD} = 0.8 \pm 0.2$  m, Mn3 in Figure 2.1) and shallower (mean depth 3.4 m). It has both a complex morphology and bathymetry caused by its morainic origin. Lake Peipsi is rather shallow and the largest transboundary water body (56% belongs to Russia, 44% to Estonia) and consists of three different parts: the northern, largest and deepest Peipsi *sensu stricto* (*s.s.*); the southernmost part Pihkva; and a river-like connection between the two, Lämmijärv. Cyanobacterial blooms are a common feature during summer. Lake Võrtsjärv is a very turbid, eutrophic, shallow lake with high water levels fluctuations. Filamentous cyanobacteria may prevail throughout the growing season. All lakes are usually ice covered for about 2–5 months every year, and Vättern only about once in three years.

**Table 2.1.** Comparison of lakes morphometric data and the bio-optical properties. Concentrations are given for the vegetation period as minimum – maximum, and median in the brackets.

	Peipsi	Võrtsjärv	Mälaren	Vänern	Vättern	Himmerfjärden Bay (Baltic Sea)	Pärnu Bay (Baltic Sea)
Area, km	3,555	270	1,140	5,648	1,856	232	700
Mean depth, m	7	2.7	13	27	40	17	7.5
Maximum depth, m	15.3	6	65	106	128	52	12
CHL, $\text{mg m}^{-3}$	2.7–122 (25.1)	3.4–72.2 (40.4)	1.2–98.2 (14)	1.2–9.5 (3.1)	0.6–9.8 (1.2)	1.2–11.6 (3.1)	0.7–10.7 (4.1)
TSM, $\text{g m}^{-3}$	1.3–61.3 (8.8)	1.6–52.7 (16)	1.4–11.2 (2.7)	0.5–0.7 (0.6)	0.4–2.3 (1)	0.5–4.8 (1.2)	5.0–24.3 (10)
CDOM(443), $\text{m}^{-1}$	1.2–7 (2.9)	1.9–8.9 (2.9)	1.2–7.7 (3)	0.5–2.8 (1.2)	0.07–1.2 (0.2)	0.2–0.8 (0.4)	0.6–3.7 (0.9)
$Z_{SD}$ , m	0.4–3.6 (1.5)	0.2–2.6 (0.75)	0.5–4.2 (1.5)	1.2–7.2 (4)	8.5–16.2 (11.5)	1.8–10 (4.9)	0.5–4.3 (1.3)

The Baltic Sea is very shallow (mean depth 60 m) semi-enclosed brackish water body. It is divided into a series of basins, mostly separated by shallow sounds or sills. The salinity is rather low (only a fifth of normal ocean waters) with a strong surface gradient and a permanent salinity stratification with depth, which declines inwards from Kattegat to the Gulf of Bothnia [79]. The slow water

renewal, in the order of 50 years for the whole basin, makes it vulnerable to pollution from the surrounding catchment area [80]. The northern sea usually freezes every winter, but the surface waters heat up in summer, in warmer years to over 20 °C. These physical properties affect the ecological conditions along the Baltic Sea, and the biodiversity declines sharply with salinity [81]. Kratzer and Tett [82] have estimated that CDOM is the most important optical component in the Baltic Sea.

The areas of investigation were Himmerfjärden Bay at the Swedish east coast and Pärnu Bay at the south-western Estonia coast of the Baltic Sea (Figure 2.1). Himmerfjärden is a shallow, fjord-like bay situated in the southern Stockholm Archipelago. It has a weak circulation and frequent summer blooms of filamentous cyanobacteria can occur [82]. Pärnu Bay is a shallow water basin in the north-eastern Gulf of Riga. The typical bottom type is fine sand which in case of strong winds and currents is suspended in the water column [83]. The main factor influencing the light attenuation is CDOM since the water quality is strongly affected by the inflow of fresh water from rivers.

The high variability of optical water types among validation sites (*e.g.* Vättern where median  $Z_{SD} = 11.5$  m,  $CHL = 1.2$  mg m<sup>-3</sup> compared to Vörtsjärv where median  $Z_{SD} = 0.75$  m,  $CHL = 40.4$  mg m<sup>-3</sup>) allowed to estimate the performance of various algorithms on lake and water type basis.

### 2.3. Field measurements and data collection

The *in situ* data used for algorithm development and validation for specific applications originates from various datasets. These are described in more detail in each publication **I–VI** separately. For the Baltic Sea coastal areas the data was measured during special cruises during 2000–2002 [48] and 2008 [84] in Himmerfjärden Bay (**III**, **VI**) and during 2006–2007 in Pärnu Bay [83] (**III**, **VI**). For inland waters, data both from Estonian (Peipsi, Vörtsjärv) (**I**, **II**, **IV**) and Swedish (Mälaren, Vänern, Vättern) (**I**, **IV**, **VI**) national lake monitoring programmes were used. Additionally, data from dedicated optical cruises from Peipsi and Vörtsjärv was used (**IV**, **VI**). For developing the transparency algorithms (**III**, **VI**) bio-optical datasets measured in inland waters (SUVI dataset, Arst *et al.* [85]) was used.

### 3. RESULTS AND DISCUSSION

#### 3.1. Validation of MERIS products over the large Nordic lakes and Baltic Sea coastal areas (Publication I, V)

Two levels of MERIS products were used for deriving water quality parameters: level 1b (calibrated radiances at the TOA) and level 2 (water-leaving reflectance and water products). Additionally flags indicating the type, quality and the validity of a given pixel were used in the validation process.

The water quality product validation with the 2<sup>nd</sup> reprocessed data (MEGS 7.4) showed best agreement between *in situ* and satellite data in case of CHL ( $R^2 = 0.52$ ,  $N = 76$ ; Figure 3 in **I**). The *algal\_2* product described well the seasonal dynamics of CHL in Peipsi, Vänern, Vättern and was able to clearly differentiate between different levels of CHL between lakes – Peipsi (high values), Vänern, Vättern (lowest values). However, there was very low correlation in case of TSM and CDOM. Both parameters were underestimated in Peipsi. In Vättern, MEGS estimated CDOM and TSM values in the same order as the *in situ* data based on only few points. Although based on the CDOM product there was no difference between Vänern (with a median of *in situ* CDOM  $1.2 \text{ m}^{-1}$ ) and Vättern (median of *in situ* CDOM  $0.2 \text{ m}^{-1}$ ).

The use of alternative Case-2 water processors, Case-2 Regional (v.1.3), EUTROPHIC (v.1.0), or BOREAL (v.1.0) improved the derivation of CDOM by the BOREAL processor, which showed good agreement ( $R^2 = 0.61$ ) with *in situ* data [86]. Each processor systematically overestimated CHL values in all lakes, and removal of invalid pixels indicated by flags did not improve the result. The correlation with TSM and CDOM product was generally low ( $R^2 < 0.50$ ), although slightly improved when pre-processing the data with ICOL.

A clear difference between MERIS standard (MEGS) and alternative Case-2 water processors was shown in the water-leaving radiance reflectance product. While the MEGS-derived reflectance product gave usually negative values in the blue and blue-green wavelengths, the AC models used in the Case-2 processors did not return negative reflectance and the spectra corresponded well with *in situ* measured spectra from Peipsi, Vänern, Vättern [86].

The water quality products from MERIS data from the 3<sup>rd</sup> reprocessing (MEGS 8.1) revealed similar patterns. MEGS 8.1 derived reflectance product was often negative in shorter wavelengths, even up to 620 nm (**III**). Both the TSM and CDOM product correlated well with *in situ* data, although there is an overestimation of TSM ( $R^2 = 0.8$ , **V**) which was more pronounced for higher concentrations, and an underestimation of CDOM. The *in situ* measured CHL values are overestimated by MERIS and results are relatively scattered around 1:1 line. Despite this, the absorption and scattering coefficients led to good approximations of total attenuation over coastal waters which was underestimated over lakes (**III**). From the Case-2 processors, the CDOM product from the BOREAL processor estimated the measured dissolved organic carbon

(DOC) ( $R^2 = 0.65$ ) reasonably well and the total absorption coefficient was a good proxy for DOC-specific absorbance at 254 nm ( $R^2 = 0.80$ ) which is a metric commonly used to assess drinking water treatability (V).

### 3.2. MERIS applications for studying phytoplankton parameters (Publication II)

In order to derive satellite-based products for inland waters where the optically in-water components exceed the training ranges of the MERIS NN and the bio-optical model, new approaches have to be developed and tested. On the basis of *in situ* data measured from Peipsi and Vörtsjärv, the potential of the Maximum Chlorophyll Index (MCI) developed by Gower [87] was investigated to derive phytoplankton parameters such as total phytoplankton biomass (TBM), cyanobacterial biomass (CY) and CHL. The MCI algorithm operates in the red and NIR spectral bands which are less affected by large amounts of CDOM typically present in the relatively humic-rich Baltic Sea and boreal lakes. Additionally, the spectral index is applicable both on MERIS L1b and L2 data. Therefore in case of highly reflective cyanobacterial blooms in the NIR, water quality parameters from L1b (TOA radiance) data could still be derived which would be saturated in case of L2 products [88] due to the possible failure in AC scheme.

By means of MERIS derived MCI we studied: 1) the linkage between MCI and TBM, CY and CHL for the quantitative mapping; 2) the performance of MCI based CHL algorithm, which would allow to derive  $CHL > 43 \text{ mg m}^{-3}$  which is the limit for MERIS bio-optical model; 3) the sensitivity of MCI to various phytoplankton species and to background conditions *i.e.* turbidity and macrophytes.

MCI is quantified by the height of the peak near 709 nm relative to a baseline extrapolated between adjacent bands at 681 nm and 753 nm [89]:

$$MCI = L_{709} - L_{681} - \left[ \left( \frac{709-681}{753-681} \right) * L_{753} - L_{681} \right] \quad (3.1)$$

where  $L_\lambda$  represents TOA radiances at wavelengths  $\lambda = 709, 753$  and  $681 \text{ nm}$ .

The spectrum in the red/NIR part is formed by the increasing water absorption, CHL absorption peak around 675 nm whereas the peak around 709 nm is formed by the combined effects of CHL fluorescence (around 685 nm) and scattering by phytoplankton cell structures [90].

In order to quantitatively map phytoplankton parameters by means of MCI, MERIS RR L1b images were used. The regression between satellite-based MCI value and *in situ* measured CHL, TBM and CY were derived (Table 3 in II). For Peipsi, it was noted that MCI derived values exhibit seasonal dependence due to typical algae present in phytoplankton. While the diatoms (*Aulacoseira*

spp and smaller centric *Cyclotella*, *Stephanodiscus*) are more abundant in spring, cyanobacteria (*Gloeotrichia echinulata* (J. S. Smith) P. Richt., *Aphanizomenon flos-aquae* (L.) Ralfs and *Aphanothece saxicola* Näg) is dominating in summer, causing blooms [91]. Correspondingly the MCI described less variation in all three parameters in spring (April–May,  $R^2$  between 0.10 to 0.30) compared to summer (June – September,  $R^2$  between 0.64 to 0.73) (Figure 7 in **II**). This can be explained by the seasonal trend in phytoplankton. While in spring the biomass of diatoms is relatively small, in summer the main bloom-formers are filamentous nitrogen fixers, with gas vacuoles, which can form dense surface cyanobacterial blooms. This results in strong absorption and backscattering of incident light in the red/NIR part of the spectrum which meets the sensitivity conditions of the spectral index [92].

Similarly to Peipsi, diatoms and cyanobacteria are present in Vörtsjärv, although the share of nitrogen-fixing cyanobacteria is negligible [93], and the dominant phytoplankton species are shade tolerant, non-nitrogen fixing species which do not form surface scum. There was no seasonal difference in the MCI describing CHL, TBM and CY values in Vörtsjärv. The regression lines describing correlation between MCI and phytoplankton parameters were almost parallel in both lakes, although always higher in Vörtsjärv (Figure 7 in **II**). This can be partly explained by higher background turbidity in Vörtsjärv (Table 2.1). Binding [88] showed the sensitivity of MCI to scattering from mineral particles which leads to an increase in reflectance at 700 nm which in turn resulted in higher value for the MCI. It was shown that the effect is most pronounced in case of low CHL values (CHL around  $10 \text{ mg m}^{-3}$ ) and it decreases significantly at higher CHL values. In Peipsi the background TSM concentration is relatively high as well, although due to different dominant algal species in summer (filamentous nitrogen fixers, which can regulate their vertical position and form surface scum during suitable conditions), it can be assumed that the pixel signal is dominated by the effect of algal cells floating on the surface rather than by the background level in turbidity. Additionally macrophytes are present in the southern and shallower parts of Vörtsjärv [94] which contribute to the reflectance in the NIR (700–1600 nm) due to scattering from cell and leaf structures [95]. This in turn adds to the peak at 709 nm and to the resulting MCI value.

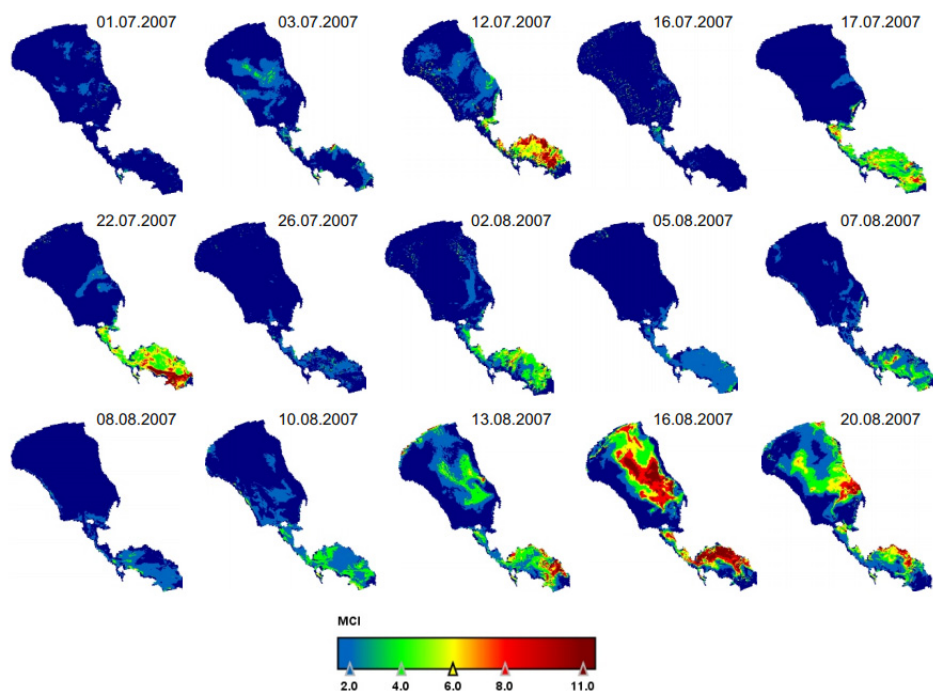
The applicability range for the MCI is wide. Gower *et al.* [87] have estimated the sensitivity of the MCI index above CHL  $30 \text{ mg m}^{-3}$  to several hundreds. Based on the *in situ* data from inland waters, Binding *et al.* [88] estimated the MCI product sensitivity for CHL already above  $10 \text{ mg m}^{-3}$ . For lower concentrations it was found that although the peak is present in the red/NIR, it is shifted to shorter wavelengths. Gilerson [90] showed that the NIR peak is dominated by the fluorescence component in case of CHL  $< 6 \text{ mg m}^{-3}$  while with an increase in CHL, the magnitude of the peak increases and shifts towards longer wavelengths. The shift of the NIR peak from 685 nm to longer wavelengths has been shown by many authors to be related to the increase of the CHL concentration [90, 96, 97, 98]. A few studies [88, 96] have described the relation-

ship between peak wavelength and CHL empirically and found better agreement between MCI and CHL when based on the observations, peak wavelength was used instead of the fixed value at 709 nm. This type of algorithms could be tested with hyperspectral satellite data.

The MCI algorithm can be applied on MERIS L1b (without AC) or L2 (after AC) data. The use of L1b data showed that MCI product provided valuable information for monitoring phytoplankton parameters. L1b product based MCI estimates are preferable in the presence of cyanobacterial blooms when it outperforms other available Case-2 algorithms *i.e.* MEGS algal\_2 and C2R [99] products. Although uncertainties due to a possible contribution from the atmosphere must be considered for quantitative mapping.

Among the three phytoplankton parameters (CY, TBM, CHL), MCI described most of the variation in cyanobacterial biomass, especially in Peipsi ( $R^2 = 0.73$ ) during the summer period (June-September) (Figure 7a in II). The coefficient of determination was lower in case of TBM ( $R^2 = 0.70$ ) and CHL ( $R^2 = 0.64$ ). As seen from the analyses of *in situ* data, all three parameters covaried in Peipsi (Figure 4, 5 in II). Thus it can be expected that all three parameters contribute to the signal quantified by MCI product. The highest correlation between MCI and CY in Peipsi during summer, can be explained by the type of algae (with gas vacuoles) which form a surface scum and therefore are easily detectable by the sensor. However the TBM and CHL are measured *in situ* from depth-integrated water samples, and therefore the biomass or concentration can be underestimated by the EO method which explains more scattered results compared to CY. In Vörtsjärv the correlation between MCI and all three parameters was lower probably due to different dominant phytoplankton species, higher background turbidity and presence of macrophytes.

To illustrate the spatial and temporal variability of phytoplankton bloom, the MCI was applied to MERIS data in Peipsi during 2007 (Figure 3.1). The MCI product indicates more rapid development of cyanobacterial blooms in the southern part of the lake, Pihkva, where it reached the first peak around 17–22 July, covering both Lämmijärv and Pihkva entirely. Stronger winds ( $\sim 5 \text{ m s}^{-1}$ ) during 23 July mixed the water column, which resulted in the decline of the surface blooms in all parts of the lake (Figure 3.1, image from 26 July). In August, the warmer air temperature ( $\sim 20^\circ \text{C}$ ) and several days of calm weather (wind speed  $< 3 \text{ m s}^{-1}$ ) provided suitable conditions for intense bloom development over the entire lake (Figure 3.1). The varying bloom locations were well described by the dominant wind directions. For example for the period 15–20 August, dominant W and SW winds carried the surface blooms to the E and NE parts of the lake. Similar conclusions can be drawn for the periods 26 July – 2 August (dominant W and SW winds) and 7–8 August (dominant E winds), which moved the surface blooms from the NE to the W coast in Pihkva.



**Figure 3.1.** Calculated MCI for cloud-free images of Peipsi during July–August in 2007.

Combining the EO data with meteorological data would allow monitoring the cyanobacterial bloom in high temporal and spatial scale [100, 101] which would not be feasible with standard monitoring methods. Kutser [102] showed the difficulties to get representative *in situ* samples due to ship induced mixing. Although *in situ* measurements of various biological and physical–chemical quality elements are essential to develop and validate the EO algorithms and also to understand the spatio-temporal patterns of algal blooms and their triggering factors [103]. Cyanobacterial blooms during summer require high frequency monitoring by means of alternative, cost-efficient methods rather than laborious and costly phytoplankton counting [104], since changes in phytoplankton abundance and composition may occur on a daily basis. Since algal blooms are indicators of ecosystem health, their monitoring for effective management is recognized by the WFD and also by the MSFD for estimating the ecological status of a water body. Here, satellite estimates during such spatially and temporally inhomogeneous conditions would provide a better overview. Besides quantitative mapping of phytoplankton parameters, EO data could be used to retrieve some of the key parameters *i.e.* spatial distribution, movement (drift) of the bloom location, frequency and intensity, duration and peak of the bloom [105, 106, 107]. Additionally MCI results could be complemented with the detection of the phycocyanin (PC) absorption from EO data [108, 109, 110, 111]; PC is a pigment rather specific to cyanobacteria [52]. This would increase

the accuracy of quantifying the cyanobacteria and allow to determine the percentage of cyanobacteria biomass of the total phytoplankton biomass which is additional parameter in WFD required to be monitored *e.g.* for Peipsi.

### **3.3. Development of the algorithms for transparency (Publication III, VI)**

Water transparency is one of the key components for describing water quality and the underwater light field which determines the biological (*e.g.* phytoplankton photosynthesis), physical (*e.g.* heat transfer, sediment resuspension) and chemical (*e.g.* nutrient cycling) processes in the water column. The first water quality measurements were made by Secchi disc [59] and date back to the 19<sup>th</sup> century. Due to the universal method, it is still used and long-time series of transparency measurements do exist globally. In optical oceanography, the attenuation of light in the water column is most commonly described by the diffuse attenuation coefficient of downwelling irradiance,  $K_d(\lambda)$ .

In the EU WFD and MSFD [6, 7] water transparency is used for ecological status classification of inland, coastal and open sea waters. It is regarded as an indicator for eutrophication in Baltic Sea management [9]. However for optically complex waters there is no standard MERIS transparency product.

#### **3.3.1. Diffuse attenuation coefficient for downwelling irradiance (Publication III)**

Semi-analytical and empirical approaches (Figure 1 in **III**) were tested and developed in order to identify the most accurate and robust  $K_d(490)$  algorithm for optically complex waters.

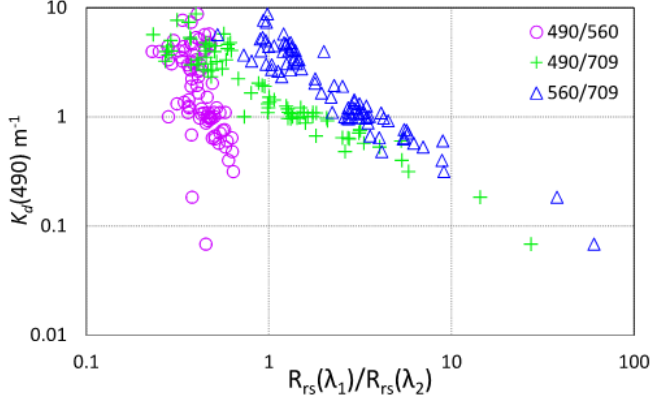
In the first approach, semi-analytical algorithms by Kirk [52] and Lee et al. [112] which derive  $K_d(490)$  as a function of the absorption, scattering coefficients and light conditions were tested. The IOPs were derived from MEGS 8.1 water products as described in the Publication **III**

In the second approach, a dataset collected from oligotrophic to hypertrophic Estonian and Finnish lakes so called “SUVI” dataset [85] was used to analyze the spectral dependence of the  $K_d(490)$  in optically complex waters based on the empirical method developed by Austin and Petzold [45]. These lakes cover a wide range of  $K_d(490)$  ( $0.1\text{--}7.7\text{ m}^{-1}$  with median  $1.2\text{ m}^{-1}$ ) and corresponding optically active substances values ( $a_{\text{CDOM}}(442)$   $0.2\text{--}6.7\text{ m}^{-1}$ ; CHL  $0.5\text{--}73\text{ mg m}^{-3}$ ; TSM  $0.7\text{--}37.5\text{ g m}^{-3}$ ). See Table 1 in **III** for the description of data used for  $K_d(490)$  algorithm development and validation.

Based on the SUVI dataset, empirical relationships between  $K_d(490)$  and various band ratios were tested (Table 2 in **III**). While the ratio  $R_{rs}(490)/R_{rs}(560)$  was relatively insensitive ( $R^2 = 0.28$ ) to changes in  $K_d(490)$ , the ratios  $R_{rs}(490)/R_{rs}(709)$  and  $R_{rs}(560)/R_{rs}(709)$  described most of the variation ( $R^2 = 0.88$ )



in the data (Figure 3.2). In general, it was noted that the further the reference band was shifted into the VIS and NIR domain, the higher was the correlation between  $K_d(490)$  and a certain band ratio (Table 2 in **III**).



**Figure 3.2.** Measured  $K_d(490)$  values regressed against various band ratios:  $R_{rs}(490)/R_{rs}(560)$ ,  $R_{rs}(490)/R_{rs}(709)$ ,  $R_{rs}(560)/R_{rs}(709)$ , based on the SUVI Dataset (Publication **III**).

Further analyses of the ratios 490/709 and 560/709 revealed that the changes in  $K_d(490)$ , in more transparent waters ( $K_d(490) \leq 2 \text{ m}^{-1}$ ) are more accurately described by the ratio 490/709 ( $R^2 = 0.88$ ,  $p < 0.05$ ,  $\text{RMSE} = 19 \%$ ) and in more turbid waters ( $K_d(490) > 2 \text{ m}^{-1}$ ) by the ratio 560/709 ( $R^2 = 0.20$ ,  $p < 0.05$ ,  $\text{RMSE} = 25 \%$ ). Additionally while the value of both ratios (490/709 and 560/709) decrease with increasing  $K_d(490)$  (Figure 3.2), the value for the 490/709 is much smaller compared to 560/709 which may lead to higher uncertainties due to possible errors in AC over optically complex waters. As a result, a combined algorithm is proposed, which switches from 490/709 to 560/709 in case of less transparent waters. Following the approach by Wang *et al.* [113], the weighting function based on band ratio 560/709 was calculated based on the SUVI dataset with  $K_d(490)$  values ranging from 2.03 to 2.76  $\text{m}^{-1}$  (where the value of  $R(560)/R(709)$  corresponds to a range of 1.796–1.519):

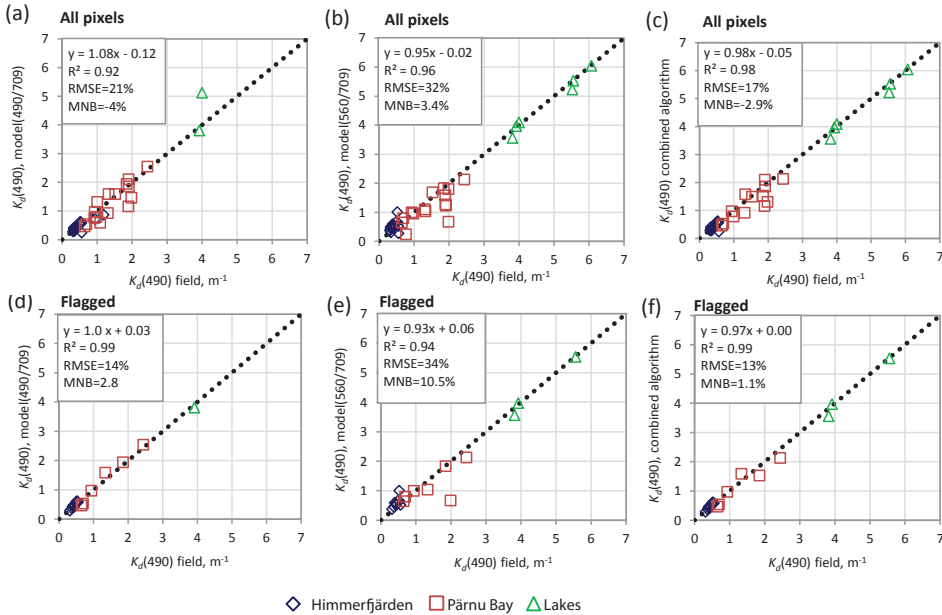
$$W = 5.098 - 2.2099 \left( \frac{R(560)}{R(709)} \right) \text{ for } 1.519 \leq \left( \frac{R(560)}{R(709)} \right) \leq 1.796 \quad (3.2)$$

The retrieved weights are then used as an input in the merged  $K_d(490)$  algorithm:

$$K_d(490) = (1 - W)K_d(490)_{(490/709)} + WK_d(490)_{(560/709)} \quad (3.3)$$

The retrieved weights from eq. 3.2 determine whether the model based on either the reflectance ratio 490/709 (calculated weight  $\leq 0$ , which will be assigned  $W=0$ ) or the 560/709 (calculated weight  $\geq 1$ , which will be assigned  $W = 1$ ).  $K_d(490)$  values will be calculated by merging the two algorithms if  $0 < W < 1$ , which corresponds to a range of  $2.03 < K_d(490) < 2.76 \text{ m}^{-1}$ .

The  $K_d(490)$  algorithms from both approaches were validated against an independent *in situ* dataset over lakes and coastal areas in the Baltic Sea. IOP-based models [52, 112] agreed well with the *in situ* measurements ( $R^2$  values between 0.55 and 0.80, and RMSE between 19% and 37%), although both models underestimated values in the lakes ( $K_d(490) > 3 \text{ m}^{-1}$ ) (Figure 4 in **III**). The site specific (lakes and two coastal sites in Himmerfjärden Bay and Pärnu Bay) validation results (Table 3 in **III**) for the empirical algorithm revealed that only the combined  $K_d(490)$  algorithm (Eq. 3.3) worked well over each site ( $R^2 = 0.98$ , RMSE = 17 %) for  $0.3 < K_d(490) < 6.1 \text{ m}^{-1}$  (Figure 3.3; Figure 6 c, f and Table 3, 4 in **III**) with very low systematic error (MNB = 1.1 %). In case of single band ratio models, the ratio 490/709 gave most accurate results for the coastal sites (for Himmerfjärden  $R^2 = 0.92$ , RMSE 9 %,  $n = 8$ ,  $p < 0.05$  and for Pärnu Bay  $R^2 = 0.98$ , RMSE = 17%,  $n = 6$ ,  $p < 0.05$ ) and the ratio 560/709 ( $R^2 = 0.98$ , RMSE = 4%,  $n = 3$ ,  $p < 0.1$ ) worked best for lakes ( $K_d(490) > 3 \text{ m}^{-1}$ ). See Figure 4, 6 and Table 3, 4 in **III** for detailed validation statistics. Examples on spatial and seasonal difference in  $K_d(490)$  and corresponding  $Z_{90}$  product over the central Baltic Sea and Nordic lakes are given in Figure 7 in **III**.



**Figure 3.3.** Validation of the  $K_d(490)$  model  $R_{rs}(490)/R_{rs}(709)$ : using all pixels (a), and after flagging (d), using model  $R_{rs}(560)/R_{rs}(709)$ : all pixels(b), and after flagging (e), and the combined algorithms: all pixels (c), and after flagging (f) (Publication **III**).

The initial input for both methods was MEGS-derived  $R_{rs}$  which is often negative in shorter wavelengths due to errors in AC over Case-2 waters. The band ratio approach resulted in reasonable estimate of  $K_d(490)$  for each lake indicating the shape of the retrieved spectra still captured the features typical for optically complex waters. While in theory semi-analytical approaches are suitable for all water types, the satellite estimations showed higher uncertainties over lakes compared to coastal waters. This could be explained by error propagation from invalid  $R_{rs}$  spectrum to IOP retrieval by the MEGS NN. Although the validation results have indicated the underestimation of CDOM and overestimation of CHL in optically complex waters by MEGS [84, 114], the use of total absorption and scattering coefficients led to good approximations of estimating  $K_d(490)$  especially over coastal areas ( $K_d(490) < 3 \text{ m}^{-1}$ ) where the derived products could be regarded as reliable.

This study demonstrates that by using band ratio algorithms,  $K_d(490)$  can be estimated reliably over optically complex waters spanning over a large range of  $K_d(490)$  values ( $0.1\text{--}6.1 \text{ m}^{-1}$ ) from MERIS data. While over non-turbid ocean waters ( $K_d(490) < 0.25 \text{ m}^{-1}$ ) the algorithm based on  $R_{rs}(490)/R_{rs}(560)$  by Mueller [115] gives reliable estimates [113], over more turbid waters a shift of the reference band towards longer wavelengths is required. As shown in this study and also by Lee *et al.* [116] at high  $K_d(490)$  values, the ratio  $R_{rs}(490)/R_{rs}(555)$  reaches an asymptotic value with increasing IOPs and loses its sensitivity, resulting in an underestimation of  $K_d(490)$  [113]. As illustrated on the *in situ* dataset measured over various optical water types, using a reference band at longer wavelengths (560, 620, 665, 709 nm) gives progressively more accurate results, resulting in a combined algorithm based on the ratios 490/709 and 560/709. In Case-2 waters there is a significant contribution from each optical component to the  $R_{rs}$  in the shorter wavelengths in the VIS spectral range. The benefit of using the band at 709 nm as a reference is that one must account mainly for the absorption by pure water and the particle backscattering to the signal. Therefore in case of highly productive waters (*i.e.* cyanobacterial blooms) or in sediment loaded waters, which adds to the signal in 709 nm, the algorithm can produce uncertainties. However the combination of two band ratios to estimate wide range of  $K_d(490)$  values resulted in strong correlation both on the calibration and validation data set. Based on the calibration data set, it can be assumed that the band ratio approach have the potential to be applicable to various Case-2 waters with wide validity range [117].

### 3.3.2. Secchi depth (Publication VI)

Three approaches were tested in order to develop Secchi depth algorithm for optically complex waters for EO applications (Figure 1 in VI).

First, empirical band ratio approach was used, originally developed by Austin and Petzold [45], by testing various MERIS band ratios to retrieve  $Z_{SD}$  estimates. Most variation ( $R^2 = 0.73$ ) was described by the ratio  $R_{rs}(490)/R_{rs}(709)$ .

Second, the regression analyses between simultaneously measured  $K_d(490)$  and  $Z_{SD}$  were performed over coastal (Himmerfjärden, Pärnu Bay) and inland waters (SUVI dataset) where the highest coefficient of determination ( $R^2 = 0.84$ ) was obtained over the coastal areas (Figure 2 in VI). Thirdly, the underwater visibility theory by Tyler [57] was used:

$$Z_{SD} = \frac{\ln\left(\frac{C_0}{C_{\min}}\right)}{K_d(PAR) + c(PAR)} \quad (3.4)$$

where  $K_d(PAR)$  and  $c(PAR)$  are the vertical diffuse attenuation and beam attenuation coefficients over the photosynthetically active radiation (PAR). In the numerator, the so called coupling constant,  $C_{\min}$  is the minimum apparent contrast perceivable by the human eye,  $C_0$  is the inherent contrast between the Secchi disk depth and the background water reflectance and calculated:

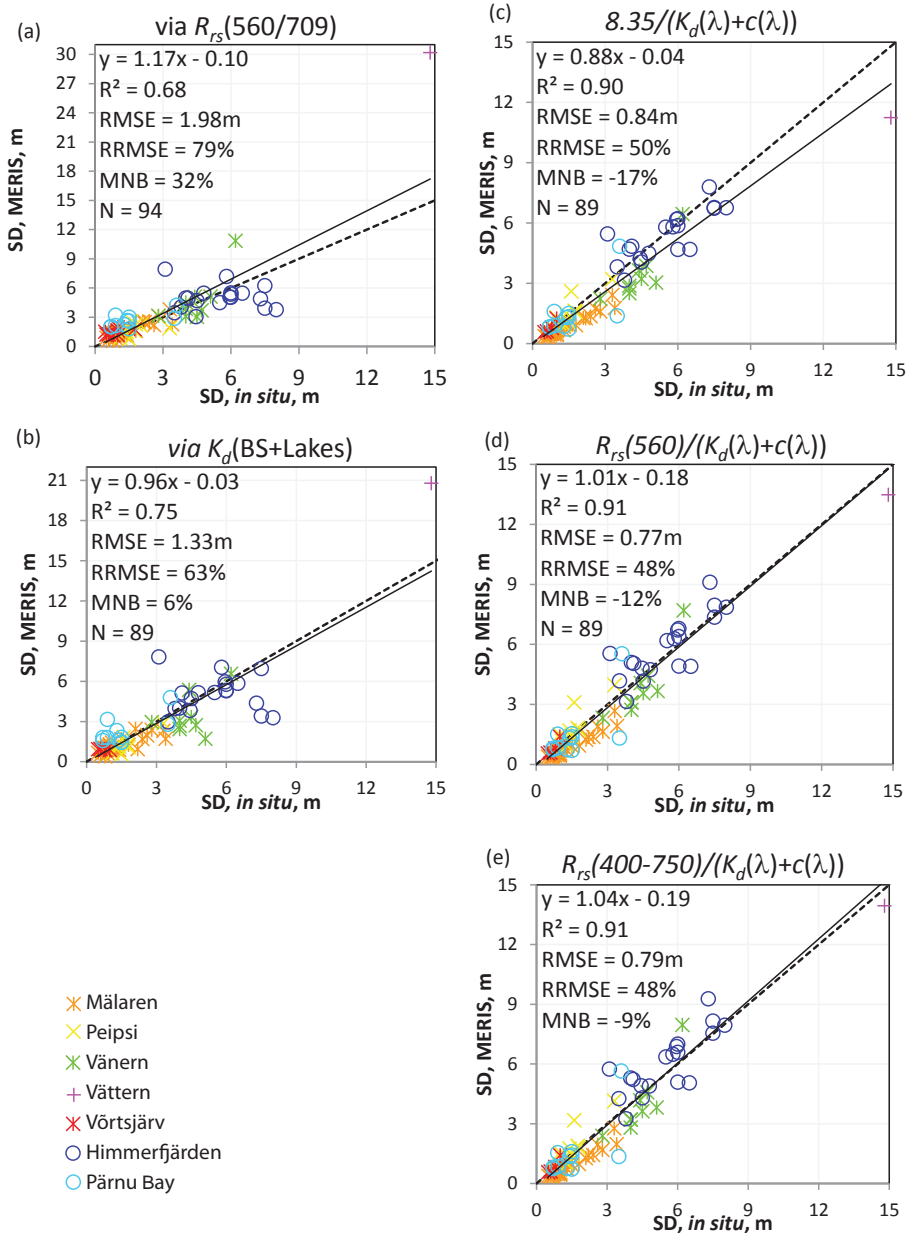
$$C_0 = \frac{R_{rs}(\text{Secchi}) - R_{rs}(\text{water})}{R_{rs}(\text{water})} \quad (3.5)$$

where the  $R_{rs}(\text{Secchi})$  is the reflectance of the Secchi disk and  $R_{rs}(\text{water})$  is the reflectance of the water, taking the sensitivity of the human eye into account [118]. For Eq. 3.4 and 3.5, a values of 0.82 was used for  $R_{rs}(\text{Secchi})$  and 0.0066 for  $C_{\min}$  according to Tyler [57]. The  $K_d(490)$  was calculated by using the combined algorithm according to Eq. 3.2 and 3.3. The beam attenuation coefficient was estimated as the sum of the total absorption  $a(490)$  and scattering  $b(490)$  as derived in III (Eq. 5, 6) from MERIS IOP data. The sums of these coefficients were then interpolated to PAR region based on the strong correlation ( $R^2 = 0.99$ ) between  $K_d(490)+c(490)$  and  $K_d(PAR)+c(PAR)$  as shown in Eq. 11 in VI.

For the underwater visibility theory, three approaches were tested to estimate the coupling constant value, more specifically the parameter  $R_{rs}(\text{water})$  in Eq. 3.5. First approach, based on the bands over the VIS spectrum with respect to the sensitivity of the human eye, showed the value of the coupling constant was ranging between 6.96 and 10.36, with an average of 8.35 based on the SUVI dataset [85]. In the second approach, similarly to Doron *et al.* [62], the MERIS reflectance value at single band (additionally to 490 nm, also bands at 510 nm or 560 nm) was used for each match-up pixel separately. Third, the MERIS reflectance values from over all visible bands with respect to the sensitivity of the human eye were used for each match-up pixel.

The validation results indicate that the band ratio algorithms had relatively high inaccuracies (RMSE = 1.98 m, RRMSE = 79%, Figure 3.4a) and all ratios tended to overestimate low (< 3 m) and high  $Z_{SD}$  values (*e.g.* Vättern *in situ*  $Z_{SD} = 14.8$  m) which was less pronounced with the ratio  $R_{rs}(560/709)$ . The accuracy increased (RMSE = 1.33, RRMSE = 63 %) when satellite derived

$K_d(490)$  was used as an input for the empirical  $Z_{SD}$  algorithm (Figure 3.4a). Independently of the conversion factors used between  $K_d(490)$  and  $Z_{SD}$  (Figure 2 in VI) the accuracy of predicting *in situ* measured  $Z_{SD}$  was very similar for each model.



**Figure 3.4.** The  $Z_{SD}$  retrievals from three main methods using MEGS data: a) via  $R_{rs}(560/709)$ ; b) via  $K_d(490)$  and via theoretical relationship between  $Z_{SD}$  and  $K_d(\lambda)+c(\lambda)$  either by using the predefined coupling constant (c),  $R_{rs}$  at single wavelength (d) or  $R_{rs}$  over the whole spectrum (e). The results are based on the flagged data (Publication VI).

The measured  $Z_{SD}$  values were predicted with the highest accuracy via the underwater visibility theory (Figure 3.4, c-e; Table 4 in VI). The accuracy depended on the approach used to calculate the coupling constant. When the predefined value (8.35) or the water reflectance at a single band (either at 490, 510, 560 nm) was used, the results indicated some dependency on the water type, where higher  $Z_{SD}$  values were slightly underestimated. The best alignment around 1:1 line (slope = 1.01, intercept = 0.18) over all water bodies (Figure 3.4d) was retrieved by using band at 560 nm to represent the water reflectance in Eq. 3.5. Although the  $Z_{SD}$  value in Vättern was derived better (*in situ*  $Z_{SD}$  = 14.8 m, model 14.4 m) by the use of  $R_{rs}(490)$  for water reflectance in Eq. 3.5. This could be explained by the maximum light penetration, which is closer to 490 nm in case of low amount of absorbing and scattering substances (as it is in Vättern) compared to other test sites which are more turbid where the maximum is shifted towards the green part of the spectrum (*i.e.* longer wavelengths). The approach to use all bands in the visible to calculate the coupling constant, for each match-up pixel separately (Figure 3.4e), was most robust for all test sites ( $R^2 = 0.91$ , RMSE = 0.79 m, RRMSE = 48%, MNB = -9%, n = 89). As the sensitivity of the human eye has the maximum at 555 nm, half-peak at 510 and 610 nm [118], the highest weight was omitted to the  $R_{rs}$  value at 560 nm which has shown, similarly to the bands at 510 and 620 nm, the highest accuracy when validated with *in situ* data over optically complex waters [84, 114].

Additionally to the coupling constant, the performance of the algorithm depends on the accurate retrieval of  $K_d(\lambda)$  and especially  $c(\lambda)$  which is in general higher than  $K_d(\lambda)$  in the visible domain. While the validation of  $K_d(490)$  algorithm has shown good agreement with *in situ* data (RMSE = 13%, MNB = 1.1%, Publication III), the retrieval of  $c(\lambda)$  has not been validated yet.

The relatively higher uncertainties in deriving Secchi depth ( $R^2 = 0.91$ , MNB = -9%) from MERIS data compared to  $K_d(490)$  ( $R^2 = 0.99$ , MNB = 1.1%) could be explained by the nature of the Secchi depth measurement technique. The actual reading is affected by many factors: 1) the person taking the measurements due to the properties of the human eye as a contrast sensor; 2) size and colour of the disk; 3) whether water telescope was used; *e.g.* Mikaelson and Aas [119] estimated an approximate 11% increase in the  $Z_{SD}$  values while taking the readings with water telescope using a 30 cm disk; 4) whether the measurement was performed on the sunlit or shadow side of the boat; *e.g.* Aas *et al.* [59] estimated the value to be 7% lower on the shadow side; 5) wind speed (the error can be in the range of 0.2–0.5 m due to wind-induced waves and ship drifting impeding the estimation of the exact depth below the waves).

Satellite data can provide a more systematic assessment of  $Z_{SD}$ . It allows to map the present state, as well the trend and anomalies based on past (MERIS), present (Sentinel-3A) and future (Sentinel-3B) ocean colour instruments for one of the most common water quality parameters. It would also provide an additional source of information for estimating transparency which is considered an important quality element that can be used to assign the ecological

status of the water body by the EU WFD [6] and MSFD [7] and may be used as an indicator for eutrophication according to HELCOM [9].

### **3.4. MERIS applications for implementing EU Water Framework Directive (Publication IV)**

The need to protect and restore ecological status of rivers, lakes, transitional and coastal waters has resulted in formulation of European Union Water Framework Directive 2000/60/EC (WFD). WFD requires the EU Member States to assess the ecological status class (ranging from ‘High’ to ‘Bad’) of a water body based on the defined parameters and their respective thresholds which have set based on the reference conditions. The fulfilment of the monitoring requirements for these parameters is an acknowledged problem [120] due to the large number of water bodies where in each case the temporal, spatial variability must be accounted to get representative data, and besides this, the accessibility to the lake might be a problem. The ecological status of a water body can be described by various biological and physical-chemical quality elements. EO approaches are available for few of them: *e.g.* 1) phytoplankton biomass; 2) chlorophyll *a* concentration; 3) water transparency; 4) frequency and 5) intensity of phytoplankton blooms. A study was performed based on the data from five large European lakes (Peipsi, Võrtsjärv, Vänern, Vättern, Mälaren) situated in Estonia and Sweden to identify if and to what extent satellite-based products could be used in the assessment. The lakes differ based on morphology and bio-optical properties (Table 2.1), representing oligotrophic (Vättern) to eutrophic (Võrtsjärv) conditions. While the monitoring and reporting of the ecological status has to be done for all inland waters  $> 0.5 \text{ km}^2$ , each member state has some flexibility in (1) the division of water bodies; (2) the set of biological and physical-chemical parameters that needs to be measured; (3) the class boundaries, *i.e.* thresholds (for assigning either ‘High, Good, Moderate, Poor, Bad’ status) of each parameter; and (4) the relevant monitoring period [121, 122].

MCI-based algorithms (Chapter 3.2) were used to derive CHL and TBM and Secchi depth algorithm (Chapter 3.3.2.) for transparency. To estimate the accuracy of the EO products, the satellite-based CHL, TBM and  $Z_{SD}$  were validated against *in situ* data from each lake (Figure 2 in IV). Secchi depth estimates were well aligned around the 1:1 line with relatively high accuracy (RMSE = 0.5 m,  $R^2 = 0.91$ ). Since the MCI-based algorithms are sensitive to  $\text{CHL} > 10 \text{ mg m}^{-3}$ , they were applied only on Peipsi, Võrtsjärv and Mälaren. CHL and TBM algorithms performed well on validation data up to  $138 \text{ mg m}^{-3}$  and  $33 \text{ g m}^{-3}$ , with highest accuracy in Peipsi.

Satellite-based products revealed seasonal trends (Figure 3 in IV), which differed from lake to lake and basin to basin, and also annually. Various seasonal patterns were detected based on CHL estimates, *e.g.* 1) linear, steep increase in CHL towards autumn 2005 in Võrtsjärv (Figure 3a in IV); 2) relatively stable during May-August followed by a steep increase in September in

2009 in Peipsi (Figure 3e in **IV**) versus high fluctuations all year round in 2007 (Figure 3c in **IV**). In Mälaren the seasonal trend of CHL showed different trend in different parts of the lake during the same year (Figure 4 in **IV**) – two pronounced peaks (up to  $45 \text{ mg m}^{-3}$ ) in Galten (western part) compared to low and stable levels of CHL ( $< 10 \text{ mg m}^{-3}$ ) all year long in Görvaln (eastern part).

For ecological status class estimation, all available measurements made during the relevant monitoring period were collected and averaged. There was better agreement on the ecological status class between satellite-based and *in situ* measured values when: 1) the inter-annual changes in CHL, TBM, and  $Z_{SD}$  were relatively small *i.e.* in clearer lakes (Vättern, Vänern, clearer parts in Mälaren); 2) the *in situ* sampling was frequent and coincided with bloom events or biomass peaks; 3) the thresholds for assigning the status class were wide (Table 2 in **IV**).

Over the years 2003–2011, both methods showed ‘High’ and ‘Good’ status based on CHL, TBM and  $Z_{SD}$  in Vänern and Vättern. In Peipsi, the annual ecological status from both methods showed that the northern parts belonged mainly to ‘Moderate’ class and according to CHL to ‘Poor’ in some years (Table 3.1). The discrepancies between the two methods are due to monitoring frequency and timing – whether bloom was observed or not (Figure 3 in **IV**). In the southern part, Pihkva, *in situ* data was only available from August which classifies the lake predominantly into ‘Poor’ and ‘Bad’ status classes (Table 3.1, with asterisk). The satellite-based evaluation agreed with this or showed better status class, especially when the data over the entire vegetation period was accounted for (Table 3.1, without asterisk). The ecological status class varied most in Mälaren, ranging from ‘Moderate’ to ‘Poor’ (Figure 5 in **IV**), and in Vörtsjärvi, from ‘Good’ to ‘Bad’ (Figure 6 in **IV**), which is due to the combination of seasonal dynamics, the effect of water level and relatively narrow class boundaries.

Various spatial variability patterns of  $Z_{SD}$  were shown well in the satellite-based maps of the studied lakes (Figures 8 and 9 in **IV**) – the optically rather homogeneous Vättern; a significant decrease in transparency towards the coastal areas in Vänern; high spatial gradient in Peipsi (N–S) and Mälaren (E–W) with only a slight annual variability in transparency. While Vörtsjärvi is regarded to be a homogeneously mixed lake where one monitoring point is considered to be sufficient to describe the whole lake [123], the spatial distribution of  $Z_{SD}$  values showed higher variability in some years and, similarly to Vänern, the inter-annual changes were more pronounced.

The seasonal and spatial trends shown by satellite-based data complemented well the *in situ* data which resulted in better description of in-water processes and water quality trends of the water body. As shown in **IV**, the assigned status class was determined by the combined effects of monitoring timing, location, ecological class thresholds and also the uncertainties, accompanying both satellite-based products and *in situ* data. The typical *in situ* sampling frequency



**Table 3.1.** Comparison of ecological status class based on in situ and MERIS data in different parts of Peipsi. In case of Pihkva \* denotes that the status class is based on the data measured in August only. The N/A indicates there was not enough data to assign an ecological status class. The ecological classes are presented: Moderate (M), Poor (P), Bad (B).

		$Z_{SD}$			CHL			TBM		
		<i>in situ</i>	MERIS		<i>in situ</i>	MERIS		<i>in situ</i>	MERIS	
Peipsi s.s.	2003	M	M		M	M		M	M	
	2004	M	M		M	M		M	M	
	2005	M	M		M	M		M	M	
	2006	M	M		P	M		M	M	
	2007	M	M		M	P		M	M	
	2008	M	M		M	M		M	M	
	2009	M	M		P	M		M	M	
	2010	M	M		M	M		M	M	
	2011	M	M		P	P		M	M	
Lämmijärv	2003	M	M		M	M		M	M	
	2004	M	M		M	M		M	M	
	2005	M	M		M	M		M	M	
	2006	M	M		M	M		M	M	
	2007	M	M		M	M		M	M	
	2008	M	M		M	M		M	M	
	2009	M	M		M	M		M	M	
	2010	M	M		M	M		M	M	
	2011	M	M		M	M		M	M	
Pihkva	2003	B*	N/A*	M	P*	P*	P	P*	P*	P
	2004	N/A*	N/A*	M	P*	P*	M	N/A*	P*	M
	2005	B*	N/A*	B	B*	P*	P	P*	P*	P
	2006	B*	N/A*	P	P*	P*	P	B*	B*	P
	2007	B*	N/A*	B	M*	P*	P	P*	P*	P
	2008	B*	N/A*	B	P*	P*	M	P*	M*	M
	2009	B*	N/A*	B	B*	P*	P	P*	P*	P
	2010	P*	N/A*	B	P*	M	M	M*	P*	M
	2011	B*	N/A*	B	P*	P*	P	P*	P*	P

is 4–6 times per year for nutrients and phytoplankton [124] which is not sufficient to describe the seasonal trends [125, 126], and the sampling frequency should be increased. Fleming-Lehtinen *et al.* [127] concluded that the ecological status assessment would benefit when scarce *in situ* data would be complemented with the data from EO and ships-of-opportunity. This would decrease the probability of misclassifying the status of water body due to the timing and frequency of data collection [128] and also allow better spatial resolution [129, 130]. As the class borders can be very narrow (*e.g.* 50 cm from 'High' to 'Bad' status class in Vörtsjärvi; Table 2 in **IV**) it requires extremely sensitive and accurate EO algorithms as well as very accurate *in situ* observation techniques and laboratory measurements. As the water retrieval algorithms can have different sensitivity for different concentration ranges, quantitative analyses of the relative performance of *in situ* versus satellite-derived products should be conducted in order to analyse the algorithm's accuracy on deriving various level of ecological status classes and therefore estimate the related uncertainties. As the EU WFD targets represent various optical water types, lake-specific and validated water quality algorithms rather than general standard algorithm should be used to assure the accuracy of the EO products required by the end-users [131]. There is an invaluable 10 year MERIS database which is now continued with Sentinel-2/MSI and Sentinel-3/OLCI products which both will be extended by S2B and S3B in the coming years. This will improve the spatial and temporal coverage of monitoring optically complex waters with more data available for algorithm development and validation. This will result in more accurate – satellite-based products usable for environmental monitoring, management and reporting purposes.

## CONCLUSIONS

Based on the results of this study, it can be concluded that:

- Standard MERIS-based water quality measuring products show underestimation (CDOM) and overestimation (CHL, TSM) of *in situ* measured values over optically-complex waters, although the use of the absorption and scattering coefficient leads to a good approximation of total attenuation. Amongst the Case-2 processors, BOREAL performs best to estimate the CDOM product and map different carbon fractions.
- MERIS-derived MCI estimates, based on L1b data, extend the detection rate for CHL up to hundreds of  $\text{mg m}^{-3}$ . The accuracy of the algorithm is dependent on the CHL concentration (the fluorescence peak value shifts with increase of CHL), background turbidity (mineral scattering contribution to NIR), submerged vegetation (scattering from leaf and cell structure), and a possible contribution from the atmosphere due to the use of TOA data.
- The MCI algorithm allows for the monitoring of the development and movement of variable cyanobacterial blooms at a high temporal and spatial scale, which would not be feasible with conventional monitoring methods, or standard EO algorithms. MCI estimates can be complemented with the detection of phycocyanin absorption. This supports the determination of the percentage of cyanobacteria biomass in the total phytoplankton biomass, which is a parameter of interest for WFD, in addition to CHL, phytoplankton biomass and transparency.
- Using a reference band at longer wavelengths (620, 665, 709 nm) gives progressively more accurate results when deriving satellite-based estimations for transparency (diffuse attenuation coefficient for downwelling irradiance or Secchi depth) over Case-2 waters. This confirms that over optically complex waters, the reference band of the respective algorithm should be in the red or infrared part of the spectrum.
- Analyses of spectral dependence of  $K_d(490)$  in optically complex waters revealed that the reflectance ratios 490/709 and 560/709 could describe most of the variation ( $R^2 = 0.88$ ), whereas the ratio 490/709 was suitable for more transparent waters and 560/709 for more turbid ones. As a result, a robust band ratio algorithm is developed, which switches from 490/709 to 560/709 over  $K_d(490)$  values of 2.03–2.76  $\text{m}^{-1}$  and is able to smoothly map  $K_d(490)$  in the ranges of 0.1–7.7  $\text{m}^{-1}$ .
- Although the MERIS standard processor MEGS derived reflectance product is usually negative in the blue-green part of the spectrum over Case-2 waters, the shape of the spectra still gives valuable information, and bands at longer wavelengths or band ratio algorithms can be applied to derive water quality parameters for such waters.
- Secchi depth can be derived with high accuracy ( $R^2 = 0.91$ , RMSE = 0.77 m, MNB = -9%, n = 89) from MERIS data over oligotrophic to eutrophic waters with good alignment around the 1:1 line (slope = 1.04, intercept = 0.19) with

pixel-by-pixel inputs of  $K_d(\lambda)$ ,  $c(\lambda)$  and the  $R_{rs}(\lambda)$  spectrum over visible wavelengths.

- The Secchi depth retrieval based on band ratio algorithms (either 490/709 for clearer coastal waters or 560/709 for more turbid waters), or by means of the previously calculated  $K_d(490)$  product, resulted in higher uncertainties due to overestimating low ( $Z_{SD} < 3$  m) and high (Vättern *in situ*  $Z_{SD} \sim 15$  m)  $Z_{SD}$  values and producing some outliers.
- MERIS-based CHL, TBM, and  $Z_{SD}$  products provide complementary information to meet the WFD assessment and reporting purposes by extending the knowledge of the seasonal and spatial variations in the data, improving the monitoring capabilities of the ecological state of the aquatic ecosystem.

## SUMMARY

This thesis presents research about applications for MERIS/ENVISAT data in order to monitor optically complex aquatic environments, such as inland and coastal waters.

Lakes and seas provide a wide range of essential ecosystem services. The assessment of the present and future state of these ecosystems is important from the regional to the global scale – for large-scale studies of the health of the environment, carbon and nutrients cycles, biodiversity maintenance, as well as for climate change studies. The substances in the water affect its transparency, productivity, food webs, and consequently, the ecological status of an entire aquatic ecosystem. Water quality varies both between different water bodies and within the same water body, on both a temporal and a spatial scale. EO provides a cost-effective means of assessing the current water quality and deriving historic information for time series analyses, or for gathering data from lakes that have not been part of conventional monitoring programmes.

Since the standard MERIS algorithms are not applicable to all water types, the algorithms have to be validated and, if needed, adapted to the specific conditions of optically complex waters. Cyanobacterial blooms are a common feature in many inland waters, as well as in the Baltic Sea. MCI-based algorithms were calibrated to estimate phytoplankton parameters (CHL, cyanobacterial biomass, phytoplankton biomass) in large Estonian lakes. The MCI-based approach allowed for the extending of the CHL detection range, as well as deriving information regarding phytoplankton biomass. Additionally, since the index is applicable on L1b images, water quality parameters can be derived in case of highly scattering cyanobacterial blooms, which are present in many of the lakes that were studied.

In addition to the standard EO water quality products (CHL, TSM, CDOM), other parameters (e.g. transparency) are required to estimate the underwater light field. It was found that while a semi-analytical approach estimated  $K_d(490)$  values rather well over coastal waters, it resulted in higher inaccuracies over inland waters. The development of empirical approaches revealed that the band ratios 490/709 and 560/709 are able to describe 88% of the variation in  $K_d(490)$  for a large range ( $0.1-7.7 \text{ m}^{-1}$ ), whereas 490/709 is more suitable for clearer waters ( $K_d(490) \leq 2 \text{ m}^{-1}$ ) and 560/709 for more turbid ( $K_d(490) > 2 \text{ m}^{-1}$ ). A combined  $K_d(490)$  algorithm was developed based on the band ratios 490/709 and 560/709, which switches based on transparency. The validation results over lakes and Baltic Sea coastal areas confirmed the high accuracy of the combined algorithm approach. In addition to  $K_d$ , Secchi depth is used to measure transparency. This is one of the oldest water quality measurements available, dating back to the 19<sup>th</sup> century. Various approaches to derive  $Z_{SD}$  in optically complex waters were developed and tested in this thesis. The best accuracy was retrieved when  $Z_{SD}$  was calculated as a function of  $K_d(\lambda)$ ,  $c(\lambda)$  and the  $R_{rs}(\lambda)$  over visible

wavelengths with pixel-by-pixel inputs, showing reliable results over oligotrophic to eutrophic conditions.

The developed algorithms were applied to the MERIS archive from 2002–2011 to identify if, and to what extent, satellite-based products could be used to monitor and assess the ecological status of inland waters as required by the WFD. The MERIS-based time series revealed the seasonal and spatial dynamics of CHL, TBM and transparency, which were complemented well by sparse *in situ* measurements that had been used for assessment and reporting of the ecological status of lakes as required by WFD. There was better agreement on ecological status class between satellite-based and *in situ* measured values when: 1) the inter-annual changes in CHL, TBM, and  $Z_{SD}$  were relatively small *i.e.* in clearer lakes; 2) the *in situ* sampling was frequent and coincided with bloom events/peaks; 3) class status boundaries were wide (*e.g.* ‘Moderate’ ecological status is assigned based on  $Z_{SD}$  when the value is between 1.5–2.5 m in Peipsi *s.s.* and between 0.6–0.7 m in Vörtsjärv). The encouraging results indicate that the EO products can be used as an additional source of information for assessment and reporting purposes. The research done in this thesis was based on MERIS/ENVISAT data, but the developed methods can be applied to OLCI/S3 data to provide EO data over optically complex waters at least until 2029.

## SUMMARY IN ESTONIAN

### Teadusuuringutest rakendusteni-optiliselt keerukate vete seire satelliitsensori MERIS/ENVISAT abil

Uurimistöö peamiseks eesmärgiks oli satelliitsensori MERIS/ENVISAT andmete kasutamisevõimaluste uurimine optiliselt keerukate siseveekogude ja rannikuvete kaugseireks.

Järved ja rannikuveed pakuvad olulisi ökosüsteemi teenuseid. Ökosüsteemi seisundi määramine on vajalik nii regionaalses kui globaalses skaalas, et mõista keskkonnas esinevaid laiaulatuslikke muutusi, tagada bioloogilise mitmekesisuse säilimine, uurida süsiniku ja toitainete ringet looduses ning modelleerida kliimamuutustega kaasnevaid protsesse. Vees olevad ained mõjutavad vee läbipaistvust, produktsiooni, toiduahelaid ning selle tulemusena ka ökoloogilist seisundit. Vee kvaliteet varieerub erinevate veekogude vahel ning samas ka ühe veekogu siseselt nii sesoonselt kui ka ruumiliselt. Kaugseire võimaldab efektiivset seire meetodit, mille abil saab hinnata vee kvaliteedi hetkeolukorda või aegriidade analüüsi abil hinnata muutusi võrreldes varasema seisundiga ning seda ka veekogude puhul, mis ei ole mõõtmistega kaetud tavaseireprogrammide raames.

Kuna MERIS standardsed algoritmid ei ole rakendatavad kõikidele veetüüpidele, peavad algoritmid olema valideeritud ning vajadusel kohandatud kohalikele oludele, et seirata optiliselt keerukaid veetüüpe. Sinivetikaõitsengud on levinud nähtus siseveekogus ning ka Läänemeres. Käesoleva uurimuse käigus kohaldati MCI indeksi [89] põhised algoritmid vastavalt suurte Eesti järvede optilistele iseärasustele, et hinnata fütoplanktoni parameetreid (klorofüll  $a$ , sinivetikate biomass, fütoplanktoni biomass). MCI põhine lähenemine võimaldab laiendada klorofüll  $a$  määramispiirkonda ning saada hinnanguid ka fütoplanktoni biomassi kohta. Kuna indeks on rakendatav MERIS L1b andmetele, lubab see hinnata vee kvaliteedi parameetreid sinivetika õitsengute korral, mille puhul standardsed atmosfäärikorrektsiooni algoritmid ei tööta.

Lisaks levinud vee kvaliteedi kaugseire tulemitel (klorofüll  $a$ , mineraalne hõljum, värvunud lahustunud orgaaniline aine), on vaja algoritme ka vee läbipaistvuse määramiseks, et hinnata veealust valgusvälja, millest sõltub veealuste organismide elutegevus. Töös testiti vee läbipaistvuse hindamist valguse difuusse nõrgenemiskoefitsiendi [ $K_d(490)$ ] ja Secchi sügavuse ( $Z_{SD}$ ) kaudu.

Selgus, et kuigi kiirguslevil põhinev algoritm hindas  $K_d(490)$  väärtusi hästi rannikuvetes siis siseveekogudes olid hinnangud ebatäpsed. Empiiriliste kanalisuhete loomisel ja testimisel selgus, et kanalite suhted lainepikkustel 490/709 ja 560/709 kirjeldasid 88% kogu muutlikkusest laia  $K_d(490)$  vahemiku puhul ( $0,1-7,7 \text{ m}^{-1}$ ), millest selgemate vete [ $K_d(490) \leq 2 \text{ m}^{-1}$ ] puhul oli tundlikum 490/709 ning sogasemate [ $K_d(490) > 2 \text{ m}^{-1}$ ] puhul kanalisuhe 560/709. Kasutamaks ühte algoritmi üle kogu andmestiku, loodi kaalufunktsioonidel põhinev kombineeritud kanalisuhte algoritm. Valideerimistulemused Läänemere ranniku- piirkonnas ning Eesti järvedel näitasid head kokkulangevust *in situ* mõõdetud

väärtustega ( $R^2 = 0,98$ ,  $RMSE = 17\%$ ,  $n = 17$ ). Vee läbipaistvuse hindamine Secchi ketta sügavuse mõõtmise kaudu on üks vanimaid vee kvaliteedi mõõtmisi ulatudes tagasi 19. sajandisse. Antud töös testiti ja arendati erinevaid lähenemisi, et hinnata Secchi sügavust optiliselt keerukate vete puhul MERIS andmetest. Parimaid tulemusi andis algoritm, mis võttis pikselhaaval sisendiks  $K_d(\lambda)$ ,  $c(\lambda)$  ja  $R_{rs}(\lambda)$  üle nähtava lainepikkuste ala. See algoritm töötas hästi samaaegselt nii vähetoiteliste kui ka eutroofsete järvede puhul.

Töös arendatud algoritmid rakendati MERIS arhiivi 2002–2011 andmetele, et välja selgitada, kas ja millisel määral saab kasutada satelliidiandmeid siseveekogude seireks ja ökoloogilise seisundi hindamiseks nii nagu on nõutud Euroopa Liidu veepoliitika raamdirektiivi poolt. MERIS andmetel põhinevad klorofüll  $a$ , fütoplanktoni biomassi ja läbipaistvuse aegread näitasid sesooneid ja ruumilisi muutusi, ja seega täiendasid hästi hõredaid *in situ* mõõtmisandmeid. Satelliidi ja *in situ* andmetel põhinev ökoloogilise klassi hinnang langes paremini kokku, kui: 1) klorofüll  $a$ , fütoplanktoni biomassi ja  $Z_{SD}$  sesoonsed kõikumised olid väikesed (st selgemates järvedes); 2) *in situ* mõõtmised olid võimalikud sagedased ning langesid kokku sinivetikaõitsengutega; 3) ökoloogilise klassi piirid olid laiad. Tulemused näitasid, et kaugseire andmeid saab kasutada täiendava infoallikana ökoloogilise seisundi hindamisel.

Väljatöötatud algoritmid ja rakendused on kohandatavad 2016. aasta veebruaris tööd alustanud Sentinel-3/OLCI andmetele, mille abil on optiliselt keerukate vete seire kosmosest võimalik vähemalt aastani 2029.



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- A. Reinart, H. Ohvril, **K. Alikas**, P. Ibrus, H. Teral, K. Valdmets, O. Okulov, “MERIS products over large European lakes – comparison with measured data about aerosol and water quality,” in: *Proceedings of ‘Envisat Symposium 2007’*, Envisat Symposium 2007, Montreux, 6 pp. 2007.



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