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MARTIN LIGI

Application of close range remote sensing for monitoring aquatic environment

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Application of close range remote sensing for monitoring aquatic environment

UNIVERSITY OF TARTU
Press

Estonian Marine Institute and Department of Zoology, Institute of Ecology and Earth Sciences, Faculty of Science and Technology, University of Tartu, and Tartu Observatory, Estonia

Dissertation was accepted for the commencement of the degree of *Doctor philosophiae* in environmental technology at the University of Tartu on February 2, 2017 by the Scientific Council on Environmental Technology, University of Tartu.

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Commencement:	Room 301, 46 Vanemuise Street, Tartu, on 28 March 2017 at 10.15 a.m.

Publication of this thesis is granted by the Estonian Marine Institute, University of Tartu

ISSN 1736-3349
ISBN 978-9949-77-353-4 (print)
ISBN 978-9949-77-354-1 (pdf)

University of Tartu Press
www.tyk.ee

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LIST OF ORIGINAL PUBLICATIONS

This thesis is based on the following publications:

I Hommersom, A., Kratzer, S., Laanen, M., Ansko, I, **Ligi, M.,** Bresciani, M., Giardino, C., Beltrán-Abaunza, J. M., Moore, G., Wernand, M., Peters, S. (2012). Intercomparison in the field between the new WISP-3 and other radiometers (TriOS Ramses, ASD FieldSpec, and TACCS). *Journal of Applied Remote Sensing*, 063615-1-063615-21.

II Kutser, T., Paavel, B., Verpoorter, C., **Ligi, M**., Soomets, T., Toming, K., Casal, G. (2016). Remote Sensing of Black Lakes and Using 810 nm Reflectance Peak for Retrieving Water Quality Parameters of Optically Complex Waters. *Remote Sensing*, 8 (497), 1–15, rs8060497.

III **Ligi, M.,** Kutser, T., Kallio, K., Attila, J., Koponen, S., Paavel, B., Soomets, T., Reinart, A. (2017). Testing the performance of empirical remote sensing algorithms in the Baltic Sea waters with modelled and in situ reflectance data. *Oceanologia*, 598(1), 57–68, 10.1016/j.oceano.2016.08.002

IV **Ligi, M.,** Kutser, T., Paavel, B., Uudeberg, K., Reinart, A., Soomets, T., Vahtmäe E. (*submitted to Boreal Environment Research*) Variability of the optical properties of the Baltic Sea coastal waters.

V **Ligi, M.,** Reinart, A., Tõnnisson, T., Reinart, A. (*submitted to Applied Optics*) First field measurements and device improvements for Multi-Spectral Volume Scattering Meter (MVSM).

Author's contribution

I The author played minor role in collecting the optical data, conducting the laboratory measurements, analysing the data and writing the article.

II The author had major contribution in collecting the data and minor contribution in analysing the data and writing the article.

III The author was responsible for analysing the data and writing the article; had major contribution in collecting the field data; model input data was received from the Finnish partner.

IV The author was responsible for writing the article and analysing the data; had a major contribution in collecting the data.

V The author collected all the field and calibration data; was responsible for writing the article and had major contribution in analysing the data.

ABBREVIATIONS

a	Absorption coefficient
aCDOM	Absorption of Coloured Dissolved Organic Matter
a_{TOT}	Total absorption of water with its constituents
b	Scattering coefficient
b_b	Backscattering coefficient
c	Attenuation coefficient
CDOM	Coloured Dissolved Organic Matter
CGLS	Copernicus Global Land Service
CHL	Chlorophyll-a
DOC	Dissolved Organic Carbon
E_d	Downwelling irradiance
ESA	European Space Agency
IPCC	International Panel for Climate Change
K_d	Diffuse attenuation coefficient of downwelling light
L_d	Downwellin radiance
L_{sky}	Sky radiance
L_u	Upwelling radiance
MSFD	Marine Strategy Framework Directive
MSI	MultiSpectral Imager
MVSM	Multispectral Volume Scattering Meter
NASA	National Aeronautics and Space Administration
NIR	Near infrared
OLCI	Ocean Land Colour Instrument
R	Reflectance
R_0^-	Irradiance reflectance just below the water surface
R_0^+	Irradiance reflectance just above the water surface
R_{rs}	Remote sensing reflectance
TSM	Total Suspende Matter
WFD	Water Framework Directive

1. INTRODUCTION

Knowing the quality of different waterbodies has been essential for human kind for thousands of years. In the last few centuries, however, the features of majority of waterbodies have been more influenced by the actions of humans rather than natural disasters or just natural variability. From the second half of the last century, policy and law makers paid most of their attention to drinking waters. In many countries managing and providing the drinking water with good quality is still the number one issue and in many regions lakes are one of the most important sources of drinking water. In other countries, where the management of drinking water resources is well regulated, the attention of monitoring has now turned to the waterbodies that are essential to fisheries, tourism, ecology, or some other purpose.

Water bodies are important for both human civilisation and natural ecosystems. They provide services in the field like transport, tourism, fisheries, they support biodiversity, and lacustrine waters are also important source for drinking water (Dudgeon, et al., 2006; Tranvik, et al., 2009; Bastviken, et al., 2011). The role that seas and oceans play in the global carbon cycle has been well recognised for some years now but the impact of lacustrine waters to this cycle has been strongly underestimated. Lakes and rivers were treated as pipes, transporting carbon from land to ocean systems. This was also the standard used in the IPCC reports prior to the 2013. More recent papers (Cole, et al., 2007; Tranvik, et al., 2009) show that lakes are actually carbon hotspots in land system as well as sentinels and regulators for carbon cycling (IPCC, 2013). There are 117 million lakes on Earth (Verpoorter, et al., 2014) and only tiny fraction of them (0.001%) is currently monitored (A. Tyler, personal communication). It is not possible to determine the role of coastal and inland waters in the global carbon cycle or monitor water quality at regional scale without using remote sensing (Palmer, et al., 2015).

Three of the main factors triggering the recent actions in European natural waters management were also triggering this work. The first is the European Union Water Framework Directive (WFD), which states, that all of the waterbodies have to reach good quality by the year 2020. To achieve this, at first the water quality parameters like transparency and chlorophyll-a concentration, have to be measured (European Union, 2000). Then the norms for all of these parameters have to be figured out. For that the natural state of the waterbody has to be taken into account as a baseline. For example, what is considered a Bad current state for naturally oligotrophic waterbody may be a Good status for naturally eutrophic waterbody. In order to take any management action in waterbodies in their jurisdiction, the governments have to determine the natural status of each waterbody, establish classification criteria for High, Good, Moderate, Poor and Bad water quality, and determine the current state. Determining the current and natural state of all the waterbodies has been a true bottle neck for this directive. In the frame of monitoring programs typically one water sample (taken in the deepest point of the lake) has to describe the state of the whole lake while natural variability within lakes may be high. Coastal waters are usually divided into large waterbodies. Legally all of them have to be monitored continuously, but in reality the sampling consists of a few measuring stations a couple of times during a year to no sampling at all. The scientists are therefore trying to convince governments to include remote sensing, as there has been an increase in accuracy of the water quality parameters that can be derived from optical data (Robinson, et al., 2008; Bresciani, et al., 2011; Palmer, et al., 2015). Remote sensing allows monitoring large number of waterbodies simultaneously over wide areas with high frequency without much human effort.

The second factor affecting the water management is the European Union's Marine Strategy Framework Directive (MSFD) that was signed in 2008. Similarly to the WFD, it sets an assignment to achieve Good ecological status of all European seas by the year of 2020 in order to maintain biodiversity and to protect the resource base upon which marine-related economic and social activities depend (European Union, 2008). In the case of the Baltic Sea, the MSFD takes the HELCOM Baltic Sea Action plan (HELCOM Ministerial Meeting, 2007) as the starting point and uses its European span to support reaching the aims set in the plan.

The third trigger of this study is the Copernicus program that provides free environmental monitoring data for everyone and for several decades to come. Sentinel-2, which data has been freely available for more than a year, and Sentinel-3, which data has been available from the October 2016, together provide detailed information about water bodies, to create regularly updated water quality applications on this data. Both OLCI on the Sentinel-3 and MSI on the Sentinel-2 are optical sensors. Therefore, it is important to understand how the optical remote sensing signal is formed in the waterbody and how it is modified by atmosphere between the water and the satellite. Several new satellites measure in off-nadir directions and the effects of the sensor viewing geometry has to be assessed (Botha, et al., 2016). Information about light behaviour and its limitations is something the scientists have to analyse in order to create the applications that provide usable and simple to read assessments about water quality for the general public and water management agencies.

There are different ways to measure water reflectance and during this study it was concentrated on three of these possibilities. To start with, the definition of reflectance has to be established as several similar but slightly different reflectance values are used in the field.

Earlier optical remote sensing studies used irradiance reflectance R. It is defined as a ratio of spectral upwelling to downwelling plane irradiances (Eq. 1). It shows how much of the radiance traveling in all downward directions is reflected upward into any direction (Morel & Smith, 1982; Mobley, 1994).

$$\boldsymbol{R}(\boldsymbol{z},\boldsymbol{\lambda}) = \frac{\boldsymbol{E_u}(\boldsymbol{z},\boldsymbol{\lambda})}{\boldsymbol{E_d}(\boldsymbol{z},\boldsymbol{\lambda})} \qquad [1]$$

R_0^+ and R_0^- are defined as irradiance reflectance above and below the water surface, respectively. R_0^- measurements should provide glint free reflectance. Unfortunately, as soon as the instrument is deeper than just below the surface, then the exact depth and amount of water constituents between the instrument and surface is needed. Therefore, the R_0^- is not achievable in the field measurements and is more of a theoretical concept.

The more popular characteristic nowadays is remote sensing reflectance (R_{rs}) which is the ratio of water leaving radiance to downwelling irradiance (Eq. 2).

$$\boldsymbol{R_{rs}(\lambda,\theta)=\frac{L_w(\lambda)}{E_d(\lambda)}} \qquad [2]$$

Water leaving radiance is calculated from upwelling (coming from water) radiance L_u and downwelling (sky radiance) L_{sky} (Eq. 3).

$$\boldsymbol{L_w(\lambda,\theta)=L_u(\lambda,\theta)-\rho_{sky}*L_{sky}(\lambda,\theta)} \qquad [3],$$

where ρ_{sky} is the air-sea interface reflection coefficient, which is dependent on the wind speed. In cases with wind speeds below 5 m/s or, where wind speeds were not measured, usually value of 0.028 is used (Mobley, 1994). However, this factor is empirical coefficient that is not working for most cases. For the perfectly smooth water surface factor of two per cent is applicable (from Fresnel law). R_{rs} is calculated as a reflectance to a certain area and therefore has a unit of sr^{-1}. In most cases, this reflectance is corrected for the effect of "white light", according to Ruddick et al. (2005), so that white light error ε (Eq. 4) is subtracted from the R_{rs} spectrum.

$$\boldsymbol{\varepsilon=\frac{\alpha*Rrs(780)-Rrs(720)}{\alpha-1}} \qquad [4]$$

where α is 2.35.

A setup where an irradiance sensor was looking directly upwards and a radiance sensor was looking directly downwards has been used for half a century. With this design the above water measurement contains reflection of sun and sky from the water surface (called glint), besides the water leaving signal. To overcome the glint problem some remote sensing spectrometers had a third – downwelling radiance channel. Such instruments were introduced in the eighties of the last century (Arst, et al., 1997). The third receiver was added to measure radiance from the zenith point of the sky that is reflected back in the upwelling radiance channel. For perfectly flat water conditions the reflectance can then be calculated (Eq. 5):

$$\boldsymbol{R=(L_u-0.02*L_d)/E_d} \qquad [5]$$

Mobley (1994) made theoretical calculations on angular distribution of sun and sky glint compared to water leaving signal and found that the optimal angle for reflectance measurements is not nadir, but 42 degrees off nadir. Based on theoretical simulations these measurements have to be taken at an azimuth angle of ~135 deg relative to the sun. In this way direct reflection effects (e.g., sun glint) that occur at the surface are theoretically minimised as much as possible (Mobley, 1994). However, calculating the reflectance from the three channel setup contains an empirical constant linking wind speed to the surface roughness and potential glint from it. Maintaining the recommended angles is also nearly impossible at sea or in a small boat. Thus, the three channel setup with tilted radiometers has also some shortcomings. The biggest problems occur on small lakes where tilted upwelling radiance sensor may measure reflection of forest (forest lakes) or buildings (urban areas) from the water surface, or in mountain lakes the sensor may measure reflection of mountains. In variable sky conditions the sky radiance measured by the L_d sensor may not match with the actual sky conditions reflected back from the area measured by the Lu sensor. Consequently, the glint contribution is under- or overestimated. Thus, the three sensor tilted option is theoretically good and works well in the open ocean, especially when equipped with automatically rotating platform adjusting azimuth based on the position of the ship against the Sun (Simis & Olsson, 2013; Brando, et al., 2016). However, it does often not work properly in coastal and especially in inland waters.

To overcome the glint problem a methodology to measure glint-free water reflectance spectra have been developed (Kutser, et al., 2013). The Ramses radiance sensor has a 5 cm black plastic tube attached to it. Besides the "normal" above and below water measurements with the two Ramses system measurements are carried out where the plastic tube of the Ramses radiance sensor is just below the water surface and is measuring the actual water leaving signal not contaminated with glint. This allows to measure glint-free reflectance spectra and the glint removal methodology based on the data collected this way (Kutser, et al., 2013) allows obtaining glint-free reflectance without making the actual glint-free measurements. The problem with this methodology is that it is hard to perform in rough conditions, especially from large research vessels.

Water reflectance data collected with field radiometers has been mainly used for satellite data calibration and validation purposes. However, handheld devices and portable autonomous systems on ferries, jetties, and buoys have become remote sensing tools in their own, as they allow collecting fast and frequent data about the state of waterbodies (Simis and Olsson 2013, Groetsch, et al. 2014, Charria, et al., 2016). An increasing trend is using the data coming from all these different platforms in one system that includes all the best possible information available. All of these instruments measure radiance or irradiance that are calculated into water leaving reflectance to remove variability in illumination conditions during the measurements. Top of atmosphere radiance and top of atmosphere reflectance are sometimes used instead of water leaving reflectance as atmospheric correction of aquatic targets, especially inland waters, is not a well solved problem. Different algorithms are then used to retrieve water parameters like the absorption by coloured dissolved organic matter (CDOM); Secchi depth, or attenuation coefficient (K_d); chlorophyll-a concentration (CHL); and Total suspended matter (TSM) concentration (Kratzer, et al., 2008).

In situ reflectance measurements can be carried out at any time and processed into concentrations or other water quality parameters in real time. Ocean colour satellites can provide info about water quality parameters only in cloud-free conditions, but they cover large areas with one image and in the case of large waterbodies can provide overview of an entire waterbody simultaneously. Cloud cover and the adjacency effects (part of signal measured above a water body originates from much brighter adjacent land) issues are present not only the case for lakes but also in the coastal waters of the Baltic Sea (Darecki & Stramski, 2004; Reinart & Kutser, 2006; Kutser, et al., 2015; Pitarch, et al., 2015). In the cloudy situations, the in situ radiometers can fill in the void (Reinart & Valdmets, 2007) in addition to using them as validation tools for satellites. The downside of the in situ devices is that some of those can be complicated to deploy by monitoring agencies, especially when the water body in question is hard to reach or a vessel has to be used to measure on the water body. The in situ radiometers can be used for point measurements (fixed on a jetty or buoy) or in transect mode (on ships of opportunity and research vessels). Thus, they cannot provide the full spatial coverage of waterbodies like satellite remote sensing can.

Only the visible part of the spectrum can potentially be used to retrieve information about properties of water bodies as water itself absorbs radiation very strongly in UV and shorter wavelengths and from red to longer wavelengths (Segelstein, 1981; Pope & Fry, 1997; Brezonik, et al., 2015). For example, the relative permittivity at the microwave region, where radar remote sensing satellites work, is so high, that the radiation does not penetrate into the water column and is reflected back from the surface and can provide information only about the surface roughness (Meissner & Wentz, 2004; Voormansik, 2014).

There are situations where the remote sensing signal outside the visible part of spectrum can be or has to be used for retrieving water quality parameters. For example, there are lakes where the CDOM concentration is so high, that most of the signal in visible part of the spectrum is almost completely absorbed (Kutser, et al., 2016a). There are also turbid lakes where the concentrations of phytoplankton (Quibell, 1992; Kutser, 2004) or the suspended matter (Doxaran, et al., 2003; Doxaran, et al., 2004) are very high. In the first case the near infrared (NIR) part of the electromagnetic spectrum has to be used and in the second case it is better to use for retrieving information about water constituents. The global inventory of lakes (Verpoorter, et al., 2014) showed that most of the lakes are situated between the latitudes of 55N and 75N. These boreal lakes have often high CDOM concentrations (Kutser, et al., 2005; Kutser, et al., 2009a; Weyhenmeyer, et al., 2014; Verpoorter, et al., 2014).

Therefore, one can assume that the number of extremely absorbing lakes is relatively high. The reason why there are only a few recent studies including these black lakes (Kutser, et al., 2009a; Brezonik, et al., 2015) is that they can be hard to reach and are extremely hard to study. Recent studies (Köhler, et al., 2013; Kutser, et al., 2015) have shown that iron bounds to dissolved organic carbon (DOC) and this way increases the absorbance resulting in CDOM retrieval complications. New remote sensing approaches are needed to retrieve CDOM concentration from radiometric measurements as the number of lakes with high CDOM is potentially high. Mapping CDOM in lakes and coastal waters is of critical importance given that the CDOM is coloured part of DOC and usually in good correlation with the DOC, which is the main pool of carbon in lakes (Wetzel, 2001) and coastal waters.

Boreal regions have four seasons and processes in lakes are influenced by ice covered period. The Baltic Sea, together with bigger lakes in the area, have two distinct blooms. The spring bloom is dominated by diatoms and summer blooms are dominated by cyanobacteria (Kahru, et al., 2016). Optical properties of these phytoplankton groups are very different (Metsamaa, et al., 2006). Moreover, cyanobacteria can move in the water column and tend to concentrate at depths most suitable for their development (Klemer, et al., 1996; Groetsch, et al., 2014) further complicating their quantitative detection by remote sensing. Vertical distribution of cyanobacteria is known to have a significant effect on the remote sensing signal (Kutser, et al., 2008).

In the remote sensing, top of atmosphere radiance is in most cases usually calculated to water leaving reflectance to remove the atmospheric contribution in the measured signal. The atmospheric correction has been a main problem in aquatic remote sensing since its early years. Even in the clear sky conditions more than 90% of radiance measured above the water bodies is actually originating from atmosphere and does not contain any information about the waterbody. Therefore, some authors have proposed methods where water constituents are estimated from top of the atmosphere radiance (Letelier & Abbot, 1996; Gower, et al., 1999; Härmä, et al., 2001; Kallio, et al., 2003; Kutser, 2004; Kallio, et al., 2008; Olmanson, et al., 2011; Kutser, 2012) or propagated the water signal to the top of atmosphere using forward atmospheric model in order not to deal with all inverse problem issues related to the atmospheric correction (Kutser, et al., 2006). However, using the top of atmosphere reflectance or radiance requires relatively strong water leaving signal in red and NIR part of spectrum (where the atmospheric signal is lower). This occurs in the case of algal blooms and in the case of optically shallow water. The problem of optically complex waters is that the assumption on zero water leaving signal in NIR part of spectrum (used in oceanic waters) is not valid. When this assumption is used for shallow or turbid water bodies, then the reflectance values are overcorrected producing negative reflectance values in the blue part of spectrum. Some atmospheric correction models assume certain water parameters. These models are mostly calibrated to lower concentrations of optically active substances but as the concentrations get higher the interaction of particles between the surface layer of water and atmosphere is increased and therefore the amount on substances in the air just above the water surface is higher resulting in the larger effect of the atmosphere. In addition to this, the types of aerosols may vary from region to region making it even harder to create general atmospheric correction approaches (Krüger, et al., 2012).

In order to develop better remote sensing algorithms and methods for optically complex waters it is useful to understand how the reflectance signal is formed in different waterbodies. Therefore, the first part of the thesis concentrates on the formation of the water leaving signal (Article IV).

The remote sensing signal measured above the water is proportional to the ratio of backscattering (b_b) and absorption (a) coefficients (Gordon, et al., 1988) (Eq. 6), where R is the irradiance reflectance just beneath the water and Q is the ratio of the upwelling radiance to the upwelling irradiance toward the zenith.

$$\frac{R}{Q} = 0.0949 * \frac{b_b}{(a+b_b)} \qquad [6]$$

The Eq.6 shows that water reflectance is proportional to absorption and backscattering coefficients. Consequently, the variability of these parameters in waterbodies has to be studied to understand the formation of reflectance. There are only a few published studies available for the Baltic Sea (Berthon, et al., 2008; Kutser, et al., 2009b). The lack of optical data is similar also in other regions of the world (Kratzer, et al., 2000; Blondeau-Patissier, et al., 2009; Gholamalifard, et al., 2013; Cherukuru, et al., 2016). Therefore, the knowledge about the variation of optical properties needs further investigation not only in the Baltic Sea but also worldwide. Most of the published Baltic Sea data is for the open parts or southern area of the sea (Woźniak, et al., 2011; Levin, et al., 2013), whereas the variation in optical parameters and concentrations is higher at the shallow coastal areas, where input from rivers, combined with the resuspension of bottom sediments, can cause significant variability in both spatial and temporal scale.

The second logical step is to understand the optical measurements to retrieve reflectance. During the data collection for this thesis, no cost effective remote sensing satellites, that were suitable for water remote sensing, were available. Therefore, this part concentrates more on in situ reflectance measurements (Article I).

The third step is testing different algorithms for estimating water quality parameters (CHL, TSM and CDOM) in optically complex waters like the coastal waters of the Baltic Sea and lakes. The articles II and III focus on this topic.

Analytical methods using the full reflectance spectrum instead of a few bands have been around for years (Arst & Kutser 1994, Kutser, et al. 2001, Doerffer & Schiller 2007, Giardino, et al., 2007; Brando, et al., 2009; Dekker, et al. 2011, Giardino, et al. 2012; Werdell, et al., 2013). The satellite sensors provide multispectral products and in situ radiometers even hyperspectral products. So at the first glance, it may not seem novel enough to suggest using band-ratio algorithms, because it raises questions why to collect so much data then.

An important aspect of simple algorithms is that this approach allows using statistical relationships in order to calculate certain parameters, whereas the analytical models have to include physical explanation of the relationship and are therefore limited by the available parameterization of inherent optical properties (IOP) (Odermatt, et al., 2012). Moreover, the empirical algorithms can be developed to estimate water characteristics that are not directly related to water reflectance or which relationship to the water colour is not well understood. For example, Kutser et al. (1995) estimated total phosphorus in Lake Peipsi from helicopter while phosphorus itself is "invisible". It just is correlated to the amount of total suspended matter of the lake which has impact on water colour. Part of DOC is not optically active, but often it is well correlated with its optically active part (CDOM) and can therefore be estimated using band ratio algorithms (Fichot & Benner, 2011; Harvey, et al., 2015). CO_2 saturation in water can be estimated with empirical algorithms whereas in lake water it is in correlation with DOC (Hanson, et al., 2003; Whitfield, et al., 2013) and in ocean waters with SST (Benson, et al., 2014) which can be mapped from satellites (Belkin & O'Reilly, 2009; Solanki, et al., 2015).

The Copernicus program offers already hundreds of different products. However, there are no ongoing products yet released for the lake water quality. In the Copernicus Global Land Service (CGLS) only one demonstration product for mapping the lakes surface areas (CGLS, 2017) with 1 km spatial resolution is currently available. There are only two Baltic Sea products in the Copernicus Marine Environment Monitoring Service (CMEMS) that are validated for the Baltic Sea – chlorophyll-a and water reflectance at a few wavelengths. There are actually two products for chlorophyll-a. One is near real time (same day) product with 1 km spatial resolution and then there is a reanalysis product that is calculated at 4 km spatial resolution with significant time delay. The latter product is based on ESA Climate Change Initiative time series that combines data from MERIS, MODIS, SeaWiFS and VIIRS sensors. The correlation between the measured and estimated chlorophyll-a is $r^2=0.20$ for the near real time product and $r^2 \sim 0.45$ for the coarse resolution reanalysis product. The relatively reasonable result for the reanalysis product is surprising taking into account that it is using a blue-green spectral ratio proven not to work in optically complex waters (Darecki & Stramski 2004). A possible explanation is that the CMEMS combines Kattegat and Skagerrak waters with the Baltic Sea despite these are optically very different. The remote sensing reflectance product works better at longer wavelengths and worse in the shorter wavelengths range (r^2 at 412nm=0.22; r^2 at 665 nm=0.57). This indicates that the atmospheric correction is most probably one of the main reasons of the failure of the near real time chlorophyll-a product as the analytical (neural network) methods require high quality reflectance data in order to provide reasonable results. It must be noted that the current CMEMS products are for aging MODIS sensor with suboptimal spectral resolution for optically complex waters. Switching to Sentinel-3 OLCI is still undergoing (CMEMS 2017).

2. THE AIM OF THE STUDY

This thesis addresses six main questions:

How much do the inherent optical properties vary in different parts of the Baltic Sea and how does this variability change the reflectance signal and therefore impact the retrieval of water constituents from remote sensing data?

Can similar outcome be expected from reflectance measurements conducted with devices that rely on different principles (different sensor configurations e.g. viewing angles)?

Is it possible to use NIR part of spectrum for retrieval of any water constituents in optically complex/absorbing waters where the water leaving signal in visible part of spectrum (typically used for water constituent retrieval) is close to zero?

Are simple empirical algorithms suitable for retrieval of water characteristics (coloured dissolved organic matter, suspended matter and chlorophyll-a) in the Baltic Sea or do analytical methods have to be used?

Can hand-held spectrometers be used as water quality monitoring devices besides being a validation tool for satellite measurements?

Is the device built in Tartu Observatory for measuring complete volume scattering function in in situ condition fulfilling its tasks and outperforming other similar (mostly laboratory) instrumentation?

3. MATERIALS AND METHODS

3.1 Study area

3.1.1 Baltic Sea and large lakes

The first group of study objects includes two major lakes in Estonia: Lake Peipsi and Lake Võrtsjärv; two in Sweden (Lake Vänern and Lake Mälaren) and the Baltic Sea coastal areas in Estonia, Latvia and Sweden. Most of the ocean colour studies keep sea water separate from fresh water. These were joined into one group as they are very similar from optical point of view as well as from biogeochemical point of view. The Baltic Sea is a brackish waterbody with low salinities in the northern and eastern parts reaching zero salinity in the Gulf of Finland and other coastal regions (Łukawska-Matuszewska & Urbańskii, 2014; Ylöstalo, et al., 2016; Skudra & Lips, 2017). CDOM dominates the optical water properties of Baltic Sea waters just as in lakes (Arst, 2003; Beltrán-Abaunza, et al., 2014). Low salinity also means, that the coastal areas are covered with ice during most of winters and the photosynthesis season starts when the ice cover gets thin enough to allow sufficient amount of light to penetrate into the water. Also the successions of phytoplankton (diatom bloom after ice melt, period of clear water, cyanobacterial bloom) are similar in these waterbodies.

3.1.2 Small lakes

The second group of waterbodies include only smaller lacustrine waters: Harku, Nohipalu Mustjärv, Meelva and Valguta Mustjärv. These lakes have been too small for the water remote sensing satellites to investigate, however, the new land remote sensing satellites Landsat-8 and Sentinel-2 are capable of retrieving information about water bodies of this size (Kutser, et al., 2016b; Slonecker, et al., 2016; Toming, et al., 2016). Harku is the example of a hypertrophic lake, where the average chlorophyll-a concentration during the vegetation period is over 100 mg/m^3. The other three are black lakes that are extreme cases of absorbing waters and as such perfect test beds for remote sensing instruments and methods. The CDOM concentration in these lakes is so high that there is no water leaving signal in almost entire visible part of spectrum. Meaning that no previously developed remote sensing algorithm can work there. Many inland and coastal water algorithms (Gitelson, 1992; Härmä, et al., 2001; Kallio, et al., 2001; Zimba & Gitelson, 2006; Hunter, et al., 2008; Gitelson, et al., 2009; Moses, et al., 2009) rely on the peak around 700–715 nm caused by the combined effect of water absorption and backscattering from particles (phytoplankton, in most of the lakes). In clear waters there is no peak in water reflectance in this spectral region as water absorption is increasing exponentially from 650 nm onwards and the number of particles is low. In phytoplankton rich waters the peak occurs as, at least in some wavelengths, the backscattering by phytoplankton can overcome the absorption by water molecules. However, in these extreme black lakes the CDOM absorption (usually assumed to be negligible in red and NIR) absorbs even stronger in the 700 nm region than the water molecules. Consequently, the most widely used piece of information about the phytoplankton abundance is also partly masked by CDOM absorption. This was the reason why the focus was on such extreme waterbodies.

3.1.3 Black Sea

The Black Sea is a waterbody with the similar size to the Baltic Sea. However, it has similar salinity level to oceanic waters. Fieldwork was conducted in the north-western part of the sea where 80% of the basin's total freshwater discharge is received (Mikhailov & Mikhailova, 2007). The fieldwork campaign conducted on the Black Sea was used, to evaluate the performance of the Multispectral Volume Scattering Meter (MVSM) and the optical properties of the Sea were not further assessed within the study.

3.2 Methods

3.2.1 Absorption and attenuation

Absorption and backscattering of light determines the water reflectance as was described above (Eq. 6). In clear oceanic waters it is possible to measure total absorption and attenuation coefficient, as well as absorption and attenuation by dissolved material, in situ. For example, WETLabs AC-S, or its predecessor AC-9, can be used with 0.2 µm filters to measure CDOM absorption directly by attaching the filters to the device, besides measuring the total absorption and attenuation. This is not possible in more turbid inland and coastal waters where the particles would clog the 0.2 µm (CDOM) or other filters almost immediately. Therefore, water samples have to be collected and analysed in the laboratory. Standard laboratory methods for absorption measurements (GLaSS, 2015) are based on measurements in spectrometer cuvettes and always include some forward scattering of light increasing the absorption values. Therefore, our latest measurements include also absorption (both total and CDOM absorption) measurements carried out with an integrating sphere absorption meter (a-sphere by HobiLabs). The path length of light in the integrating sphere is indefinite meaning that the scattering errors are theoretically excluded.

The AC-S instrument, used in field measurements, has 86 bands to cover wavelengths from 400 to 730 nm with a resolution of ~4 nm. It uses a proven flow-through system with a pump to allow faster profiling through the water body and elimination of air bubbles from the flow cells. There are two cells, one for attenuation and one for absorption and the measurements are taken simultaneously. Standard AC-S cells are 25 cm long. Light cannot penetrate so long distance in optically complex (turbid or strongly absorbing) waters. Therefore, an instrument with 10 cm cells was used in this study. The instrument produces results where clean water values, taken from Pope and Fry (1997), have been subtracted from measured values. Therefore, the output is attenuation and absorption coefficient of all additives in the water. In order to retrieve total absorption and attenuation coefficient values (e.g. for comparison with laboratory results or using in some models) clean water data has to be added back to the final product. The calculation of the products is more thoroughly explained in article IV.

3.2.2 Backscattering

It is hard to create a device that can measure the volume scattering function at all angles with high speed. Therefore, the instruments designed for fast in situ backscattering measurements use one to three measuring angles and certain assumption about the volume scattering function. Two such devices were in use in this study. The first instrument is ECO-BB3 which measures backscattering coefficient at three different wavelengths: 412, 595 and 715 nm. The ECO-BB3 contains a single-angle (124 degrees) sensor for determination of optical backscattering. This angle was determined through modelling as the minimum convergence point for variations in the volume scattering function (VSF) (Sullivan, et al., 2012), induced by suspended materials and water itself. Using 124 degree angle results in the measured signal that is less determined by the type and size of the materials in the water, and is more directly correlated to the concentration of the materials (WETLabs, 2010). The second sensor is the ECO-VSF3 that measures the volume scattering function at three angles (100°, 125° and 150°) and three wavelengths (470, 532 and 660 nm). The wavelengths in use can be selected when manufacturing the instrument. Therefore, the wavelengths of the two instruments were chosen so that they complement each other. The three-angle measurement allows determination of specific angles of backscattering through interpolation. Conversely, it can also provide the total backscattering coefficient by extrapolation and integration from 90 to 180 degrees (Sullivan, et al., 2012).

The issue with measuring backscattering is that the signal in CDOM rich waters is underestimated due to strong absorption that weakens the signal scattered backwards towards the sensor. Meaning that at shorter wavelengths (where the CDOM absorption is stronger) the measured backscattering is lower than the actual one because part of the radiation is absorbed on the way back to instrument. In strongly absorbing environments this is significant despite the volume where backscattering is measured is within a few centimetres next to the instrument. Therefore, additional correction is needed in strongly absorbing waters and the absorption measurements from AC-S can be used for that (Article IV).

3.2.3 Volume scattering function

The volume scattering function describes the angular distribution of light scattered from an incident beam. Although, it is a fundamental inherent optical property of the aquatic environment, and for the correct calculations of the radiate transfer, it is essential to know the variations of the phase function, there is little known about the range of variability in the VSF in the aquatic environment. The main reason for it is that the VSF measurements are difficult to perform. Therefore, a lot of currently used radiative transfer models are based on a very limited set of measurement campaigns, which were conducted more than 40 years ago (Petzold, 1972). These measurements were conducted with wideband spectral response sensors which can cause mismatch between modelled data and measurement conducted with modern narrow band sensors (Pitarch, et al., 2016). Instruments, which have previously been used for measuring VSF, were complicated, bulky and most importantly: not able to take measurements of the VSF in full angular range (Tartu Observatory, 2015).

There are a couple of prototype instruments, that tackle this issue (Tan, et al., 2015), and one is used in this study. With the support from ESA and EC, Tartu Observatory has been working on the Multispectral Volume Scattering Meter (MVSM) that is capable of measuring Volume Scattering Function at eight different wavelengths (362, 400, 465, 525, 590, 625, 660 and 740 nm) at the angles from 2 to 178 degrees, with the maximum angular resolution of 0.1 degrees. This is made possible as the signal is directed to the sensor by rotating prism (Figure 1). The smaller angles are not accessible due to the signal from the direct beam. At the larger angles, the prism itself is blocking part of the beam. The rotation of the prism takes time; therefore, 0.5 degree step is used at the moment. The VSF at angles near to 90 degrees are more stable, but the differences near the 0 and 180 degrees are in orders of magnitude. It is planned to introduce dynamic step, in order to retrieve more information at the edges and at the same time, to reduce the measurement time.

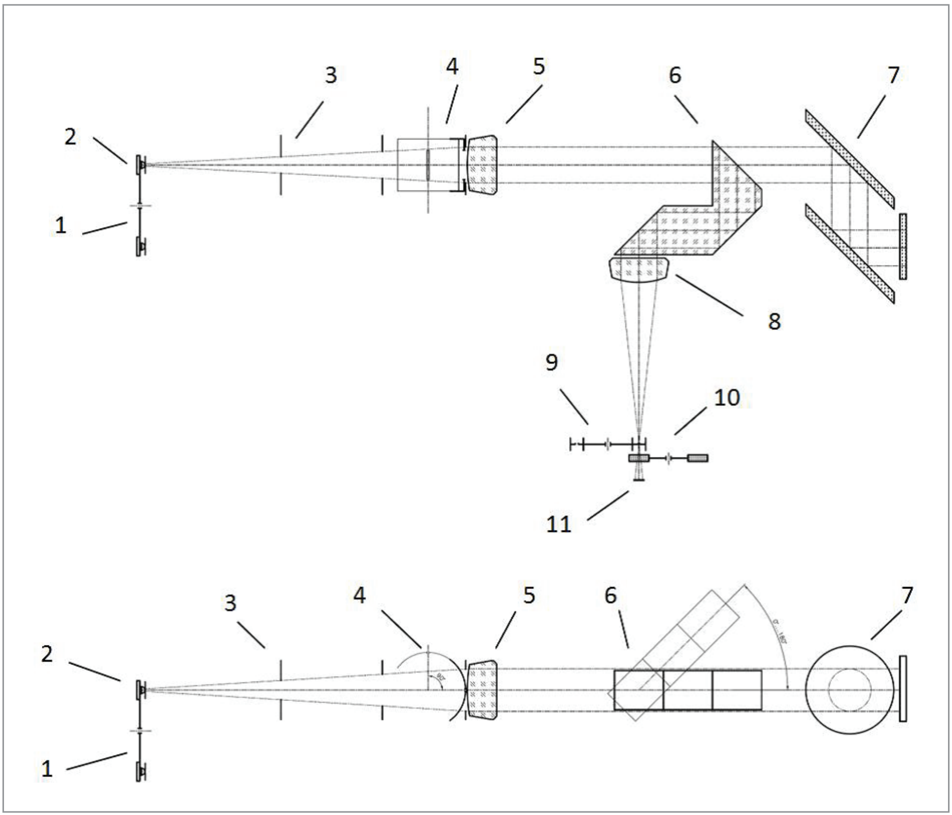

Figure 1. Schematic outlines of main optical components of the Multi-spectral Volume Scattering Meter: 1 – radiation source (LED) disc, 2 – radiation source (LED), 3 – diaphragm, 4 – diaphragm disc, 5 – collimating lens for the radiation source (LED), 6 – periscope prism, 7 – light trap, 8 – collimating lens for the detector (photomultiplier), 9 – diaphragm disc, 10 – optical filter disc, 11 – detector (photomultiplier)

3.2.4 Reflectance measurement sets

To standardise the reflectance measurements, ESA has signed a contract in 2016 for project FRM4SOC, which core action is to ensure that ground-based measurements of ocean colour parameters are traceable to SI standards in support of ensuring high quality and accurate Sentinel-2 MSI and Sentinel-3 OLCI products. Therefore, only radiometers that were available for the PhD study are compared here. All radiometers used in the field can be divided into two subsections: radiance and irradiance sensors. Radiance sensors measure light in a narrow angle while irradiance sensor collects data from hemisphere.

The radiance sensors in use were the TriOS RAMSES ARC-VIS's. They have a 256 channel silicon photo diode array detector that is covering the range from 320 to 950 nm. Pixel dispersion is 3.3nm and wavelength accuracy is 0.3nm. Number of usable channels is 190. The integration time for measurements is

4 ms – 8 s depending on the available signal. Field of view is 7 degrees in the air and accuracy better than 6%. Irradiance sensors were the TriOS RAMSES ACC-VIS that are similar to radiance sensor, but have a cosine collector and accuracy of 6–10% (TriOS, 2017).

WISP-3, which is a handheld instrument, has two radiance and one irradiance sensor all in one device. It contains three Ocean Optics, Inc., JAZ radiometers (with 2048 channels calibrated to 350–800 nm), a processor and a battery. The three radiometers are, via optical fibres, connected to, respectively a cosine corrector to measure the downwelling irradiance, and two Gershun tubes, with a viewing angle of 3 degrees for the radiance measurements. The radiance sensors have a band width of 4.9nm and the irradiance sensor 3.9 nm (Water Insight, 2017). The tubes are fixed to 42 degree angle from the zenith to measure the downwelling radiance from the sky and at 42 degrees from the nadir for the total upwelling radiance. These three radiometers and the angles are chosen according to Mobley's (1994) theoretical guidance on above-water radiometric measurements in order to minimise the effect of sun and sky glint.

During the study, two TriOS RAMSES setup (an irradiance sensor looking directly upwards and a radiance sensor looking directly downwards) was used for above water measurements, similarly to the approach used for almost half a century. The same two RAMSES instruments were used for the glint free measurement technique (Kutser, et al., 2013). The WISP-3 and three sensor TriOS RAMSES setup (an irradiance sensor looking directly upwards and two radiance sensors looking at 42 degrees from nadir and zenith respectively) were used to follow the methodology by Mobley (1994) that should theoretically minimise the amount of glint in measured signal.

3.2.5 Laboratory measurements

Water samples from the surface layer were collected at every station where optical measurements were conducted (Study area described above). The remote sensing signal is also received from the same layer.

To retrieve the chlorophyll-a (CHL) concentration (mg/m^3), water samples were filtered through the 0.7 mm pore size Whatman GF/F-filters. The filters were then soaked in 96% ethanol and studied spectrophotometrically according to the ISO standard method (ISO, 1992). Finally, CHL was calculated using the Lorenzen (1967) method.

For the retrieval of total suspended matter (TSM), the samples were filtered through pre-weighed and pre-combusted (103–105 °C for 1 h) GF/F filters. Filters were then measured gravimetrically. The weighed filters were then put to the combustion oven at 550 °C for 30 min. The leftovers were then weighed again to get the inorganic fraction of suspended matter (SPIM). The organic fraction (SPOM) was determined by subtracting the SPIM from TSM (ESS, 1993).

Absorption by coloured dissolved organic matter (CDOM) was measured with a spectrometer (Hitachi U-3010 UV/VIS, at the range of 350—750 nm) in water filtered through a Millipore 0.2 mm filter. Measurements were carried out in a 5-cm cuvette against distilled water and corrected for residual scattering according to Davies-Colley and Vant (1987). The second device for CDOM measurements in use was a-Sphere spectrometer described in 3.2.6.

Phytoplankton pigments were measured with the dual-beam spectrophotometer with the integrating sphere. First the GF/F filter with filtered water was measured then the filter was bleached with oxidizing agent sodium-hypochloride (NaClO). After the bleaching, the filter was again measured in the sphere and the result spectrum was subtracted from the original measurement to retrieve the spectrum of pigments. More thorough description of the method is available in Tassan and Ferrari (1995).

3.2.6 a-Sphere spectrometer

The total absorption coefficient, a_{TOT}, and CDOM absorption was measured with an a-Sphere spectrometer (spectral range 360–764 nm, HOBI Labs, Bellevue, USA). Light entering through an aperture reflects of the wall many times and creates a uniformly diffuse internal light field. The multiple reflections cause photons to travel a total distance much greater than the dimensions of the cavity. This greatly increases the absorption path length and therefore the sensitivity of the measurement. Thus, it doesn't require scattering correction, even in highly turbid waters. For the CDOM measurements filtered water was used.

3.2.7 Model

Hydrolight radiative transfer software was used to produce a spectral library of Baltic Sea waters. HydroLight and the lighter version, EcoLight, are modelling software produced by Sequoia Scientific, Inc. More thorough overview about the software is given in article IV. Here it is important to point out, that the software is well recognized in water optics community already for decades and is currently the most used software to model the behaviour of light in the water.

4. RESULTS AND DISCUSSION

4.1 Inherent optical properties

The absorption values in the Baltic Sea differed greatly from values of other European seas (Article IV). The cleaner waters of Swedish coast had ten times lower absorption values than the highest values from the Estonian coast (Figures 2 and 3 in article IV). To enhance the readability, only the samples from Estonian coast are shown in the Figure 2. All of these were collected in an area with 50km radius. The absorption values near the coastal areas were similar to the values of Lake Peipsi (Figure 2 and Figure 3). Only some of the coastal values were lower than typical Lake Peipsi values and some Lake Peipsi values were higher than typical coastal values. To demonstrate the variability of CDOM absorption in different waterbodies then the examples of two clear waterbodies (Lake Äntu and Baltic Sea) were compared with three average lakes (Lake Peipsi, Lake Mäleren and Lake Võrtsjärv), one hypertrophic lake (Lake Harku) and one extremely absorbing lake (Nohipalu Mustjärv) (Figure 4). The comparison of the AC-S and a-Sphere measurements (Figure 5) shows that there are forward scattering effects in the AC-S measurements leading to overestimation of the absorption values. Note that on the graphs the absorption coefficients are given not as total absorption coefficient spectra that go into Eq. 6, but as an absorption coefficient of water constituents. For the total absorption, pure water values have to be added to these measurements.

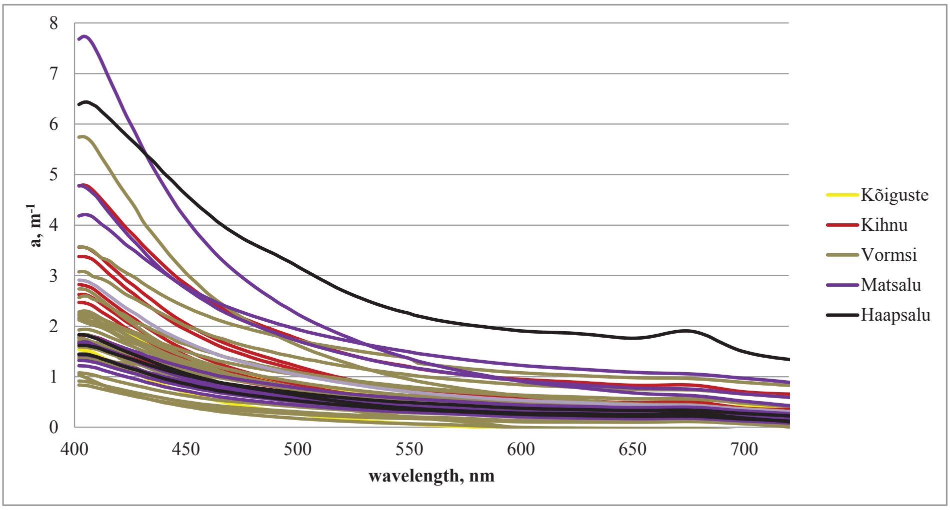

Figure 2. Station average absorption coefficients of water constituents from 5 regions at the Estonian coast

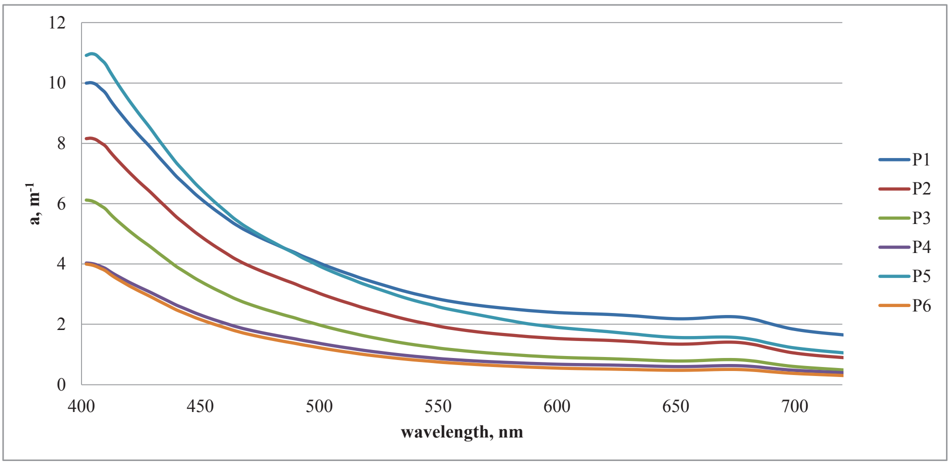

Figure 3. Station average absorption coefficients of water constituents from 6 Lake Peipsi stations in 27.07.2016

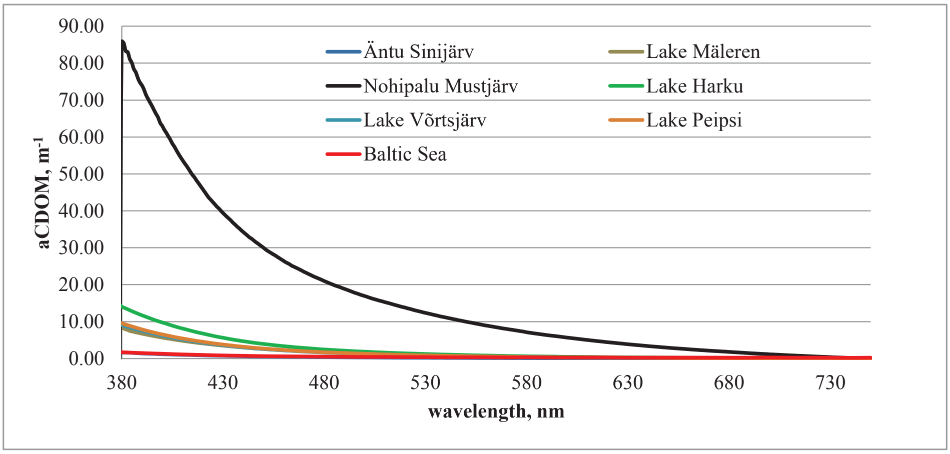

Figure 4. CDOM absorption coefficient spectra measured during the summer period in the Baltic Sea and 6 different lakes in 2010–2013.

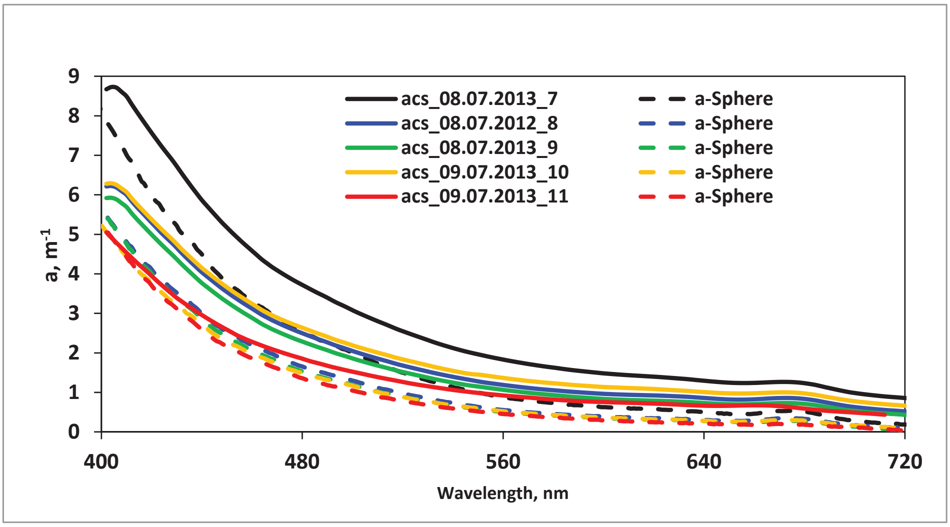

Figure 5. AC-S and a-Sphere station average absorption coefficients of water constituents' measurements from the Lake Peipsi in July 2013

It is also important to know how the absorption coefficient behaves in the water column. The mixed layer of the Baltic Proper is typically around 25–30 meters in the summer period (Elken & Matthäus, 2008). Most of the coastal stations were in much shallower water. The water column was usually well mixed in the Estonian coastal areas (Article IV), as can also be seen in Muhu Väin stations 1–3 on Figure 6. This means that the concentrations estimated from remote sensing signal are valid for the whole mixed layer. Results from Matsalu Bay (Mat 3, Figure 6) show that the water column consists of two layers: strongly absorbing river Kassari waters on top, and less absorbing marine waters below it. In this location the optical depth (from which originates the signal captured by remote sensing sensors) was less than the physical thickness of the top layer. This means that the concentrations retrieved from that signal were not representing the whole water column. For the bigger rivers, this effect can be visible far from the river mouth, as can be seen on Figure 7. The river Danube waters were still not mixed with the Black Sea waters 25 km offshore. Brodie et al. (2010) have shown a potential river input induced phytoplankton bloom even 150 km offshore. Problems related to strong stratification occur not only near rivers. Unlike other phytoplankton, cyanobacteria can regulate their buoyancy and migrate to the water depth optimal for their growth. In calm weather this may result in a very strong stratification close to the water surface. In sunny and hot conditions the maximum biomass layer may be a few meters below the water surface, but lower illumination creates optimal condition just below the water surface. The situation, where the maximum amount of cyanobacteria is concentrated to a depth of few meters, results in maximum values of the absorption and attenuation coefficients peaking at the same depth (Figure 11 in article IV).

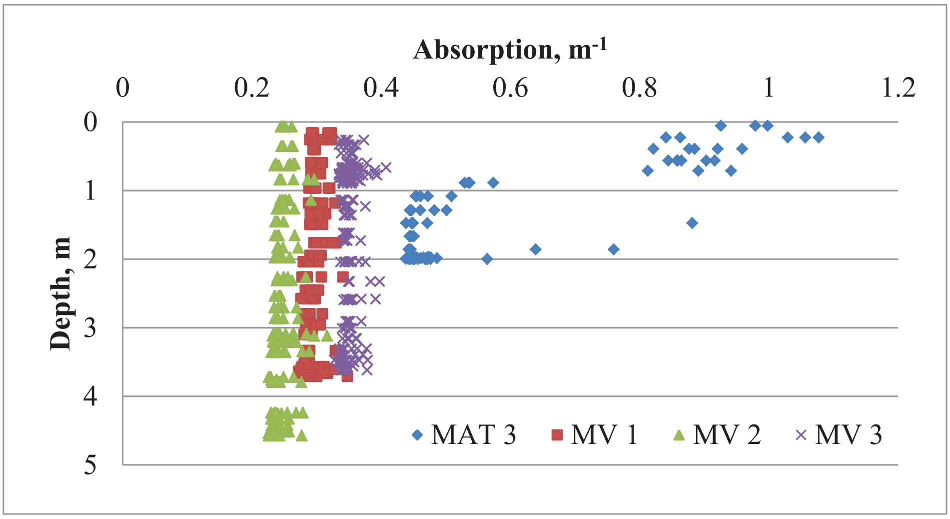

Figure 6. Vertical distribution of the absorption coefficient of water constituents at 665nm. MV stands for Muhu Väin and MAT for Matsalu bay

Figure 7. Surface effect on the Black Sea by the Danube river (water on the left side of the photo), 25km away from its mouth. Picture is taken 17.06.2016

In strong bloom, it means that water properties below the bloom layer cannot be studied by remote sensing. On the other hand, this also means that the data collected with flow through instrument does not represent the actual bloom conditions in the sea (Kutser, 2004). For example, the flow-through (FerryBox) systems on ships of opportunity take water from about 5 m depth whereas the whole cyanobacterial biomass is often above this layer and the rest of the water column is relatively clear. Moreover, in the last phases of blooms cyanobacteria lose their buoyancy and form surface scum. No water properties can be estimated through the scum. Estimating biomass of the scum is also not possible as the thickness of the scum is unknown, but also because the surface layer chlorophyll-a may be completely decomposed in bright sunlight while the scum itself may contain plenty of chlorophyll-a.

During the next phases of the study, specific absorption of particles needs to be measured as many radiative transfer models use this as their step towards concentrations. It is important to Figure out how different these variables are and how the changes affect the reflectance. The specific absorption of phytoplankton can vary strongly within the same location during one vegetation period, as seen in Figure 8. Sampling station under investigation was in Lake Peipsi and the measurements were taken during the year 2015.

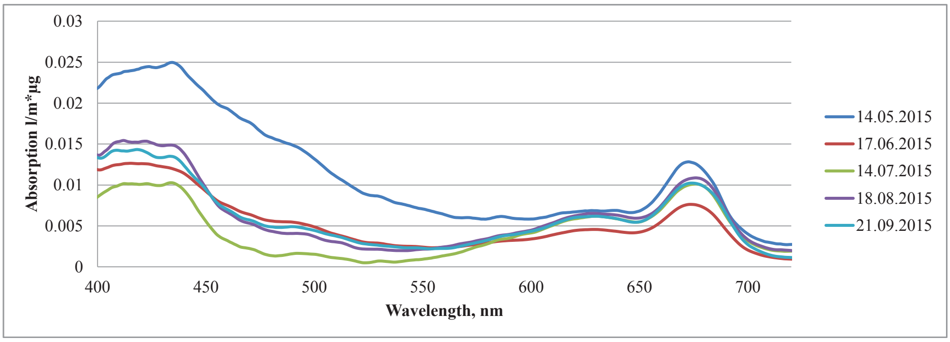

Figure 8. Phytoplankton specific absorption coefficient in station 11 in Lake Peipsi in the year 2015

Not only the absolute values of backscattering change due to the changes in its concentration, but also the spectral shape of backscattering may change (Article IV). For example, the organic to mineral ratio in the suspended matter impact the backscattering as these particles scatter light differently (Article IV).

The overall results of backscattering can be seen on Figures 8 and 9 in article IV. The Estonian coastal area covered the same variability (Figure 9) that was in the factor of 5 even if the most extreme samples are removed.

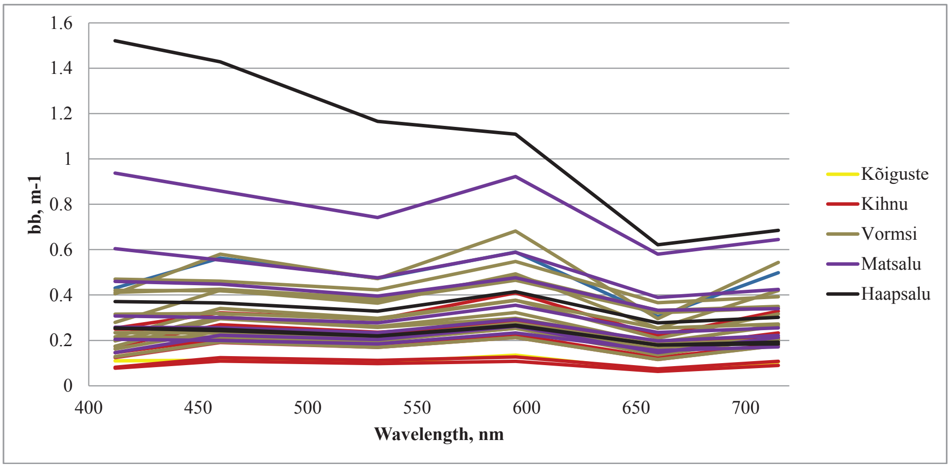

Figure 9. Station average backscattering coefficients of water constituents from 5 regions at the Estonian coast

The MVSM, built in Tartu Observatory, was tested in the field conditions for the first time in the Black Sea in 2016. Although the device is still going through the development phase, it is possible that the device can be used for the Baltic Sea in 2017. The fieldwork at the Black Sea was conducted at the coastal areas in Romanian and Bulgarian waters. The water properties of this area are strongly influenced by incoming rivers and depth changes (water depths at stations varied from 20 to 1400 meters). The optically different waters, where Secchi depth varied from 0.8 to 15 meters, provided necessary input for the device's development. The MVSM measurements stability was confirmed with the series of measurements with MQ water throughout the campaign. The MVSM managed to measure also the samples of more absorbing waters (Secchi depth less than 1 meter) that suggests the device is not only capable of measuring oceanic waters but also lacustrine waters like the Lake Peipsi. The results from station 64 in the Black Sea are shown as an example in Figure 10. More information about the cruise can be found in article V.

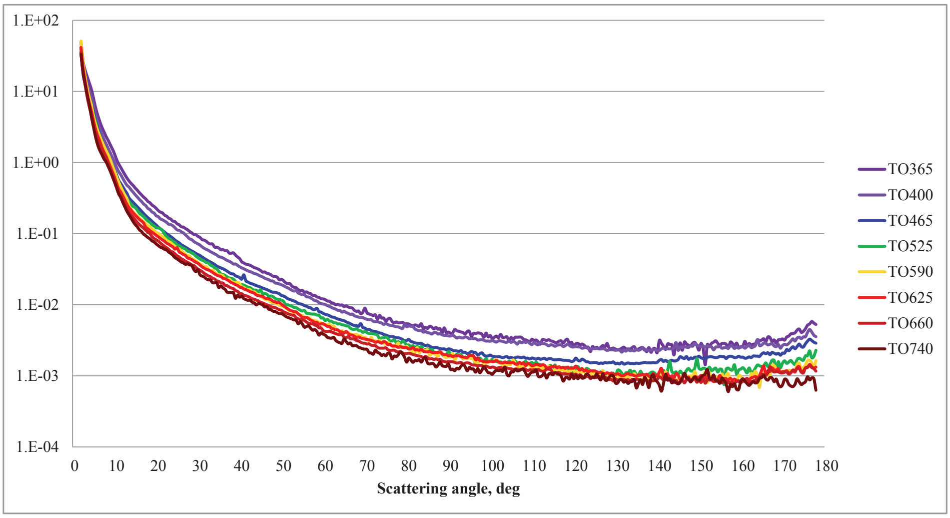

Figure 10. Angular distribution of VSF in the Black Sea station 64. Latitude 44.0002 and longitude 28.8870

4.2 Comparisons of reflectance measurements methodologies

Measurements made with three sensor setups (WISP-3 and RAMSES 3) provided similar results (Article I). Exactly the same results are impossible to achieve even with perfect calibrations because the sensors cannot look at exactly the same area of water and sky. There is also difference in area under investigation as RAMSES radiance sensors have 7 degree viewing angle whereas WISP-3 radiance sensors have a 3 degree viewing angle. The latest results show, however, that WISP-3 is underestimating the reflectance values, after all the corrections (Figure 11). The values registered by WISP-3 were lower for sky irradiance and water leaving radiance measurements when all three sensors are compared. The sensor measuring the sky radiance was showing similar results to the RAMSES instrument (Figure 12). It may have been that the calibrations for the two underestimating sensors was a bit off and a new calibration will bring the results of the reflectance measurements closer to the RAMSES measurements. This will be tested before the new field season.

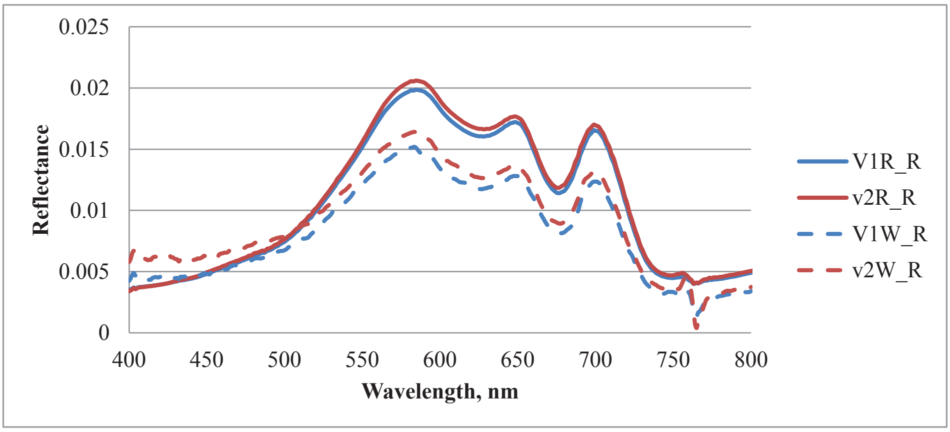

Figure 11. Example of WISP-3 underestimating the reflectance compared to the 3 sensor RAMSES setup on Lake Võrtsjärv. R stands for RAMSES and W for WISP-3 measurements

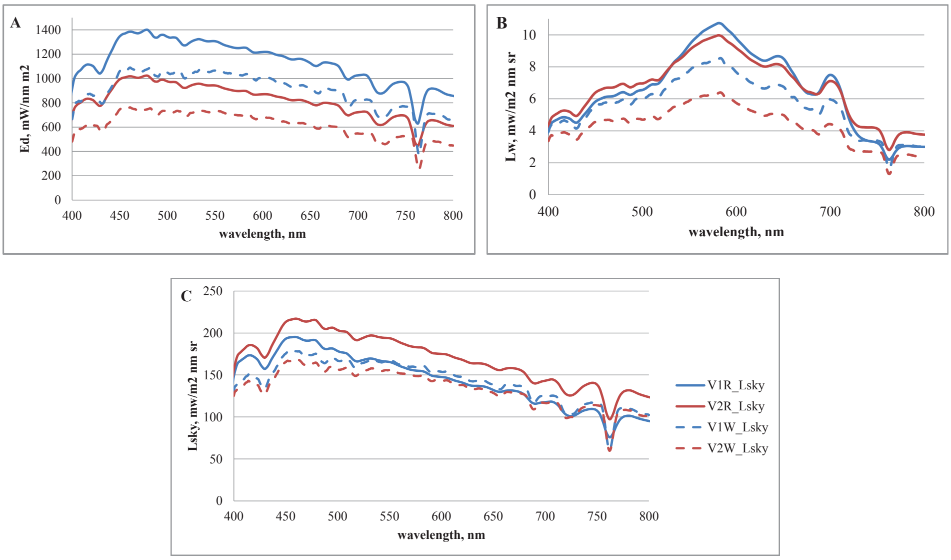

Figure 12. Comparison of three sensors for WISP-3 and RAMSES set-up at two Lake Võrtsjärv stations. R stands for RAMSES and W for WISP-3 measurements. A is irradiance, B is water leaving radiance and C sky radiance.

The similar underestimation of the signal can also be seen when WISP-3 was compared to the two sensor RAMSES setup (Figure 13). Note that these RAMSES sensors were not the same as the ones used in the three sensor setup. One important aspect that was pointed out in article I, is that the weather conditions make a great impact to possible measurements and different instruments can handle these conditions differently. One reason is that when the same amount of measurements or the same timeframe is used for averaging into one output spectrum, then instruments with higher sensitivity or bigger field of view are having shorter measurement time or larger number of measurements available. For example, as shown in the article I, the root mean square error (RMSE) difference between WISP-3 and RAMSES 3 sensor setup was only 1-3%, when measurement conditions were perfect, but with worse conditions, this error increased to around 20%.

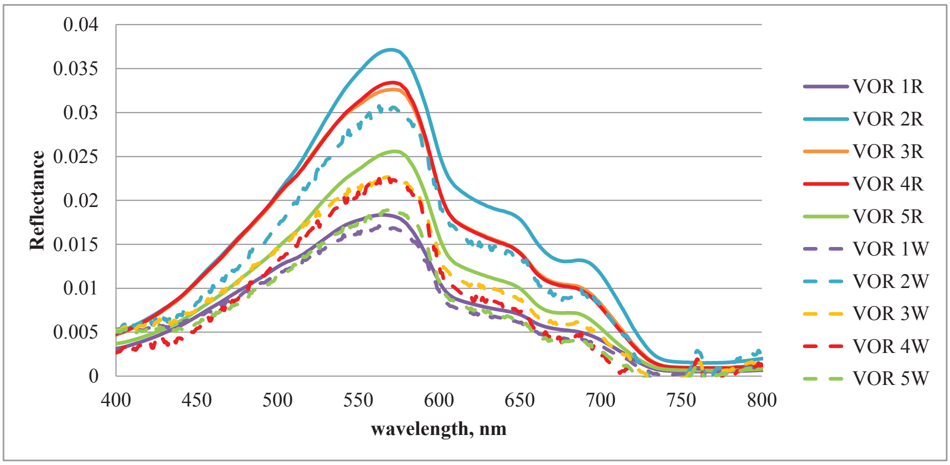

Figure 13. Example of WISP-3 underestimating the reflectance compared to the RAMSES setup at five stations near Vormsi Island.

The results showed that different instruments can provide similar results when following the same measurement protocols. However, the calibration of each instrument has to be up to date. This is extremely important with WISP-3 as its outputs are concentrations of chlorophyll-a, suspended matter, attenuation coefficient, and cyanobacterial pigment phycocyanin that are calculated with simple band ratio algorithms directly from the reflectance. Thus, users will get wrong outputs even without knowing this, if there are any calibration problems of the instrument. The target market of WISP-3 includes municipal agencies that often do not have the knowledge and skills needed to calibrate the device or may not be aware about the potential errors and need in calibration.

4.3 Empirical algorithms testing

The results for all the algorithms tested within this study are presented in articles II and III. For example, it is shown in article III that widely used approaches for ocean waters, like OC4v6 algorithm based on blue-green ratio (Anon, 2015), do not work in the Baltic Sea. This is not surprising and is one of the reasons why the scientific community treats natural waters as case-1 (optically simple waters where CHL is defining all water properties) and case-2 (optically complex). On the other hand, it was surprising that the algorithm produced for Baltic Sea southern area (Kowalczuk, et al., 2005) performed badly for the central Baltic. This also proves, that there is still work to do, to find even regional algorithm that provide stable results and the algorithms suggested in articles II (use of the reflectance peak at 710nm) and III (R705/R675 for CHL; R705 for TSM; and R665/R490 for CDOM) for Sentinel-2 and Sentinel-3 need to go through thorough validation, before these can be used for public products. One algorithm that was published already decades ago (Yacobi, et al., 1995) is still looking to future in remote sensing point of view (Figure 14). It is using the spectral range up to 850 nm. Very few satellites have spectral bands in the 850 nm region as in clear waters reflectance is assumed to be zero already below 700 nm and in phytoplankton rich waters reflectance becomes negligible at around 750 nm, except at certain wavelengths like 810 nm (Article II). The Baltic Sea has a strong seasonal component in the phytoplankton composition and it was clear from the modelled data that this seasonality has its effect on reflectance values. The spring bloom is dominated by diatoms and the summer bloom, typically in July-August, is dominated by cyanobacteria. Therefore, many Baltic Sea remote sensing studies (Kutser, 1997; Simis et al., submitted) suggest, that different remote sensing algorithms may be needed during the two distinct seasons for better performance of remote sensing. Results of this study showed the same (red and blue points on Figures 13–15). Nevertheless, there are algorithms that can produce reasonable results over the entire vegetation period as can be seen below.

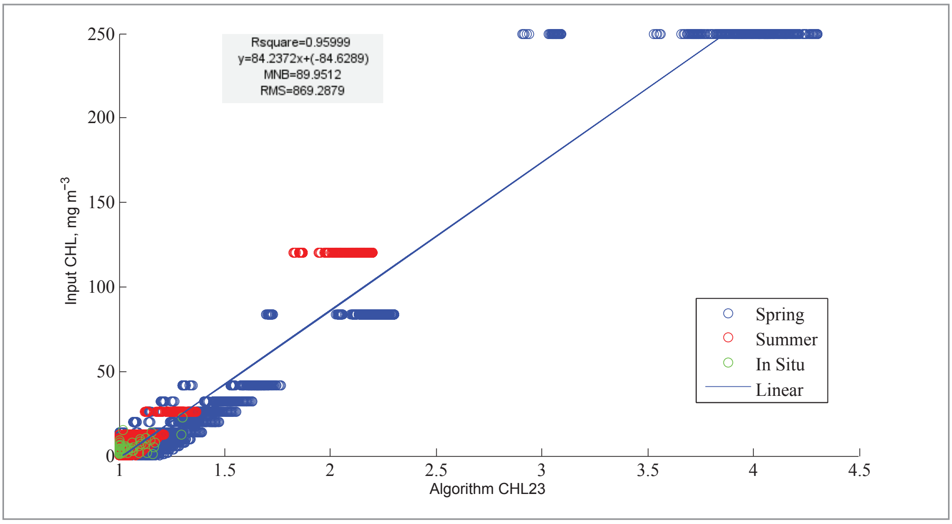

Figure 14. Correlation between the chlorophyll algorithm No. 23 (Rmax(670–850)/R670) (Article II) and chlorophyll concentrations measured in situ (for green circles) or used in the model simulations (red circles-summer and blue circles-spring samples).

The best results for the TSM retrieval were obtained with algorithm introduced in article II. However, this is based on the spectral region from 770 to 840 nm and there are no currently available satellites that have appropriate bands to use this algorithm. Sentinel-2 MSI has a band at 783 nm that captures part of the peak, but suitability of this band has to be tested further before any conclusions can be made. NASA is planning the HyspIRI mission (expected launch 2022) that would have a band in that region (Devred, et al., 2013). This mission should be suitable for water remote sensing (Hestir, et al., 2015). Meanwhile, hyperspectral data (airborne or ship borne) has to be used to capture the 810 nm peak. Results from this study recommend using the algorithm from Härma et al. (2001) that is based on red part of the spectrum when current satellite sensors are used. It means that this algorithm should also provide reasonable results for CDOM rich lakes besides the Baltic Sea coastal areas. One thing that makes it harder to retrieve TSM concentration in the Baltic Sea is the variation in TSM composition (article IV). In the open parts of the sea most of the TSM is phytoplankton and its degradation product detritus while in the coastal areas the TSM may be dominated by mineral or organic particles of terrestrial origin. Optical properties of these groups are quite different and may vary even within each group complicating the retrieval of the TSM.

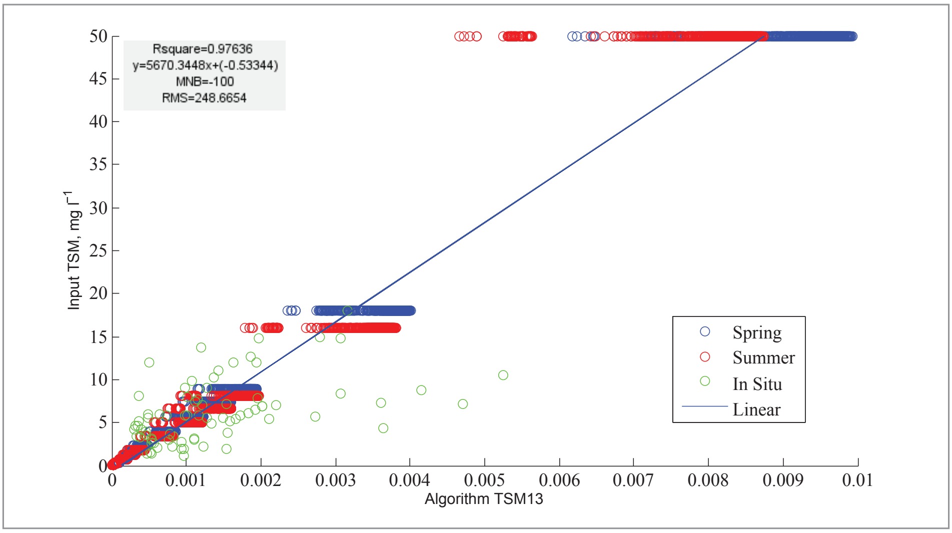

Figure 15. Correlation between TSM algorithm No. 13 (R705-R754) (Härmä, et al., 2001) and the TSM values used in model simulations (red circles-summer and blue circles-spring samples) or measured in situ (green circles).

The absorption of CDOM is the strongest in the blue part of the spectrum and decreases with increasing wavelength. When the CDOM concentrations are not very high then the absorption in the red region is negligible and blue to green ratios are used for CDOM retrieval (Doxaran, et al., 2004; Kowalczuk, et al., 2005). In more CDOM rich waters the signal in the blue is very low due to CDOM itself and phytoplankton that absorbs also in the blue part of spectrum (maximum around 430 nm). Meaning the blue to green ratios (used in oceans for chlorophyll-a retrieval) are not useable for neither chlorophyll nor CDOM retrieval. In such waters green to red band ratios have to be used for CDOM retrieval (Ammenberg, et al., 2002; Kutser, et al., 2005; Menken, et al., 2006; Kallio, et al., 2008; Olmanson, et al., 2016). In more extreme cases, like the CDOM rich lakes presented in article II, the signal in almost entire visible part of the spectrum becomes negligible and estimating CDOM concentration from remote sensing data becomes complicated, if not impossible. Optical properties of the Baltic Sea are also CDOM dominated. Therefore, it was a bit surprising that the best results were obtained with an algorithm using blue to red ratio (Article III). However, it must be noted that most of the data used in the analysis was modelled with HydroLight and did not contain glint. In real life the marine signal contains a lot of glint and the glint signal is strongest in the blue. The atmospheric correction is the most difficult in blue, where the atmospheric contribution to the measured signal is the highest. Also calibrating the sensors in blue is the most complicated as many light sources used for calibration do emit very little blue light, but the Sun, on the other hand has maximum emission in blue. Consequently, it will be very difficult to get results comparable to the modelling exercise when real Baltic Sea reflectances are used. Therefore, the results from this study suggest using the red to green band ratio for retrieval of CDOM. The algorithm from Ammenberg et al. (2002) and in many similar lake CDOM remote sensing papers (Kutser, et al., 2005; Menken, et al., 2006; Kallio, et al., 2008; Olmanson, et al., 2016) with slightly variable central wavelengths (depending on the sensor used in each of the studies) gave similar results to the best blue-red ratios (Figure 16).

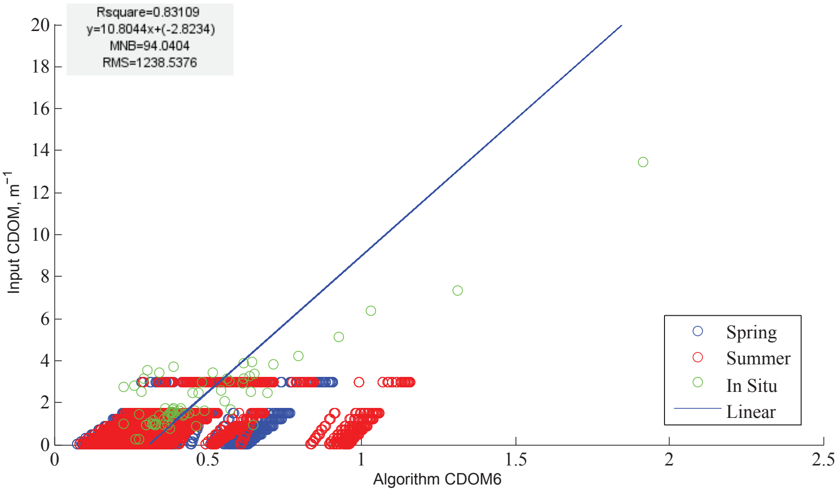

Figure 16. Correlation between CDOM algorithm No. 6 (R664/R550) (Ammenberg, et al., 2002) and the CDOM values used in model simulations (red circles-summer and blue circles-spring samples) or measured in situ (green circles).

At present the Copernicus Land Service is not providing any water quality products as the inland water part is in the very early stages of development. The marine service, CMEMS, has quite long legacy as it is based on the MyOcean and MyOcean-2 projects. Despite that, the CMES provides only two validated near real time products (chlorophyll-a and reflectance) and one reanalysis product (chlorophyll-a) for the Baltic Sea. To a certain extent, the results of this PhD study contradict with the CMEMS findings. For example, several band ratio type algorithms were found that had very high (r^2 up to 0.96) correlation with chlorophyll-a while the CMEMS chlorophyll-a product has a very low correlation ($r^2=0.20$) with measured chlorophyll-a. Moreover, the CMEMS chlorophyll-a reanalysis product is using a blue-green band ratio known not to work in optically complex waters, especially in the Baltic Sea, where the signal in blue is determined by the amount of CDOM and the impact of chlorophyll-a is negligible (Härma, et al., 2001; Darecki & Stramski 2004; Darecki, et al., 2005; Koponen, et al., 2007). The CMEMS chlorophyll-a reanalysis product had correlation with in situ data that is not high ($r^2=0.45$), but still significantly better than our results ($r^2=0.005$) despite mainly modelled reflectance was used that should provide better results than the actual in situ data. To a certain extent, these discrepancies can be explained by the different study area. The CMEMS uses Kattegat and Skagerrak data to validate its Baltic Sea products. These waterbodies are actually optically very different from the Baltic Sea. This may explain the much better performance of the clear ocean chlorophyll-a algorithm in the CMEMS reanalysis product than our results or other Baltic Sea remote sensing studies show (Darecki & Stramski 2004; Darecki, et al., 2005). The modelling results used in the thesis were also for the open parts of the sea, but all the Baltic Sea in situ data was from coastal waters. The CMEMS validation data comes from large research vessels that cannot go close to the shore. Our data was collected from smaller boats and often in coastal areas not accessible by large ships. Therefore, the optical properties of waters used for validation of the CMEMS products and used in this study were very different. It must be also noted that the CMEMS products do not cover the actual coastal areas where this study was carried out. In order to avoid mixed pixels the satellite data collected close to islands, islets or shallow areas has to be masked out. Meaning that the CMEMS products start many kilometres from the shore or archipelago areas, especially in the case of 4×4 km reanalysis products. Consequently, the in situ study area of this study and the part of the Baltic Sea covered by CMEMS products are different (except for the modelled reflectances) and complete match cannot be expected. It was also shown that there are other products (CDOM and TSM) that can be estimated in lakes and the Baltic Sea using different algorithms (Article III). These products are not currently provided by any Copernicus services.

CONCLUSIONS

Three different set-ups of radiometers were tested to measure water leaving reflectance. Two of these devices used instruments from the same company just in different setup. The approaches resulted in slightly different reflectance values. If the measurement procedure was correctly followed and the conditions were not too rough, then the values of different approaches were coherent allowing using them for water quality monitoring and/or for validation of satellite measurements. The variation within a satellite pixel is usually greater than the differences between the two in situ sensors (as long as the calibrations are up to date). However, the differences between the reflectance spectra obtained with different sensor set-ups need further investigation.

The absolute values of IOPs in the Baltic Sea vary over one order of magnitude. Examples from Swedish coastal areas are more similar to the open parts of the sea. The variation in IOPs in sandy and shallow areas from Estonian coast was much higher and the IOPs differ significantly from the open Baltic Sea waters. The difference comes most probably from the bottom and coastline structure. Swedish waters are mostly deep not allowing resuspension of sediments in windy conditions. Meaning that the suspended matter in Swedish waters is primarily phytoplankton while in Estonia it is a mixture of phytoplankton and mineral particles. Mineral particles may even dominate in shallow areas in windy days. The results suggest that the same remote sensing algorithms can be used for open parts of the Baltic Sea and rocky shores with deep water (Sweden and probably Finland), but not in shallow sandy shores (Estonia and probably Latvia, Lithuania, Russia, Poland, Germany and Denmark).

The new Multispectral Volume Scattering Meter, developed in Tartu Observatory, enables measuring scattering in water with the angular resolution that is not possible with any other in situ measuring device. Although the device is not yet production ready, then after some design flaws and calibration issues are overcome, then it is possible to use the prototype to measure VSF values in the Estonian waters and compare those with the modelled values. Something that has not been done before.

Our and previous studies have shown that the optical properties of phytoplankton assemblages present in the Baltic Sea and lakes in spring and summer are quite different. This suggests that either different algorithms have to be used for different seasons or analytical methods coping with the whole range of optical variability have to be used. It was shown that the seasonal variability in the coefficients of algorithms exists. However, several empirical algorithms that work reasonably well during the whole ice free season were found.

We have shown that in optically dark waters NIR part of the spectrum can be used to retrieve info about water constituents. The results show that in the extreme CDOM rich waters, the reflectance signal in the visible part of spectrum is too weak to retrieve information about CDOM. Surprisingly, it is possible to estimate the amounts of CHL and TSM using the signal at longer wavelengths, namely at 810 nm. The peak around 810 nm was present in all our measurements (also in the Baltic Sea). Most remote sensing scientists ignore the signal at wavelengths longer than 750 nm. Even if the reflectance data has been presented for longer wavelengths in some papers then it was not used in any way. Based on this study, these wavelengths should not be ignored and, if possible, a satellite sensor channel around this area should be implemented. For the black lakes, the 810 nm peak is preferred for phytoplankton (chlorophyll-a) retrieval as the signal at 710 nm (typically used for chlorophyll-a retrieval) is significantly affected by CDOM. It was also found that the height of the 810 nm peak allows to estimate chlorophyll-a, if the particles in water are primarily phytoplankton (like it is in many lakes).

Some of the simple empirical algorithms for calculating CHL, TSM and CDOM provided very good results for the Baltic Sea, especially when computed from modelled data. There were also approaches that were promising for the total vegetation period. However, it is still recommended to use different algorithms for spring and summer periods, as the species composition, including the dominating species, is not the same for these two seasons. The good results obtained with the simple algorithms mean that these can be used for real time concentration retrieval with in situ devices (like WISP-3), especially when the algorithms are regionally tuned. This information can then be used to decide whether additional measurements or samples are needed. For example, the collection of in situ samples (that are expensive and time consuming to analyse) is only carried out when something extraordinary is observed with a remote sensing device. Another alternative is using remote sensing devices on monitoring vessels in transect mode. Then the locations of in situ sampling stations can be decided based on the remote sensing products. Laboratory analyses are expensive and ships/boats are mostly rented with hourly-rate. This way, the cost of a monitoring or research cruise can be reduced or the money is spent more efficiently.

The number of lakes or coastal sampling stations is usually low in national monitoring programs due to the limited budget and manpower. Using WISP-3 like devices, that are easy to handle and give a concentration output immediately after the measurement, a large number of stations could be measured during a short period of time. Consequently, the number of expensive analysis can be reduced and the number of stations in the program and or the measurement frequency can be increased. This is especially useful when cyanobacterial blooms are expected to emerge. Frequent measurements allow warning general audiences (or fish farmers) about the appearing threat. OLCI on Sentinel-3A provides data about Estonia on two out of three days and the launch of Sentinel-3B will double the number. The MSI on Sentinel-2A provides data every 4–5 days, but the launch of Sentinel-2B will allow to get 10 m resolution free imagery every second day. Thus, the near real time monitoring of lakes and coastal waters, where the 10–20 m spatial resolution is necessity, will become possible in the very near future. “Hand held” radiometers on buoys, jetties, ships, boats or hands of scientists will play crucial role in calibration of these new satellites data and validating the satellite products. However, the hand held radiometers allow filling in the data gaps occurring due to the cloud cover (frequent at our latitude) and can be effectively used as water quality monitoring tools in their own right.

As the title indicates, the focus of this study was on the use of close range remote sensing in coastal and inland water quality research and monitoring. However, the data collected will be very valuable for product development of both Copernicus land and marine services. The reflectance data collected allows calibrating satellites and improving atmospheric correction methods while the concentrations and underwater optical data will allow better understanding of the formation of remote sensing signal in coastal and inland waters. Consequently, this study contributes to the developing of robust remote sensing products for coastal and inland waters that will be useful for scientists and water quality managers.

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SUMMARY IN ESTONIAN

Lähi-kaugseire meetodite arendamine veekogude seisundi hindamiseks

Veekogude kvaliteedi hindamine on inimkonnale oluline olnud juba tuhandeid aastaid. Vee kehv kvaliteet on põhjustanud palju terviseprobleeme ja seetõttu keskenduti esialgu nendele veekogudele, kust ammutati joogivett. Kuigi puhta joogivee kättesaadavus on globaalses skaalas endiselt suur probleem, siis arenenud riikides on olukord selles vallas piisavalt hea, mistõttu on tähelepanu pööratud kõikidele veekogudele, juhtides tähelepanu nii bioloogilisele mitmekesisusele kui ka jätkusuutlikusele. Euroopa Liidus on veekogude kvaliteedi hindamise aluseks kaks dokumenti: Euroopa Liidu veepoliitika raamdirektiiv (allkirjastatud aastal 2000) ja Euroopa Liidu merestrateegia raamdirektiiv (allkirjastatud aastal 2008). Mõlemad dokumendid seavad sihiks saavutada Euroopa veekogude „hea“ konditsioon aastaks 2020.

Sõltumata millisest suurusest alates lugeda veekogu järveks, on nii maailmas kui Euroopas nende hulk liiga suur, et riiklikud seireprogrammid suudaksid nende kõigi kohta ülevaadet anda. Lisaks koguvad sellised programmid andmeid proovivõtupunktide tasemel, millega ei saa ülevaadet terve veekogu dünaamikast. Läänemere puhul jääb sellistel juhtudel uurimispiirkonnast välja kogu rahvusvaheline tsoon. Rohkemate veekogu seiramiseks ja kogu veekogust ülevaate saamiseks tuleb appi võtta kaugseire.

Pärast pikka teadus- ja arendustegevust on Euroopa Kosmoseagentuur (ESA) Copernicus programmi raames orbiidile lähetanud esimesed Sentinel seeria satelliidid. Veel olulisem on otsus samasuguste satelliitide jätkuvale orbiidile lennutamiseks. Programmis on mitu erinevat satelliiti, millest veekogude seireks pakuvad enim huvi Sentinel-2 ja Sentinel-3 seeriad. Eesmärgiks on võetud, et igal ajahetkel peaks orbiidil olema vähemalt kaks ühe seeria satelliiti, mis tagaks piisava katvuse ja ajalise järjepidevuse. Kuivõrd mikrolaineline kiirgus ei ole võimeline tungima veesambasse, siis ei ole võimalik kasutada selle programmi radarsatelliite ja tuleb piirduda elektromagnetkiirguse nähtava spektriosaga.

Satelliiditulemeid saab kasutada ainult määral, mis on valideeritud maapealsete spektraalmõõtmistega. Selleks eesmärgiks kasutatavad sensorid on juba kujunemas täiesti iseseisvateks seirevahenditeks ning neid paigaldatakse nii poidele, kauba- ja reisilaevadele, ning on võimalik operatiivselt kasutada soovitud asukohtades.

Arendamaks selliste seadmete võimekust valideerida satelliidiandmeid, anti käesoleva töö käigus hinnangu järgnevatele küsimustele:

- Kui palju mõjutab Läänemere erinevates osades otseste optiliste omaduste varieeruvus peegeldustegurit ja seeläbi kaugseiresignaalist vee koostisosade määramist?
- Kas võib oodata sarnast peegeldusteguri tulemit, kui kasutatakse erineva ehitusega sensoreid?

- Kas lähisinfrapunane spektriosa on kasutatav vee koostisosade määramiseks optiliselt keerukates vetes?
- Kas lihtsate kanalisuhte algoritmidega on võimalik hinnata Läänemere karakteristikuid (klorofülli, heljumi ja lahustunud orgaanilise aine kontsentratsioon) või peab kasutama analüütilisi meetodeid.
- Kas käsispektromeetritel on rohkem rakendusi või sobivad nad ainult sateliiditulemite valideerimiseks?
- Kas Tartu Observatoorium on suutnud ehitada välitöödel kasutatava hajumismõõtja, mis suudab mõõta kogu nurkjaotust, samas kui teised sarnased seadmed on ainult laboris mõõtmiseks või suudavad mõõta üksikutes nurkades?

Töös leiti, et Läänemere optilised omadused varieeruvad enam kui kümme korda. Pehme merepõhjaga Eesti rannikuvetes on varieeruvus suurem kui graniitse põhjaga Soome ja Rootsi rannikuvete erinevus Läänemere avaosast. Lisaks tugevale jõgede sissevoolule mõjutab varieeruvust ka veekihi väike sügavus, mistõttu tekitab tuul pidevat resuspensiooni põhjakihist pinnalähedasse kihti. Kui valdav osa kaugseirealgoritme eeldab vees oleva heljumi ühtlast jaotust mineraalse ja orgaanilise fraktsiooni vahel, siis Eesti rannikuvetes on ka see suhe äärmiselt muutuv, mis mõjutab omakorda ka veest väljuvat kiirgust ja sellega ka peegeldumisspektri väärtusi.

Uurimistöös testiti kolme erinevat seadmete komplekti (WISP-3 ja kaks erinevat TriOS RAMSES komplekti) peegeldumisteguri mõõtmiseks. Kuigi oodatult andsid kõik need veidi erinevaid tulemusi, oli see erinevus niivõrd väike, et sateliidisensori ühe piksli sees võiks üldjuhul oodata isegi suuremat variatsiooni, seega võib antud uurimistöö põhjal soovitada erinevate instrumentide kasutamist, juhul kui jälgitakse korralikult mõõtmisprotokolle ja seadmete kalibratsioonid on ajakohased.

Kaugseirealgoritmid kasutavad sisendina elektromagnetkiirguse nähtavat osa, sest lühemad lainepikkused on neelatud juba atmosfääri poolt ja pikematel lainepikkustel on probleemiks puhta vee enda neeldumine. Optiliselt keerukates järvedes on tihti väga kõrge lahustunud orgaanilise aine konsentratsioon, mis tähendab, et selles spektripiirkonnas puudub piisav signaal arvutuste adekvaatseks teostamiseks. Uurimustööst selgus, et sellistel juhtudel on vee koostisosade hindamiseks võimalik kasutada peegeldumisteguri väikest maksimumi 810 nm juures. Vastupidiselt ootustele andis see sama lähenemine häid tulemusi ka Läänemeres, kus lahustunud orgaanilise aine poolt põhjustatud neeldumine on märkimisväärselt väiksem.

Kuigi varasemalt on näidatud, et fütoplanktoni koosseis ja seetõttu ka optiline signaal Läänemeres on sesoonselt erinev, siis antud töös on tuvastatud ka lihtsaid kanalisuhte algoritme, mis võimaldavad rahuldaval tasemel hinnata vees sisalduvate ainete (klorofüll, heljum, lahustunud orgaaniline aine) kontsentratsioone kogu vegetatsiooniperioodi jooksul. Sellegipoolest on soovitatav võimalusel kasutada aastaajapõhiseid algoritme. Töö tulemusena leiti kanalisuhte algoritme mida on võimalik rakendata satelliidiandmetele. Eelistatum oleks olukord, kus need algoritmid on sisendiks rohkem arvutusvõimsust nõudvatele analüütilistele mudelitele, sest kui piirata võimalike väljundite vahemikke, väheneb oluliselt ka vajaminevate iteratsioonide arv ja need lähenemised oleksid kiiremad. Samuti saab neid algoritme kasutada käsispektromeetrites reaalajas tulemite andmiseks.

Lisaks sateliidisensorite valideerimisele, on käsispektromeetritel oma roll ka seireprogrammide ja -agentuuride igapäevatöös. Sellised seadmed muutuvad järjest odavamaks ja lihtsamini kasutatavaks ning võimaldavad saada kiirelt esmase ülevaate, mille põhjal on võimalik otsustada laboriproovide võtmise vajalikkus. Viimased on kõige ajamahukamad ja kulukamad etapid veekogude seireprogrammides. Laborimõõtmisi vähendades on seireprogrammidesse võimalik kaasata rohkem veekogusid ja sama aja jooksul on võimalik ülevaade saada oluliselt rohkematest veekogudest.

Kuigi Tartu Observatooriumis valminud vee hajumismõõtja prototüüp ei ole veel täielikult tootmiskõlbulik, siis võimaldab see välitingimustes mõõta vee hajumist mahus, mida teised välitööde seadmed ei suuda. Pärast teatud muudatusi seadme disainis saab eeldatavasti juba 2017. aasta suvel sooritada mõõtmisi Eesti vetes, kogudes seega vee hajuvuse mudelarvutustega võrdlemiseks andmeid, mida varasemalt siinses regioonis tehtud ei ole.

ACKNOWLEDGEMENTS

This study was supported by the Republic of Estonia Ministry of Education and Research grants SF0180009As11 and SF0180009Bs11, Estonian Science Foundation Research Grant ETF7725, the BONUS program project FerryScope, the European Comission programs GLaSS and WaterS; and the Finnish national project EOMORE.

I am deeply grateful for my supervisors, Dr. Tiit Kutser and Dr. Anu Reinart, who invested a huge amount of time and effort over the years to counsel me on my way to becoming a scientist.

I would like to thank my colleagues in Tartu Observatory and Estonian Marine Institute, as without them, there would not be enough data and discussion in order to complete this thesis. For the same reason I would like to send out my gratitude towards my international partners, especially the group from SYKE, Finland.

Finally, I would like to point out the fact that this thesis would still be a work in progress, unless my little daughter Marta, with help from my wife Teele, would not have provided me with the necessary motivation boost to get my act together!

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Publications:

Ligi, M., Kutser, T., Kallio, K., Attila, J., Koponen, S., Paavel, B., Soomets, T., Reinart, A. (2017). Testing the performance of empirical remote sensing algorithms in the Baltic Sea waters with modelled and in situ reflectance data. *Oceanologia*, 598(1), 57–68, 10.1016/j.oceano.2016.08.002

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Other publications:

Ligi, M.; Kutser, T.; Paavel, B.; Reinart, A.; Kauer, T.; Vahtmäe, E. (2014). Läänemere rannikuvete optilised omadused. Aan, A.; Narusk, K. (Editors). *Kaugseire Eestis 2014* (12–21). Tallinn: Keskkonnaagentuur.

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DISSERTATIONES TECHNOLOGIAE CIRCUMIECTORUM UNIVERSITATIS TARTUENSIS

1. **Sille Teiter.** Emission rates of N_2O, N_2, CH_4 and CO_2 in riparian grey alder forests and subsurface flow constructed wetlands. Tartu, 2005, 134 p.
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