REMOTE SENSING IN OPTICALLY COMPLEX WATERS -water quality assessment using MERIS data

José M. Beltrán-Abaunza



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© José M. Beltrán-Abaunza, Stockholm University 2015 Cover image by Ana Sofia Beltrán-López Light in the ocean (9 years old)

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This thesis is dedicated to:

Marcela Ana Sofia y Andrea Nicole Marie

Mamá and Papá.

"The life of photons"

"If emission may be called, somewhat poetically, the birth of photons, absorption may be called their death, although their spirit (energy) lives on in whatever absorbs them".

Between birth (emission) and death (absorption) photons are scattered"

"Between birth (emission) and death (absorption) photons are scattered"

Craig F. Bohren (2006)

Abstract

This PhD study focusses on the use of ESA's MEdium Resolution Imaging Spectrometer (MERIS) data for reliable and quantitative water-quality assessment of optically-complex waters (lake, brackish and coastal waters). The thesis is divided into two parts: A. intercalibration of reflectance measurements in different optically-complex water bodies (Paper I), and validation of various satellite processing algorithms for the coastal zone (Paper II). B. Applications: the use of MERIS data in integrated coastal zone management mostly using Himmerfjärden bay as an example (Paper III and IV).

Himmerfjärden bay is one of the most frequently monitored coastal areas in the world and it is also the recipient of a large urban sewage treatment plant, where a number of full-scale nutrient management experiments have been conducted to evaluate the ecological changes due to changes in nutrient schemes in the sewage plant.

Paper I describes the development and assessment of a new hyperspectral handheld radiometer for in situ sampling and validation of remote sensing reflectance. The instrument is assessed in comparison with readily available radiometers that are commonly used in validation.

Paper II has a focus on the validation of level 2 reflectance and water products derived from MERIS data. It highlights the importance of calibration and validation activities, and the current accuracy and limitations of satellite products in the coastal zone. Bio-optical in situ data is highlighted as one of the key components for assessing the reliability of current and future satellite missions. Besides suspended particulate matter (SPM), the standard MERIS products have shown to be insufficient to assure data quality retrieval for Baltic Sea waters. Alternative processors and methods such as those assessed and developed in this thesis therefore will have to be put in place in order to secure the success of future operational missions, such as the Sentinel-3 sensor from the Copernicus mission from ESA.

The two presented manuscripts in the applied part B of the thesis (paper III and IV), showed examples on the combined use of in situ measurements with optical remote sensing to support water quality monitoring programs by using turbidity and suspended particulate matter as coastal indicators

(manuscript III). The article also provides a new turbidity algorithm for the Baltic Sea and a robust and cost-efficient method for research and management. A novel approach to improve the quality of the satellite-derived products in the coastal zone was demonstrated in manuscript IV. The analysis included, the correction for adjacency effects from land and an improved pixel quality screening. The thesis provides the first detailed spatio-temporal description of the evolution of phytoplankton blooms in Himmerfjärden bay using quality-assured MERIS data, thus forwarding our understanding of ecological processes in in Swedish coastal waters.

It must be noted that monitoring from space is not a trivial matter in these optically-complex waters dominated by the absorption of coloured dissolved organic matter (CDOM). These types of coastal waters are especially challenging for quantitative assessment from space due to their low reflectance. Papers III and IV thus also provide tools for a more versatile use in other coastal waters that are not as optically-complex as the highly absorbing Baltic Sea waters. The benefits of the increased spatial-temporal data coverage by optical remote sensing were presented, and also compared to in situ sampling methods (using chlorophyll-a as indicator).

Sammanfattning

Den här avhandlingen fokuserar på tillämpningen av den optiska sensorn MEdium Resolution Imaging Spectrometer (MERIS) från Europeiska rymdbyrån för en tillförlitlig och kvantitativ bedömning av vattenkvalité i optiskt komplexa vattentyper (såsom sjöar, bräckt- och kustvatten). Avhandlingen är uppdelad i två delar; där den första delen, A) behandlar interkalibrering av reflektionsmätningar i olika optiskt komplexa vattendrag (Artikel I), och validering av olika algoritmer satellit data inom kustområden (Artikel II) medan den andra delen, B) fokuserar på tillämpningar av MERIS data för en integrerad kustzonsförvaltning med Himmerfjärdens kustområde som huvudexempel (Artikel III och IV). Himmerfjärden är ett av de mest undersökta kustområdena i världen och är även recipient för ett stort urbant reningsverk. I området har ett flertal fullskaliga förvaltningsexperiment utförts för att utvärdera de ekologiska förändringarna som orsakats av utsläppen av näringsämnen från reningsverket.

Artikel I beskriver utvecklingen och utvärderingen av en ny handhållen hyperspektral radiometer för in situ provtagning och validering av reflektionsdata. Instrumentet granskades i jämförelse med sedan tidigare väletablerade radiometrar, vilka vanligen används inom satellitvalidering.

Artikel II fokuserar på validering av reflektions och vattenkvalitetprodukter som beräknats från MERIS data. Artikeln betonar vikten av kalibrering och validering med in situ data, och utvärdering av noggrannheten och begränsningar av satellitmetoden i kustzonen. Bio-optiska in situ data är en viktig komponent för att bedöma tillförlitligheten av nuvarande och framtida satellitprodukter. Förutom för suspenderat material (SPM), har MERIS standardprodukter visat sig vara otillräckliga för att säkerställa pålitlighet av Östersjöns vattenkvalitetsmätningar från rymden. De alternativa processorer och metoder som har utvärderas och utvecklats i den här avhandling var viktiga att kunna säkerställa för att att kunna säkra framgången av framtida operativa fjärranalysprogram, som t.ex. den kommande Sentinel-3 sensorn inom Copernicusprogrammet från Europeiska rymdbyrån.

De två presenterade manuskripten i den tillämpade delen (B) i avhandlingen , visade exempel på en kombinerad tillämpning av in situ mätningar och optiska fjärranalysdata. I artikel III utvecklades en ny algoritm för grumligheten i Östersjön och, som i kombination med fjärranalytiska metoder ger en robust och kostnadseffektiv metod för forskning och kustzonsförvaltning. Grumlighet och suspenderat material som använd som

indikatorer för vattenkvaliteten inom kustvatten och stödjer således de nationella övervakningsprogrammen (artikel III).

I artikel IV presenteras en ny metod för att förbättra kustzonsövervakningen med hjälp av satellitprodukter. I analysen ingick en korrektion för reflektion från land och en förbättrad screening av pixelkvalitet. Satellitbilderna ger en detaljerad rumslig och-temporal beskrivning av utvecklingen av växtplanktonblomningar i Himmerfjärden med hjälp av kvalitetssäkrade data, vilket förbättrar vår förståelse av de dynamiska ekologiska processerna i kustvattnen.

Det bör noteras att övervakning från rymden inte är en enkel företeelse eftersom optiskt-komplexa vatten domineras av absorptionen från färgat löst organiskt material (CDOM). På grund av deras låga reflektion är dessa typer av kustvatten utmanande, speciellt för en kvantitativ bedömning från rymden. Papers III och IV demonstrerar nya verktyg för en mer global tillämplig i andra kustvatten som inte år lika optiskt-komplexa som de vattentyperna i Östersjön. Fördelarna med den rumsliga och temporala datatäckningen med optisk fjärranalys diskuterar, och också jämfördes med in situ provtagningsmetoder (med hjälp av klorofyll-a som indikator).

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Abbreviations

Abbreviation	Description	Unit/version
CHL, chl-a	Phytoplankton pigments with Chlorophyll-a as	mg m ⁻³
	proxy	
SPM	Suspended particulate matter	g m-3
CDOM	Coloured dissolved organic matter	m-1
ESA	European Space Agency	
IOP	Inherent Optical Properties	
AOP	Aparent Optical Properties	
WISP-3	Water Insight spectrometer	
TACCS	Tethered attenuation coefficient chain-sensor	
TriOS	TriOS Ramses radiometer	
AERONET-OC	Aerosol Robotic Network-ocean colour	
MERIS	MEdium Resolution Imaging Spectrometer	
OLCI	Ocean and Land Colour Instrument	
MODIS	Moderate Resolution Imaging Spectroradiometer	
SeaWiFS	Sea-viewing Wide Field-of-view Sensor	
MERMAID	MEris Matchup In-situ Database	
FR	Full Resolution	
ENVISAT	ENVIronment SATellite	
MEGS	MERIS ground segment development platform	v.8.1
FUB	Freie Universität Berlin Water processor	v.1.2.10
C2R	Case 2 Regional	v.1.5.3
ICOL	Improved Contrast between Ocean and Land	v.2.9.1
VIS	visible light of the electromagnetic spectrum	
NIR	Near Infrared	
MIR	Mid Infrared	
TIR	Thermal Infrared	
Rrs	Remote sensing reflectance	sr-1
TOA	Top of Atmosphere	
SMHI	Swedish Metereological and Hydrological Institute	
NIST	National Institute of Standards and Technology	
NIOZ	Royal Netherlands Institute for Sea Research	
WFD	Water Framework Directive	
MSFD	Marine Strategy Framework Directive	
IAPSO	International Association of the Physical Sciences	
	of the Ocean	

Scope of the thesis

This thesis mainly focuses on satellite-based optical remote sensing, as it is applied for marine ecology. It covers topics from in situ radiometry to assess water quality, followed by image processing algorithms to validate water quality products in coastal waters of the Baltic Sea. Examples of applications for water quality monitoring, using turbidity, suspended particulate matter and a time series of chlorophyll-*a*, demonstrate the advantages in terms of spatial and temporal resolution and also provides tools for assessment of other coastal areas.

List of Papers

The following papers, referred to in the text by their Roman numerals, are included in this thesis.

Part A. Method development and validation

I. Hommersom, A., Kratzer, S., Laanen, M., Ansko, I., Ligi, M., Bresciani, M., Giardino, C., Beltrán-Abaunza, J. M., Moore, G., Wernand, M. and Peters, S. Intercomparison in the field between the new WISP-3 and other radiometers (TriOS Ramses, ASD FieldSpec, and TACCS). J. Appl. Remote Sens., 6(1), 63615 (2012). DOI: doi:10.1117/1.JRS.6.063615

Contributed to collection and lab analyses of field data during the international field campaign in Lake Vänern. TACCS deployment and its data processing (deriving reflectance). Co-write later versions of the manuscript and revisions.

II. Beltrán-Abaunza, J. M., Kratzer, S. and Brockmann, C. Evaluation of MERIS products from Baltic Sea coastal waters rich in CDOM. Ocean Science, 10(3), 377–396 (2014). DOI: doi:10.5194/os-10-377-2014.

Contributed to planning, collection and analysis of field data during the field campaign in 2010. Satellite data processing and analysis. Statistical analyses. Document writing/revision of the manuscript.

Part B. Algorithm development and applications

III. Kari, E., Beltrán-Abaunza, J. M., Harvey, E.T., Kratzer, S. Retrieval of Suspended particulate matter from MERIS data- Algorithm development and validation. Manuscript in review by Remote Sensing Environment.

Contributed to collection of field data during 2010, manuscript planning with major contribution to satellite data processing and analysis. Contribution to discussion of the results, co-writing of the manuscript

IV. Beltrán-Abaunza, J. M., Kratzer, S. and Höglander, H. Using MERIS data to assess the spatial and temporal variability of phytoplankton in coastal areas. Manuscript in preparation for International Journal of Remote Sensing.

Contributed to planning, satellite data processing and analysis. Data evaluation. Statistical analyses. Document writing/revision of the manuscript.

Reprints of the published articles were made with permission from the publishers.

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Introduction

"There is no single cause for the colours of the sea" Bohren (2001)

Sunlight drives the environment conditions in the aquatic ecosystem. It is the main source of heat that drives the ocean and atmosphere circulation. Light is one of the most important signals that organisms use to obtain information from their surroundings (Depauw et al., 2012). Light, directly or indirectly, affects most of marine organisms that rely on its energy to fuel their biological processes and set up their physical environment. It is a primary ecological factor of photosynthesis (Shirley, 1935; Thomas, 1955), especially for communities of aquatic plants and photosynthetic organisms, like phytoplankton, that needs to manage fluctuating light conditions that vary in intensity and wavelengths as light travels and interacts with and within the water column (Kirk, 1994; Thomas, 1955).

Globally, the light-harvesting capacity of plant communities in the marine ecosystem accounts for half of the net primary production (Behrenfeld et al., 2001; Gregg et al., 2003). With unfavorable light conditions (light intensity of less than 4%, Shirley, 1945), healthy cells may turn into unhealthy cells that leak soluble constituents like dissolved organic matter or their chloroplast content to the surrounding water, thus losing their photosynthetic capacity (Børsheim et al., 2005). This may cause starvation of the photosynthetic organisms (Shirley, 1945). If other conditions are favorable for the survival of aquatic plants, i.e. carbon dioxide, water temperature, concentration of particular nutrients like nitrogen, phosphorous or potassium; the actual light intensity required for their survival is between 1 to 5% approximately the value at which photosynthesis balances respiration (Kirk, 1994; Shirley, 1935). Light availability in the aquatic ecosystem is therefore an ecological factor important to assess, as it directly influences the growth rate of the basis of the marine food web (primary producers) and hence the upper trophic levels in the aquatic ecosystem (see Figure 1).

PRIMARY PRODUCTIVITY = Light Find Productivity BIOMASS RATE Nutrients Sinking Nutrients Supply Concentration Temperature

Figure 1 Primary productivity is the product of phytoplankton biomass (regulated by import, export, sinking, mortality, nutrient supply, and growth rate) times phytoplankton growth rate (regulated by light, temperature, and nutrient concentrations, credits Cloern et al. (2014) with permission of Copernicus Publications under Creative Commons Attribution 3.0 Licence).

Water is blue

As a marine ecologist it is important to know about the intrinsic colour of water, which is blue (Braun and Smirnov, 1993). Although to appreciate its intrinsic blueness, water requires to be free of dissolved and suspended particulates, i.e. it should not include any impurities; and light has to travel through it in a distance of several meters (see Fig. 2). The strong absorption of water at the red end of the visible electromagnetic spectrum (VIS) promotes vibrational transitions to higher energy states, which combined with the primarily blue light that has been scattered back, is perceived as blue. More formally, underwater, the spectral distribution of light (solar radiation) changes markedly with depth (Kirk, 1994). Basically, the wavelength of the photon that can penetrate deeper into the water (not being absorbed) is also more likely to be scattered back to the surface and determine the water colour. However, referring to colour as a property of an object is misleading. Colours are caused by differing qualities of light, i.e., the superposition of different wavelengths in the visible spectrum. Wavelength, however, is not a synonym of colour (Bohren, 2006). Wavelength is the wave size of a travelling wave. In marine optics, this wave is mainly associated with the

solar energy reaching the aquatic medium and interacting with it. Therefore and summarized by (Bohren, 2001):

"The colour of the sea is merely shorthand for colours of the light coming from different patches of the sea under various conditions of illumination and observation".

In this thesis this definition is used when referring to the colour of an object.

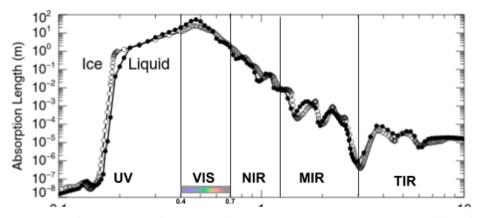


Figure 2. Absorption length (inverse absorption coefficient) of pure ice and liquid water from ultraviolet (UV), visible (VIS) to infrared (NIR-near, MIR-mid, TIR - thermal). Modified and reprinted with permission from John Wiley and Sons, license number 3767020654903 (Figure 2.2, Bohren, 2006). Rendered Spectrum by Spigget. Licensed under CC BY-SA 3.0.

Why are some water bodies not blue

Knowing that pure water is blue, is the first step towards our understanding of the light interactions in the aquatic medium. However, it is even more important to understand why a specific water body is not blue. The water and substances, either dissolved or suspended particulate matter in the aquatic medium, have distinct optical characteristics. These optical signatures occur when two physical process, absorption and scattering are triggered by light interacting with them. This interaction works together, i.e. the separated values of either absorption or scattering do not determine the brightness, nor the perceived colour of any object or medium. It is the ratio

of scattering to absorption that we perceive as the brightness and colour of an optically thick multiple-scattering medium (Bohren, 2001). Light is absorbed by water and optically active pigments, like chlorophyll or carotenoids, and it is scattered by particles while penetrating the water column. Furthermore, all kind of suspended particles, breaking waves, ocean bubbles, whales, shoaling or schooling fishes, even sunken ships and shallow bottoms may contribute to the colour change. Anything that reduces the path length of the photons on their way out of the sea will be combined in the ratio of scattering to absorption to yield what is observed as the colour of the sea.

More formally, optical properties that are not affected by the distribution of the light field and are dependent on the concentration, type and morphology of the substance are known as Inherent Optical Properties, i.e., absorption and scattering properties (Preisendorfer, 1976). Inherent optical properties (IOP's) are different among groups of optical water constituents, and three groups are considered to be responsible for significant changes in the optical properties of the water: phytoplankton, non-algal particles of biological or terrestrial origin and coloured dissolved organic matter (CDOM), see Figure 3. Each group is also subject to a certain variability (Prieur and Sathyendranath, 1981).

Optical Properties that depend both on IOP's and also on the light field distribution in a medium at a given observation point are called Apparent Optical Properties - AOP's (Smith and Baker, 1981). AOP's describe the rate of change of radiometric quantities with depth (Zaneveld et al., 2007). Formal descriptions and derivations of both IOP's and AOP's can be found in several papers in the literature, but the key stones are the works of Preisendorfer (1976), Morel and Prieur (1977), Kirk (1994), Mobley (1994) and Morel and Maritorena (2001). More recently the Ocean Optics Web book provides the background and references for this marine field of research freely accessible (Mobley, 2010).

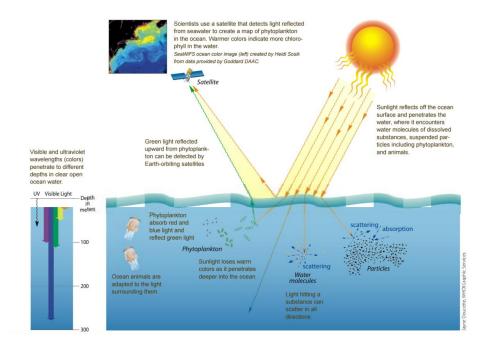


Figure 3. Light in the ocean. Reprint with permission from Oceanus Magazine • Vol. 43, No.2, 2004.

Formally, the optical information of the water body is contained in the water-leaving radiance, L_w , but equally important it is dependent on the incident sun light that has reached the ocean, the downwelling irradiance, E_d , at the surface. By knowing the amount of energy arriving and leaving the water surface, *i.e.* the diffuse reflectance of the upper ocean, $R(\lambda)$, we can estimate the component of incident light that is missing in the up-welled light field that represents the light that has been absorbed or scattered by water constituents (Twardowski *et al.* 2007).

The wide range of possible combinations of optical properties of the water constituents, are not only complex, they exhibit a large range of variations (Doxaran et al., 2006). When the optical properties have major contributions from inorganic particles and yellow substances, besides from phytoplankton, it is **an optically-complex water body**, also known as optical Case-2 waters. When the optical properties are dominated by phytoplankton and associated biogenous materials, the water body is commonly referred as optical Case-1 water, i.e. clear natural waters such as clear ocean waters (Morel and Prieur, 1977, Morel and Maritorena, 2001).

Extended concepts of radiometric definitions and properties that describe the light in aquatic environments are given in detail in Kirk (1994), Mobley (1994), Mueller et al., (2003a, 2003b). The latter two studies described the NASA protocols for optical and radiometric measurements relevant for satellite remote sensing of ocean colour (see following sections). Nonetheless, a practical handbook on remote sensing, like the work by Lavender and Lavender (2015), would be recommended for the non-specialist marine ecologist before attempting to dive into the bio-optics works of Kirk or Mobley, for instance.

Measuring the available light in the water

Light is a difficult parameter to measure. It is a stream of packets of electromagnetic energy, called photons. Photons carry energy, with linear and angular momentum, but no mass. However, the physical importance of sunlight arriving at the ocean surface is in its energy transport, not in its momentum, i.e. "sunlight heats us up rather quickly, but it does not push us around" (Mobley, 2010). Photons are considered to be of one kind and only different in energy and momentum (Bohren, 2006). The photon has an associated frequency, ν , that corresponds to a wavelength, λ , endowing the photon with wave-like properties (Mobley, 2010). Photons (as electromagnetic waves) move through empty space with the same speed, c, about 3 x 10 8 m s⁻¹. The simplest kind of waves, a plane harmonic, in free space can be characterized by its wavelength, related to its frequency expressed by $\lambda \nu = c$ (Bohren, 2006). We can detect the wave properties of light by measuring the wavelength (e.g. using diffraction gratings), or we can detect its particle nature involving absorption and scattering by its photoelectric effect.

In order to measure the available light in the water we need to know the light source (e.g. sunlight or a built-in calibrated light source combined with a photodetector), how much light impinges upon an illuminated area (usually at the sea-air interface) and how much light is reflected from it. Note that a change in the light source implies that the light scatter will be different (Kemker, 2014). This may be combined with deployed instruments that measure light attenuation by depth, i.e. the loss of intensity due to absorption and scattering by the water and particles within it. The scatter can be in any direction (see Figure 4), and it is dependent on the light source, wavelength and on the concentration, type and morphology of the substance as we have mentioned before. Thus when considering the light interaction with matter, a first question to consider is how large the electromagnetic waves are (Bohren, 2006).

SMALL PARTICLES
SMALLER THAN 1/10 THE WAVELENGTH OF LIGHT
SYMMETRIC SCATTERING

MEDIUM PARTICLES
APPROXIMATELY 1/4 THE WAVELENGTH OF LIGHT
SCATTERING CONCENTRATED IN FORWARD DIRECTION

LARGE PARTICLES
LARGER THAN THE WAVELENGTH OF LIGHT
EXTREME SCATTERING IN FORWARD DIRECTION

Figure 4. Representation of light scattering depending on size of particles in relation with wavelength. Reprinted with permission of Fondriest Environmental, Inc. Credits (Kemker, 2014)

The accuracy and usefulness of methods and designs of light meters, i.e. radiometers, or simple devices to measure light transmission or its attenuation in the aquatic environment varied for specific applications (Paper I). Therefore, there is a need of inter-comparisons of data products and methods used from simultaneous measurements and optical sensors inter-calibrated through the same light source (absolute radiometric calibration), usually a traceable lamp from a National Institute of Standards and Technology (NIST), and using the same standards and methods (Zibordi et al., 2012). Note that the recommended nomenclature, symbols and definitions follow the Committee on Radiant Energy in the Sea of the International Association of Physical Sciences of the Ocean (IAPSO) given in (Morel and Smith, 1982).

Historical instruments used to visually describe the transparency and colour of water have been summarized by (Wernand, 2010; Wernand and van der Woerd, 2010). For example, a standard method to determine water clarity (transparency) used since the end of the nineteenth century, is the Secchidisc method (Wernand 2010). This widely and still used method consist of lowering a 30 cm white (matt) painted disk into the water column until the

disk is perceived to disappear. The disk is termed 'Secchi disk' as the method was first introduced by Father Pietro Angelo Secchi in 1865. Another common and still in use method from the 19th century is the Forel-Ule (FU) scale. This scale is based on 21 specific chemical solutions reassembling a scale of colours of natural waters that were sealed in glass tubes and used to match the observed colour of the sea. The method was proposed by Francois Alphonse Forel and Willi Ule as a colour comparator scale (Novoa *et al.*, 2013, 2014; Wernand, 2010; Wernand and van der Woerd, 2010). In this thesis a method to measure turbidity has been applied in Paper III, that uses a handheld device with a light source and a photodetector at 860 nm that are placed at a 90-degree angle to each other to maximise the sensitivity of scattering regardless of particle size (Kemker, 2014).

Due to its simplicity and robustness, the Secchi disk depth method continues to be one of the most frequently used measurements in optical oceanography to estimate the optical depth of light within a water body; it is one of the largest AOPs dataset available, but limited in spatial and temporal coverage (Arnone et al., 2004). Nevertheless, the Forel-Ule scale marks the beginning of the ocean colour classifications and it is one of the oldest oceanographic data sets available covering up to the year 2000, more than a century of observations (Novoa et al., 2013, 2014; Wernand, 2010; Wernand and van der Woerd, 2010).

Based on radiometric measurements in the euphotic zone (i.e. spectral transmittance of the light (from 350-700 nm), Jerlov (1977) provided a water classification. In the same year, Morel and Prieur (1977), using measurements of in-coming and out-coming light (downwelling and upwelling irradiance) in relation to turbidity and pigment content, introduced the terms Case-1 and Case-2 waters, which has been mentioned here before. Based on Gordon et al. (1975) and Morel and Prieur (1977) a simple relationship which is a function of the ratio of the backscattering and absorption coefficients has been used to estimate optical parameters from the irradiance reflectance (Gordon et al. 1988; Morel 1988; Gordon 1989; Morel and Gentili 1991) and it has been the base of further ocean colour algorithms and developments. Summarized in the International Ocean Colour Coordinating Group (IOCCG) reports (IOCCG 2000; IOCCG 2006; IOCCG 2011) key examples of above and in-water instrumentation and platforms and Ocean Color Remote Sensing Applications can be found.

Optical remote sensing

Sensors capable of measure the radiant energy in the visible (VIS) [380 nm – 750 nm] and near infrared (NIR)[750 nm - 1400 nm] parts of the electromagnetic spectrum are referred to as optical sensors. These optical sensors are frequently mounted on moored platforms, aeroplanes or satellites, but can also be optical close-range instruments used as hand-held devices for field measurements in situ (Paper I and Paper III). When the targets are oceans and seas the discipline in question is called 'ocean-colour remote sensing'. Furthermore, when considering all types or water bodies, i.e. coastal, inland or open sea waters, we refer to aquatic remote sensing. Ocean colour remote sensing instruments register those photons that have reached the water body after travelling through the atmosphere, interacted within the aquatic medium and then were backscattered through the atmosphere, and finally reached the satellite sensor.

A key objective of ocean colour remote sensing is the estimation of the IOPs and concentrations of the in-water constituents to derive useful information about the marine environment. Over the past 40 years, Ocean Colour Remote Sensing has increased its accuracy to estimate the concentrations of optical constituents such as chlorophyll-a (Chl-a), which has been successfully used as a proxy for phytoplankton over the open ocean. Ocean colour revealed intricate spatial patterns of phytoplankton dynamics, showing their complexity and variability (Gordon et al. 1980). Since then, several studies detailing the chemistry and biology of the oceans through global observation from space have become available (McClain 2009; McKinna 2015; Odermatt et al. 2012). The validity of such studies relies on high quality of field measurements at sea that are used as reference values (i.e. sea-truthing data) to validate the satellite data (Paper I, II and Paper III). The validation analysis requires coincident measurements (both in space and in time) of in situ and satellite observations, with data sets (both satellite and in situ), derived from a well-defined standards used to determine the quality of the measurements, i.e. quality control and exclusion criteria (Mueller et al. 2003). This is not trivial as it requires software to predict the orbit of the satellite in question and also extensive experience with field-validation techniques.

How satellites sensors measures light from the water and retrieve its information

Satellite-based ocean colour remote sensing is a passive technique, where sunlight is the primary source of energy and light is used as information carrier. Ocean colour remote sensing data provides a synoptic view of the emerging radiance from a water body, from which higher level products can be derived. Remote sensing is based on inversion modelling which is the estimation of IOPs, i.e. absorption and scattering properties and the subsequent estimation of the concentration of optical water constituents from the IOPs when the spectral characteristics of the water-leaving radiance are known (Zaneveld et al., 2007). The inverse problem has no unique solution, different combinations of optical active constituents may result in the same spectral signal measured by the sensor, making this signal difficult to interpret and not possible to invert accurately for all ranges of IOPs found in natural waters. Furthermore, the entire radiant distribution at the surface is unknown, and often a full characterization of the IOPs is difficult to obtain due to the complex composition of in-waters constituents. Thus, inversion models depend mostly on semi-analytical approaches that relate the water constituents and IOPs to the remote sensing signal rather than on empirical relationships where the uncertainties cannot be predicted or analysed (IOCCG, 2000). The accuracy of the models depends also on the training range of the model. If it does not cover the actual range of all optical constituents in a given water body, the accuracy of the retrieved products may decrease.

Empirical algorithms are based on statistical regressions of satellite bands or band ratios. Those algorithms use specific IOPs (e.g. the spectral chlorophyll-specific absorption coefficient) that are often location-dependent thus require parameterization to work in different regions (Twardowski et al., 2007; Matthews, 2011). Semi-analytical methods use empirical relationships, along with a theoretical model to invert the remote sensing reflectance and derive the inherent optical properties, scattering, absorption and backscattering (Twardowski et al., 2007). While empirical methods (usually based on band ratios) are mostly applied to clear oceanic waters, semianalytical algorithms are mostly used in optically-complex waters such as coastal waters and lakes. Several examples of analytical models can be found in the literature (Odermatt et al., 2012), to derive water products such as chlorophyll (Carder et al., 1999; Garcia et al., 2006; Gordon et al., 1988; Roesler and Perry, 1995; Siegel et al., 2002); total suspended matter (Fettweis and Nechad, 2010; Lavender, 1996; Nechad et al., 2010; Siegel et al., 2002); coloured dissolved organic matter (Carder et al., 1999; Kutser et al., 2005; Morel and Gentili, 2009; Siegel et al., 2002; Zhu et al., 2014); ocean transparency (Doron et al., DEC 15 2011; Lewis and Kuring, 1988; Woodruff et al., 1999); inherent optical properties (Garver and Siegel, AGU 15 1997; Gould and Arnone, 1997; Hoge and Lyon, 1996; Kahru et al., 2013; Le et al., 2013; Mélin et al., 2005, 2011; Morel and Maritorena, 2001; Roesler and Boss, 2008; Tilstone et al., 2012).

The satellite geophysical products derived from the inversion algorithms are known as level 2 products. Level 2 data are processed from level 1B data (physically calibrated Top of Atmosphere radiance data without any atmospheric corrections) to provide geophysical measurements such as atmospherically corrected water-leaving reflectance and values of the water quality constituents. Level 3 products, are derivatives of level 2 MERIS data over a given time period (binned products). The image processing algorithms used for atmospheric correction and to derive level 2 products from level 1B are called processors.

In order to retrieve information related to the in-water optical properties, the atmosphere signal has to be removed first so that the quality of light (shape of the observed spectra) is characteristic of the observed target. Otherwise the atmosphere may affect the observed spectra of the target and limit the accurate retrieval of water constituents (Saulquin et al. 2016; IOCCG 2010; Philpot 1991). For example, in the visible part of the electromagnetic spectrum, the measured signal at the top of atmosphere TOA is dominated by the atmosphere (IOCCG 2010) and the total radiance, L_T , is generally an order of magnitude larger than the water-leaving radiance, L_w .

In situ data is a fundamental requirement for ocean colour products validation and for confirming the reliability of the satellite products. Frequent field observations combining different regions and independent sources are required to produce large datasets representative of various marine bio-optical regimes (Werdell et al. 2003). However, the use of various field instruments with a variety of calibration sources, diverse sampling methods and protocols, and application of different processing schemes may increase the uncertainty of radiometric measurements. Intercomparison of data products with benchmark sensors is the preferred method to reduce the increase in uncertainty (Datla et al. 2010). In this theses paper I and paper II deal with the reliability of satellite data and the evaluation of uncertainties in high absorbing waters. A lot of the coastal processors in use were not primarily developed for highly absorbing waters such as the Baltic Sea and Lake Vänern, and it is therefore important to test if the methods work in these waters types.

The development of the ENVISAT Medium Resolution Imaging Spectrometer (MERIS), the European Space Agency (ESA) provided a new tool for the monitoring of coastal waters (Doerffer et al. 1999; Rast et al. 1999).

Launched in 2002, the ENVISAT satellite, successfully delivered MERIS data world-wide every two-three days (depending on latitude). A communication failure with the ENVISAT in April 2012 left the data-user community with a legacy of 10-year satellite data archive to be exploited (Laur 2012). MERIS data improved the spatial and spectral resolutions (~ pixel size of approximately 290 m x 260 m and 15 spectral channels in the visible/near infrared region-VIS/NIR) compared to other ocean colour sensors like MODIS and SeaWiFS. In the work reported in this thesis we used MERIS data, which will in the very near future be replaced by ESA's Ocean and Land Colour Instrument (OLCI) on Sentinel-3. The Sentinel 3 operational mission, will provide continuation of the MERIS legacy with the Ocean & Land Color Instrument (OLCI). OLCI will use the same spectral bands and radiometric performances as MERIS, plus 6 additional new bands (see Table 1), to cover the range from 400-1020 nm (Regner 2013), with the aim to improve atmospheric correction procedures and retrieval of water quality products in coastal waters.

Examples of remote sensing with focus in the Baltic Sea

Natural and regular phenomena occurring in the Baltic Sea are the spring and summer phytoplankton blooms. The summer blooms are of special environmental and health interest because in the open sea they tend to be dominated by the potentially toxic nitrogen-fixing filamentous cyanobacteria, *Nodularia spumigena* and non-toxic *Aphanizomenom sp* Examples of remote sensing with focus in the Baltic Sea (Kahru et al. 1994; Rud and Gade 1999). Due to the high spatial and temporal variability of cyanobacteria blooms, conventional shipboard monitoring cannot assess the extent or dynamics of surface blooms, thus in the Baltic Sea region the literature on remote sensing of the Baltic Sea is dominated by several studies for detection of algal blooms based on chlorophyll retrieval (Kahru et al. 1994; Håkansson and Moberg 1994; Rud and Gade 1999; Siegel et al. 1999; Ennet et al. 2000; Lavender and Groom 2001; Kutser 2004; Reinart and Kutser 2006; Kahru et al. 2007; Kutser 2009; Park et al. 2010; Kahru and Elmgren 2014).

Cyanobacteria can regulate their buoyancy and form dense aggregations (packaging effect) having a non-uniform distribution vertically and horizontally, thus it is difficult to estimate their concentration, either in situ or by satellite methods (Kutser 2004). Satellite remote sensing frequently underestimate chlorophyll concentrations during heavy blooms, but provide good estimates in the early development of a bloom (Kutser 2004; Reinart and Kutser 2006).

Table 1. Ocean & Land Color Instrument (OLCI) spectral channels. Highlighted in blue are the additional bands not included in the Medium Resolution Imaging Spectrometer (MERIS) sensor (Regner, 2013).

Channel	Central wavelength (nm)	Width (nm)
1	400	15
2	412.5	10
3	442.5	10
4	490	10
5	510	10
6	560	10
7	620	10
8	665	10
9	681.25	7.5
10	708.75	10
11	753.75	7.5
12	761.25	2.5
13	764.375	3.75
14	773.75	5
15	781.25	10
16	862.5	15
17	872.5	5
18	885	10
19	900	10
20	940	20
21	1020	40

Recent comparisons of satellite sensors to detect harmful algal blooms have been carried out by Reinart and Kutser (2006) assessing SeaWiFS, MODIS/Aqua and MERIS sensors and by Park et al. (2010) using MERIS and MODIS with quasi-coincident data. Both studies found good capabilities of MERIS and MODIS to detect the blooms, but caution is suggested about data consistency and quality. Differences among MERIS and MODIS sensors were significant in turbid coastal waters and during heavy blooms, where high variability in the chlorophyll estimates were found. Reinart and Kutser (2006), mention that high chlorophyll concentrations during the peak of a bloom might lead to measurements being out of range of the standard satellite processing algorithms, leading to atmospheric correction failure. By looking at the spatial distribution of the differences of chlorophyll values Park et al. (2010) found that MODIS is also contaminated by backscattering from inorganic suspended particles with values 50% higher compared to MERIS in optical case 2 waters. Standard chlorophyll-a algorithms fail in the Baltic Sea (Reinart and Kutser 2006; Darecki and Stramski 2004), and it is generally attributed to the optical properties of the Baltic Sea that are dominated by CDOM absorption (Kutser 2009; Kratzer and Tett 2009). A report on the validation of algorithms for chlorophyll-a retrieval from satellite data in the Baltic Sea was presented by the Helsinski Commission and prepared by the European Commission's Joint Research Centre, improving the knowledge and use of the satellite information in the Baltic Sea (HELCOM 2004).

Ocean colour remote sensing in the Baltic Sea has focused also on the study of mesoscale features, like upwelling and ocean fronts (Gade et al., 2012; Semovski et al., 1999; Vahtera et al., 2005) or monitoring dredging plumes (Kutser et al., 2007). Fundamental studies related to ocean colour remote sensing include in situ characterization of the inherent and apparent optical properties and the quantification of water constituents for different regions in the Baltic Sea. Such as Siegel et al., (1999), who studied optical in-water constituents (i.e. Chl-a, SPM and CDOM) and provided values for their specific absorption coefficients from the Northern Baltic Proper to the Skagerrak region. Furthermore, Siegel et al., (2005) expanded the work to the Baltic Proper and Southern Baltic Proper, including the Gulf of Gdansk. Sørensen et al. (2007) provided the backscattering and specific absorption coefficients for the Skagerrak and Kattegat. The optical properties in the Gulf of Finland were characterized by Kutser (2004) and Krawczyk et al. (2007). The Mahu Strait in The Gulf of Riga was studied by Kutser (2009) where the authors provided an IOP characterization of the area and presented a new method for mapping CDOM distribution in a coastal area. Kowalczuk et al., (2005) also focused on the analysis of optical properties of CDOM in the southern Baltic Proper, for different seasons, and provided empirical relationships for CDOM and apparent optical properties.

The Northern Baltic Proper along the Swedish Coast is optically described by Kratzer et al. (2003, 2008) and Kratzer and Tett (2009). Høkedal et al. (2005) presents the similarities of optical properties of the Oslo Fjord with those of the Baltic Sea along the Swedish coast. Berthon et al. (2006) provides a comprehensive study on the bio-optical properties, mostly on the Southern Baltic Proper, which complements the work of Babin (2000). Berthon and Zibordi (2010) focused on the bio-optical properties of the Bothnian Sea, the Quark and the Bothnian Bay in northern Baltic Sea, and due to the special optical properties it was suggested that this area is suitable for studies on atmospheric corrections and vicarious calibration of ocean colour sensors in coastal waters. The most recent and cross-site consistent characterization study of in situ radiometric measurements for satellite ocean colour applications is presented in the work by Zibordi et al. (2011). In their study, comparisons of the regional average of inherent and apparent optical properties were provided for the Baltic Sea region, the Eastern Mediterranean Sea, the Ligurian Sea, Adriatic Sea, Black Sea and English Channel.

Sea-truthing studies for validation of satellite data play a key role assessing the reliability of different sensors and algorithms to retrieve optically inwater components and their concentrations. Zibordi et al. (2006) showed how stationary tower-based radiometric measurements, using the SeaWiFS Photometer Revision for Incident Surface Measurements (SeaPRISM) mounted on the Gustav Dalén Lighthouse Tower in the North-western Baltic Proper, could be used to validate the retrievals of normalized water leaving radiance from the MODIS sensor. Zibordi et al. (2009) used data from the Aerosol Robotic Network (AERONET-OC) to validate satellite ocean colour products from MODIS/aqua, SeaWiFS and MERIS, mostly in the Northern Baltic Proper. Darecki and Stramski (2004) evaluated the performance of the standard bio-optical algorithms of MODIS and SeaWiFS and found that both sensors showed poor agreement in the normalized water-leaving radiance when compared with in situ measurements, mostly due to atmospheric correction failure.

The uncertainty of the remote sensing reflectance of MERIS was evaluated with field observations and the SeaWiFS data Analysis System (SeaDAS) by Melin et al. (2011). They found that, in the Baltic Sea, the mean absolute relative difference between satellite and field data was much higher for the blue bands characterized by low amplitudes.

In the Himmerfjärden region, along the west coast of the Northern Baltic Proper, Kratzer et al. (2008) assessed the use of the full resolution data of MERIS to monitor the coastal zone. For the same area Kratzer and Vinterhav (2010) compared three MERIS processors for retrieval of water constituents with in situ data, where they found that the water processor of the Freie Universität of Berlin (FUB) provided the best estimates. Validation of the

MERIS water products and the bio-optical relationships for the Skagerrak and the Kattegat region was reported by Sørensen et al. (2007), while Doron et al. (2011) focused on validation of water transparency algorithms for estimating Secchi depth by MERIS, MODIS and SeaWiFS in the same region. Other key topics relevant in ocean colour remote sensing in the Baltic Sea are related to the water transparency Kratzer et al. (2003) or water quality (Erkkilä and Kalliola, 2007; Ferraro et al., 2009; Karabashev et al., 2006; Krawczyk et al., 2007; Kutser et al., 1998; Neumann et al., 2004). Furthermore, the assessment of the extent of the coastal zone has been studied in the central and eastern Gulf of Finland, by using remote sensing estimates of chlorophyll-a (Lessin et al., 2009). Bio-optics and the inorganic fraction of the suspended particulate matter were used to distinguish coastal waters from open sea in the Himmerfjärden area (Kratzer and Tett, 2009). Harvey et al. (2015) showed that in Himmerfjärden, comparable concentrations of chlorophyll-a from ship-based measurements can be derived from satellite remote sensing for water quality monitoring.

Central Findings and discussion

This thesis shows examples of the workflow that needs to be considered when assessing the water quality using optical remote sensing in the coastal zone. Paper I and II, addressed data collection in the field. Calibration and validation activities are highlighted as keys for the success of operational satellite missions.

Intercomparison of both in situ radiometers and the methods on how to use them (Paper I), allows us to define the reliability and the practicality of their use in field measurements as well as to both quantify and qualify their uncertainties. Furthermore, evaluation of the best remote sensing algorithms is made possible by measuring the spectral reflectance in situ.

Although inter-comparison campaigns are challenging, due to the involved high costs and logistic coordination, calibrations of radiometers need to be done, either by sending the instrument to the manufacturer, or to specialized calibration facilities, that use a traceable lamp (NIST lamp). Furthermore, an intercalibration of radiometers using the same traceable light source and standard methods was highly recommended to be carried out in (Zibordi et al., 2012). Because, only then, if both intercomparison and intercalibration are performed carefully, it is possible to fully quantify the uncertainties of each radiometer and to make the produced data comparable. Well calibrated instruments, allow us to move forward and to ensure the accuracy of satellite products. The derived and quality-assured satellite products may then be used e.g. for operational monitoring of water quality, or to improve sensor design for future missions, or for ecological modelling and climate change studies, or to forecast. Both, radiometry and water-derived products, such as chlorophyll-a (CHL), suspended particulate matter (SPM) and colored dissolved organic matter (CDOM) are key remote sensing products, and recommended to be evaluated during sea truthing campaigns, which was done in paper I-III.

Semi-analytical ocean colour algorithms usually use specific IOPs (e.g. the spectral chlorophyll-specific absorption coefficient) and are therefore often location-dependent, and require parameterization to be applicable in different water bodies/ optical regions (Twardowski et al. 2007; Matthews 2011; Paper III). Validation of standard and alternative ocean colour algorithms is

thus required, to assess the reliability of the method (Paper II, Paper III). In situ validation makes it possible quality-assured remote sensing applications for marine ecology studies and for reliable monitoring of coastal waters (Paper III and Paper IV).

Results of the intercomparison of instruments

In paper I (Hommersom et al. 2012), the intercomparison of the radiometer WISP-3 was performed over one coastal site and two lakes. The coastal site was located on the island of Texel at the boundary between the North Sea and the Wadden Sea in the Netherlands. The two lakes included in the study were two boreal lakes, Lake Peipsi in Estonia, and Lake Vänern in Southern Sweden. The results presented in paper I, have demonstrated that the WISP-3 is comparable with other well-known instruments. Root mean squared percentage errors relative to those of the TriOS system were generally between 20% and 30% for the WISP-3. The comparison in three optically different water bodies showed the potential of the WISP-3 to observe interesting features in the Rrs spectra related to water constituents. The study also demonstrated the reliability of the instruments even in waters with high CDOM and Chl absorption. In general, the greatest discrepancies of the Rrs spectra relative to the TriOS system were mainly due to differences in environmental conditions encountered during data collection. The intercomparison in lake Vänern was the most relevant for this thesis. It covered a wide sampling scheme under different physical settings, environmental conditions and variable concentrations of optical water constituents. The central part of lake Vänern showed the most stable physical and environmental conditions for the intercomparison. Similar Rrs shape spectra characterized the instruments but differences in magnitude were observed. Rrs were consistently lower in WISP-3 than the TriOS (used as reference), along the spectrum, except in the blue where WISP-3 showed higher noise. The other two in water radiometers, the TACCS and ASD, showed reflectances that were consistently higher than the reference.

The comparison of in situ concentrations in Lake Vänern and Lake Peipsi derived from band ratios from TriOS, WISP-3 showed a good correlation for the three water quality parameters (SPM, Chl and CDOM). Using a linear model and a single band at 708 nm, SPM was the best retrieved water quality parameter with a correlation coefficient R²=0.98 using TriOS, and R²=0.88 for the WISP-3. The chlorophyll ratio Rrs(708)/Rrs (665) was best retrieved by WISP-3 with R²=0.86, however it showed higher scattering for in situ values above 15 mg m⁻³ (same as TriOS) and below 4 mg m⁻³, but TriOS was more stable. The conditions during the field were not ideal to perform

an inter-comparison radiometers. In the study of Zibordi et al. (2012) an inter-comparison was done in almost perfect conditions, i.e. with clear skies, moderate low sea state and relatively low sun zenith angles. Above-water instruments such as the TriOS, were deployed under controlled geometry, mounted on grounded platforms. The in-water radiometers, e.g. the TACCS, were deployed following the same protocols as described in paper I. The use of ships or small boats was avoided for above-water instruments as small boats tend to be affected by drift and roll. All of the compared instruments were also inter-calibrated in the same laboratory against a traceable NIST lamp which presumable helped to reduce potential bias in the derived radiometric products due to inaccurate calibrations. Such favourable conditions are more of an exception rather than the rule. Hence, an inter-comparison of instruments showing its reliability under different physical setting of the deployment and variable environmental conditions is valuable. However, in Hommersom et al. (2012) it was not possible to perform an inter-calibration against a traceable NIST lamp that reduced the uncertainties due to different lab calibrations of instruments. Instead, the TriOS system, was used as a reference. The TriOS system from Tartu Observatory used during the Lake Vänern and Lake Peipsi campaigns, had also been characterized under favourable conditions, together with the TACCS, and its uncertainties are well described (Zibordi et al. (2012). The main advantages of using the WISP-3 are that it is the instrument that is most easy to handle. Less experienced operators would be able to perform measurements with a similar accuracy, provided the follow the sampling protocol correctly. The WISP-3 can be programmed to use band ratios adapted for local conditions, which allows for real-time water quality estimations.

Ocean colour algorithms

Field campaigns in optically-complex waters are critical to increase the amount of in situ data that is the basis of semi-analytical satellite algorithm. Studies in optically complex waters are recommended in the mission requirements for future ocean colour sensors (IOCCG 2012), "since the primary vicarious calibration site is usually an open ocean environment care should be taken to obtain sufficient in situ data from turbid waters". However, to obtain the required ideal match-up in space and time for the validation of ocean-colour algorithms, is not trivial since the in situ measurements should be collected at the same time as the radiometric measurements (Santamaría-del-Ángel et al., 2011). However, depending on the hydrodynamics of the water body, it is recommended to be as close as possible to the time of the satellite overpass, usually from 30 min to 2 hrs (Doerffer, 2002;

Mueller et al., 2003b), in order to be sure of sampling the same water mass as captured by the satellite sensor (Paper II).

Our study in paper II, contributes towards setting the standards for validation in Baltic Sea waters, with a new dataset and validation of the MERIS 3rd reprocessing version level 2 data-derived products. Four different level 2 processors were evaluated in coastal waters and a new implementation of the ICOL processor for land adjacency corrections was applied. It was found that due to the relatively low currents a sea-truthing window of +/- 2 hours was adequate for Baltic Sea validation. In the North Sea, however, the tidal currents are very strong, and the recommended sea-truthing window in the MERIS protocols (Doerffer, 2002) is therefore +/-30 min.

The use of common macro pixels (i.e. 3x3 matrix used by processors assuring the same pixels and observing conditions to derive the respective geophysical products) for the comparisons after applying the macro pixel quality and exclusion criteria, allow us to make a fair evaluation of the processors, as the common macro pixels guarantee that the same locations are used to address their differences. The methodology used in paper II was an improvement of the previous study of Kratzer and Vinterhav (2010), on which this study is based upon. In our study, the modification to the homogeneity test, proposed by Bailey and Werdell (2006) to minimize the impact of geophysical variability within macro pixels; allowed us to have a minimum horizontal heterogeneity and avoid validating the satellite retrievals by assuming oligotrophic conditions in the coastal zone. Heterogeneity is also avoided in our truthing protocol as detailed in the MERIS protocols (Doerffer, 2002). In our validation campaigns, we usually used the Baltic Algal Watch System (BAWS) developed by SMHI to keep track of potential surface accumulations of cyanobacteria in the Baltic Sea, combined with information from weather forecasts, to avoid surface blooms during validation campaigns.

Overall, the coefficient of variance within the macro pixels was below 25% for CHL retrievals by FUB and MEGS and for SPM less than 10%. A high range of variability within the macro pixels (50%-90%) were found for CHL during algal bloom events, and within Himmerfjärden bay (stations H3 and H4). Himmerfjärden bay was more frequently affected by land adjacency effects, mixed pixels contamination (land/water) and non spatial homogeneity of the atmosphere (variable aerosols), which increased the variability within a macro pixel, thus impacting the retrieval of water products by a given processor.

Higher uncertainty in the blue spectral region, often caused by inadequate atmospheric correction, is likely to impact the retrieval of CHL and CDOM. Furthermore, the low MERIS reflectance values in the blue bands - due to high CDOM absorption - may produce an overestimation of CHL (Darecki and Stramski, 2004) at low CHL concentrations. As the main attribution of

the total absorption is towards pigment absorption (Heim et al., 2008), it may lead to an underestimation of CDOM by the processors. Furthermore, a nonhomogenous atmosphere with highly variable aerosols may artificially increase the MERIS reflectance towards the blue, therefore CHL is more likely to be underestimated as there is an apparent decrease of absorption in the blue wavelengths. In our study area, relatively low concentrations of SPM and CHL were found. Higher uncertainties dominate the measured remote sensing signal when relatively low SPM loads occur in the presence of relatively high CDOM absorption (Doerffer and Schiller, 2008). For improvement of the accuracy analysis, it would be necessary to have a higher number of chlorophyll and SPM match-up data. However, increasing the number of match-up data is not trivial, considering the high frequency of clouds in the region, and also the lack of coordination between marine monitoring programmes with satellite overpasses. Furthermore, the Northwestern Baltic Sea was one of the few European coastal water sites in the ESA MERIS Match-up In situ Database (MERMAID, http://mermaid.acri.fr/) the validation data base that gave a sufficient number of real match-ups from shiptruthing campaigns to ensure validation and data quality evaluation.

Overall, the studied processors improved the retrievals of MERIS reflectance when the latest MERIS FR 3rd reprocessing was used along with equalized and "smile" corrections, corrections for the land adjacency effects by using the improved contrast between ocean and land (ICOL), and confirmed the findings by Kratzer and Vinterhav (2010). However, the successful application of ICOL for coastal and inland waters is highly related to the geomorphology of the region of study. Water bodies with a predominant geomorphology where the adjacency effect is most dominant in the direction of the forward scattered sun light (i.e. the direction where the sun is), like in Himmerfjärden (south-north direction), may be more successful as ICOL is working in the principal plane (Santer and Zagolski, 2009).

Marine remote sensing applications

Coastal waters are optically diverse (Mélin and Vantrepotte, 2015), providing for versatile opportunities to exploit their optical signatures in a wide range of marine applications (e.g. algal bloom monitoring or monitoring the effects of dredging) with clear societal benefits (IOCCG, 2008). Two manuscripts included in this thesis, showed examples on the combined use of in situ measurements with optical remote sensing to support water quality monitoring programs.

Dissolved and particulate matter, cause a reduction of the transparency of the water column. When the reduced transparency is due to suspended particulate matter (SPM), turbidity occurs. Turbidity increases the scattering of photons and thus affects the light penetration in the water column, hence primary production (Doxaran and Lavender, 2003). In manuscript III, we validated a model development to retrieve SPM from turbidity and provided an example of its application, using both in situ and MERIS data. SPM is not a mandatory variable in conventional monitoring programs to assess water quality. However, turbidity is listed as a mandatory parameter in Annex III of the European Union's Marine Strategy Framework Directive (European Commission, 2008). This emphasizes the relevance of manuscript III to support water quality monitoring in coastal waters by providing a new algorithm for the Baltic Sea. As the algorithm can be applied to the whole MERIS mission, it is possible to retrieve reliable SPM data for coastal areas from the start of the mission in early 2002.

Using an in situ data set with water samples collected in Swedish coastal waters (northwestern Baltic Sea) during 2010-2014, we found a linear and high correlation (r=0.97) between SPM and turbidity measured by a portable turbidity. The linear model was then used to retrieve SPM from MERIS with a reflectance-based turbidity model. It was found that SPM model had higher accuracy and lower bias than the MERIS SPM standard product. Providing a robust and cost-efficient method for research and management to determine in situ and remote sensing derived SPM.

In manuscript IV, the benefits of the increased spatial-temporal data coverage by optical remote sensing were presented and evaluated in comparison to in situ monitoring programs for the assessment of water quality in the coastal zone (using chlorophyll pigments as indicator). A novel approach to increase the quality of the satellite-derived products in the coastal zone was included in the analysis, by using a satellite data density mask on top of the standard quality flags of the product and improved quality flags from the CoastColour project datasets (http://www.coastcolour.org/). Himmerfjärden like no other coastal bay, is one of the most frequently monitored coastal areas in the world, where several major changes in nutrients loads have been performed as part of several full-scale adaptive management experiments. The description of the spatial and temporal evolution of phytoplankton blooms in Himmerfjärden bay was presented. Climatology maps of satellite-derived Chlorophyll-a over 8 complete years, allowed to assess the spatial distribution of chlorophyll-a concentration (based on median values) in Himmerfjärden and adjacent areas, along with their monthly anomalies. MERIS data was here first used for the integration of chlorophyll-a over different water bodies, previously classified by the Swedish Meteorological and Hydrological Institute (SMHI). This made it possible to evaluate how representative the in situ monitoring stations were for each water body, and to compare chlorophyll-a

maxima estimates from in situ sampling directly with weekly MERIS-derived chlorophyll-a measurements. The results presented here complement the established monitoring efforts in Himmerfjärden, and may serve as additional as input to ecological or dynamical models. The remote sensing method also provides useful visualization of the phenology of phytoplankton blooms, showing areas of early blooms on a yearly basis, and helps to identify areas that are insufficiently monitored by ship. It may also be useful for identifying areas where the chlorophyll values do not differ much from the median value of the MERIS time series, and thus maybe not requiring such intensive ship-monitoring efforts. The methodology presented here can be easily adapted to other coastal regions world-wide as it is computed using Python code that can be easily modified as required by the Open Science Initiative.

Conclusions and Outlook

Ocean colour can no longer be considered as an emerging field of science. Varies studies have confirmed the reliability and the versatility of the method, from chlorophyll quantification and primary production studies, to sediment transport, water transparency, turbidity, and light attenuation, which all are providing useful ecological indicators of the water quality. Now, the optical remote sensing field is moving beyond chlorophyll quantification and becoming more accurate also in the coastal zone. New methods are arising towards the identification of phytoplankton taxonomic groups that were out of the scope of this thesis, but worth mentioning here. Better understanding of the bio-optical properties of aquatic ecosystems has encouraged the use of absorption and scattering as satellite-derived optical properties rather than the use only of derived water products concentrations. Ahead of us, new dedicated ocean colour missions like Sentinel, may bring an even wider range of coastal applications closer to the users.

However, one must not forget that quality-assured in situ data is one of the key factors for the reliable use of current and future satellite missions. It is advisable to increase bio-optical sea-truthing datasets, especially in the coastal zone, with a strong participation of national monitoring programs for water quality assessment. The sea-truthing data sets must include information on the exact sampling dates and times and could also be synchronised with satellite overpasses. Bio-optical measurements of SPM, CDOM and turbidity should be included as mandatory parameters, especially in the coastal zone and with the aim to better fulfil the requirements of EU legislation (e.g. the Water Framework Directive-WFD and the Marine Strategy Framework Directive-MSFD).

Regional algorithms need to be developed in order to retrieve quantitative and reliable information from ocean colour sensors. This is mandatory for the Baltic Sea region, which is characterized by high CDOM absorption and thus requires algorithms that are able to resolve the relatively high optical contributions of CDOM absorption.

The validation of reflectance measurements are not trivial and require highly trained staff. The planned operational Sentinel-3 mission will make the continuous assessment of all marine waters possible. However, as the standard products have shown to be insufficient to insure data quality retrieval for Baltic Sea waters, alternative processors and methods such as developed and evaluated in this thesis will have to be put into place.

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