Bio-optic, satellite remote sensing and Baltic Sea ecosystems
- Applications for monitoring and management

Therese Harvey
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Cover photo by European Space Agency, ESA. It displays an Envisat MERIS image on 13 January 2012 of a phytoplankton bloom in the South Atlantic Ocean, situated about 600 km east of the Falkland Islands.


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ABSTRACT

Earth observation satellites cover large areas with frequent temporal repetition and provide us with new insight into ocean and coastal processes. Ocean colour measurements from satellite remote sensing are linked to the bio-optics, which refers to the light interactions with living organisms and dissolved and suspended constituents in the aquatic environment. Human pressures have changed the aquatic ecosystems, by, for example, the increased input of nutrient and organic matter leading to eutrophication. This thesis aims to study and develop the link between bio-optical data and the remote sensing method to the monitoring and management of the Baltic Sea. The results are applied to the European Union’s Water Directives, and the Baltic Sea Action Plan from the Helsinki commission. In paper I indicators for eutrophication, chlorophyll-a concentration and Secchi depth were evaluated as a link to remote sensing observations. Chlorophyll-a measurements from an operational satellite service (paper I) were compared to conventional ship-based monitoring in paper II and showed high correlations to the in situ data. The results in paper I, II and IV show that the use of remote sensing can improve both the spatial and temporal monitoring of water quality. The number of observations increased when also using satellite data, thus facilitating the assessment of the ecological and environmental status within the European Union’s water directives. The spatial patterns make it possible to study the changes of e.g. algae blooms and terrestrial input on larger scales. Furthermore, the water quality products from satellites can offer a more holistic and easily accessible view of the information to decision makers and end-users. In paper III variable relationships between in situ bio-optical parameters, such as coloured dissolved organic matter (CDOM), dissolved organic carbon, salinity and Secchi depth, were found in different parts of the Baltic Sea. In paper IV an in situ empirical model to retrieve suspended particulate matter (SPM) from turbidity was developed and applied to remote sensing data. The use of Secchi depth as an indicator for eutrophication linked to the concentrations of chlorophyll-a and SPM and CDOM absorption was investigated in paper V. The variations in Secchi depth were affected differently by the mentioned parameters in the different regions. Therefore, one must also consider those when evaluating changes in Secchi depth and for setting target levels for water bodies. This thesis shows good examples on the benefits of incorporating bio-optical and remote sensing data to a higher extent within monitoring and management of the Baltic Sea.
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<tr>
<td>$\lambda$</td>
<td>Wavelength (nm)</td>
</tr>
<tr>
<td>$a$</td>
<td>Absorption coefficient (m$^{-1}$)</td>
</tr>
<tr>
<td>$b$</td>
<td>Scattering coefficient (m$^{-1}$)</td>
</tr>
<tr>
<td>$b_b$</td>
<td>Backscattering coefficient (m$^{-1}$)</td>
</tr>
<tr>
<td>$b_f$</td>
<td>Forward scattering coefficient (m$^{-1}$)</td>
</tr>
<tr>
<td>$c$</td>
<td>Beam attenuation coefficient (m$^{-1}$)</td>
</tr>
<tr>
<td>Radiance, $L$</td>
<td>The light intensity or radiant intensity is the power incident on or radiated by a surface in a given direction, per unit surface area and solid angle, denoted $L$ (W m$^{-2}$ sr$^{-1}$)</td>
</tr>
<tr>
<td>Irradiance, $E$</td>
<td>Also termed flux of density. Defined as the power incident on or radiated by a surface per unit area, denoted $E$ (W m$^{-2}$)</td>
</tr>
<tr>
<td>$E_u$, $E_d$</td>
<td>Upwelling and downwelling plane irradiance (W m$^{-2}$)</td>
</tr>
<tr>
<td>Reflectance, $R$</td>
<td>The ratio between the upward irradiance to downward irradiance, just below the sea surface, $R = E_u / E_d$ (sr$^{-1}$)</td>
</tr>
<tr>
<td>$R_{RS}$</td>
<td>Remote sensing reflectance (sr$^{-1}$) from the sensor, the upward reflectance reaching the satellite sensor</td>
</tr>
<tr>
<td>$K_d$</td>
<td>Diffuse attenuation coefficient for downwelling plane irradiance (m$^{-1}$)</td>
</tr>
<tr>
<td>$L_w$</td>
<td>Water-leaving radiance (W m$^{-2}$ sr$^{-1}$)</td>
</tr>
<tr>
<td>Optical case 1 waters</td>
<td>Waters where the optical properties are influenced by the optical properties of water itself, phytoplankton and associated CDOM. Most open sea waters</td>
</tr>
<tr>
<td>Optical case 2 waters</td>
<td>Waters where the optical properties are influenced by the optical properties of water itself, phytoplankton (and associated products) and other optical factors, such as CDOM and/or SPM. Most coastal and inland (e.g. lakes) waters</td>
</tr>
<tr>
<td>ESA</td>
<td>European Space Agency</td>
</tr>
</tbody>
</table>

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1. Physical definitions from Morel and Smith (1982) and IOCCG (2010)
ENVISAT  ESA satellite
MERIS  MEdium Resolution Imaging Spectrophotometer
NASA  National Aeronautics and Space Administration
MODIS  MOderate Resolution Imaging Spectrophotometer
Chl-a  Chlorophyll a concentration (µg l⁻¹)
SPM  Suspended particulate matter (g m⁻³)
Tripton  Suspended particulate matter
SPIM  Suspended inorganic particulate matter (g m⁻³)
SPOM  Suspended organic particulate matter (g m⁻³)
CDOM  Colour dissolved organic matter (m⁻¹)
DOC  Dissolved organic matter (mg l⁻¹)
Pixel  The smallest part of a digital satellite image
Sea-truthing  To validate satellite measurements of ocean colour by concurrently measure in situ parameters in order to verify the satellite image
WFD  European Union’s Water Framework Directive
HELCOM  Helsinki Commission on the Protection of the Marine Environment of the Baltic Sea Area
BSAP  HELCOM’s Baltic Sea Action Plan
LIST OF PAPERS


V Harvey, E. T., Kratzer S., Walve J., Karlson B. and Andersson A. The effect of optical properties on Secchi depth and implications for management. Manuscript (in prep.).

My contribution to the papers:
I Involved in SPICOSA meetings. Data analyses of temporal and spatial resolution of chlorophyll-a concentrations. Co-wrote later versions of the manuscript.
II, III; IV Contribution to planning, collection of field data and lab analyses.
IV Contributed to in situ data analyses, evaluation and discussion of the results and co-authoring of the manuscript from start.
V Major contribution to planning and collection of the data. Conducted CDOM lab analyses for Gulf of Bothnia and Baltic Proper, SPM analyses and parts of the chlorophyll-a analyses for Baltic Proper.
II, III, V Prime responsibilities for data selection, data evaluation, statistical analysis, and writing/revision of the manuscript.

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SCOPE OF THE THESIS

Ocean colour remote sensing and bio-optics is an interdisciplinary field, bringing together physics, oceanography, ecology, mathematics and engineering. As my background is in marine ecology, the work with this thesis has given me a new insight and new perspectives into the fields of physical oceanography and aquatic remote sensing and how they can be linked up with ecology. The first part of the summary chapter places the thesis into a larger context of monitoring and management of coastal and optically-complex waters. Moreover, some of the fundamental bio-optical and remote sensing theory is described in order to provide a basis for those readers that are not familiar with it. The central findings and conclusions of the five papers are described and discussed together with the limitations of the results and future aspects.

The aim of this thesis was to study and develop the link to, and use of, bio-optical data and remote sensing for monitoring and management of the pelagic. The focus has been on understanding the complex coastal systems in the Baltic Sea, with respect to eutrophication caused by human pressures acting on the ecosystems.

The specific objectives are:


- Develop the use of remote sensing and bio-optical measurements as indicator for monitoring and assessment of eutrophication (papers I, II, V).

- Contribution to increased knowledge and development of bio-optical parameters within the Baltic Sea region (papers III, IV, V).
INTRODUCTION AND BACKGROUND

The coastal zones are the most inhabited areas of the world. Due to the high biological productivity and the access to rich food resources, these ecosystems produce invaluable services related to human health (MA 2005), and are important recreation sites. On a global average the population density is about three times higher in coastal regions, as 23% of the world’s population live within 100 km distance from the coast and less than 100 m above sea level (Nicholls et al. 2007), and 71% of those within 50 km of estuaries (MA 2005). As a result, coastal zones are strongly affected by human impact and the rapid urbanisation has many consequences and causes many changes of the environment (MA 2005; Newton et al. 2014). Figure 1 shows a map of the human footprint and pressures upon the world, where the coastal and densely populated areas are clearly under higher pressures (Diaz and Rosenberg 2008). The drivers are for example; agriculture; aquaculture; fishing; damming; dredging; urbanisation and industrial development, causing for example; nutrient increase; phytoplankton blooms; changes in ecosystem diversity and species composition; changes in bird and fish communities and pollutions (Newton et al. 2014; MA 2005). Human actions are shaping the complete earth systems and we are presently living in the geological epoch Anthropocene (Crutzen 2002; MA 2005). The ability of coastal systems to continue to provide valuable ecosystem services depends a lot on the health of the system, which is affected and linked to the health of the adjacent freshwater, marine or terrestrial systems, shaped by human activities (MA 2005; Newton et al. 2014). In order to continue having a good health of coastal systems and rich ecosystems that can nurse the species living there and provide the human needs and services, several actions need to be taken. The actions include wiser decisions for regulation and protection for the use of ecosystem services, and by improved actions aiming to limit negative effects and the degree of changes, such as overexploitation of the ecosystems (MA 2005). Knowledge about the systems and the changes within are key factors for managing the coastal zones as well as the knowledge transfer to decision makers (MA 2005; HELCOM 2007; Jutterström et al. 2014; Newton et al. 2014). To assess the water quality more efficiently, good and reliable monitoring methods need to be in place. New methods that can provide data with high spatial and temporal coverage, which are cost-effective, are a good complement to conventional monitoring by e.g. ships.
Figure 1 The human footprints over the world and the areas with hypoxic systems due to eutrophication. The map clearly shows that most areas with the highest human pressures are close to or connected to coastal areas. The locations with hypoxic systems are obviously linked to coastal areas, including the Baltic Sea in northern Europe. Figure from: Diaz and Rosenberg (2008). Reprinted with permission from The American Association for the Advancement of Science (AAAS).

Several ocean global processes could not have been observed without the synoptic data and the high temporal resolution provided by Earth observation satellite missions. Remote sensing, and especially ocean colour applications, for monitoring of open pelagic seas have given us a new perspective and important understanding of the global ocean systems and the dynamics within, e.g. accurate sea surface temperature measurements and the spatial and temporal extent of algae blooms (Platt and Sathyendranath 2008), and El Niño-La Niña periods (McClain 2009). Marine optical remote sensing, is also, due to the high spatial resolution and improved temporal resolution, a very suitable method for studying the dynamics in coastal and estuarine areas, and the complex processes taking place in the boundary between (Brockmann et al. 2004; Andrefouet et al. 2008; Kratzer et al. 2011; Matthews 2011, papers I and II). For coastal observations high-resolution sensors are needed, like the remote sensing data used for this thesis, from the sensor “MEedium Resolution Imaging Spectrometer” (MERIS) from the European Space Agency satellite ENVISAT. Remote sensing and bio-optical data makes it possible to study transports of dissolved and suspended matter from both terrestrial run-off and river inputs, their influence on water transparency, as well as surface chlorophyll-a concentrations in the coastal zones (Siegel et al. 2005; Cui et al. 2010; Kratzer et al. 2011; papers I, II, III, V). Applications of remote sensing can therefore offer more effective monitoring and management, since they provide a synoptic view over a wide range of waters and are a very cost-effective method for detecting changes in aquatic systems (Brockmann et al. 2004; Chen et al. 2004a; Chen et al. 2007a; Andrefouet et al. 2008; papers I, II, IV). The use of remote sensing and bio-
optical data contributes to ecosystem-based management by improving the
best available knowledge about the ecosystem for management of the re-
sources (Nobre and Ferreira 2009). However, the use of remote sensing and
bio-optical data within the coastal zone is still rather sparsely used (but
steadily increasing) compared to open ocean applications and studies.

In northern Europe the world’s second largest brackish sea is found, the Bal-
tic Sea (Figure 2). Only the Black Sea is larger (Chen et al. 2004b). The Bal-
tic Sea is semi-closed with changing physical and biological properties in a
north-south gradient as well towards the Danish Straits in the west. The Bal-
tic Sea consists of several basins separated by sills and shallow areas. The
sills and the narrow Danish Straits lead to a restricted water exchange with
the North Sea and a low water turnover rate. Furthermore, the high run-off
from land and freshwater input from several large rivers cause a strong salin-
ity gradient. The surface salinity is very low in the Bothnian bay basin (0-4),
increasing to the south in the Bothnian Sea to about 5-6 and further increas-
ing in the central Baltic Proper basin with a salinity around 7. In the southern
basins, the inflow from the North Sea is more pronounced with higher salini-
ties of 8-10, and the highest found in Kattegat of 28 (Voipio 1981;
Leppäranta and Myrberg 2009; Deutsch et al. 2012). The changing physical
gradients determine several of the characteristic features of the Baltic Sea,
such as the formation of sea ice during the winter months, the pronounced
haloclines with higher salinity in the bottom waters in all basins and summer
thermoclines, causing a rather strong stratification (Voipio 1981; Leppäranta
and Myrberg 2009). These changing conditions affect the ecology of the
Baltic Sea, by accommodating only a restricted number of species, especial-
ly in the north. Moreover, the drainage basin is remarkably large (about 4
times) compared to the area of the sea. About 85 million people, from 14
countries, nine of which are riparian water states, inhabit the catchment area.
Almost half of the population, around 40 million, live in the coastal areas
and in the big cities along the coast (Sweitzer et al. 1996; Leppäranta and
Myrberg 2009). The large population and the physical features makes the
fragile marine ecosystem Baltic Sea especially sensitive to changes and envi-
ronmental pressures, such as anthropogenic stressors, nutrient enrichment
causing eutrophication, overfishing, maritime activities and climate change
(Jutterström et al. 2014; Newton et al. 2014).

About a century ago the nutrient condition in the Baltic Sea was very differ-
ent compared to today with oligotrophic conditions and low values of an-
thropogenic additions of nitrogen and phosphorus. The nutrient status
changed drastically when urbanisation and the change to large-scale agricul-
ture took place in the 1950’’s (Gustafsson et al. 2012), altering the system to
eutrophic conditions (Conley et al. 2009; Savage et al. 2010). The strong
pressures onto the Baltic Sea have made it one of the most polluted seas in
Figure 2 Map over Europe and the Baltic Sea. The Baltic Sea area and the regions studied in this thesis are marked up with red squares and names; the Bothnian Sea in the north (paper III and V); the North Western Baltic Proper (paper I, II, III, IV and V) in the central parts; the Skagerrak (paper V) at the northern West Coast.

the world, and eutrophication is considered one of the most serious problems (Cederwall and Elmgren 1990; HELCOM 2007). Nixon (1995) defines eutrophication as “an increase in the rate of supply of organic matter to an ecosystem”. Increased nutrient input stimulate the growth of phytoplankton and macroalgae (e.g. filamentous benthic species) that cause an imbalance of the functions in the aquatic ecosystem. In turn this leads to numerous negative processes, which all interact with one another, such as larger algal blooms that occur more frequently, which lead to a production of excess organic material consuming more oxygen when being decomposed, leading to hypoxia (oxygen depletion) in the sea bottoms. The changing conditions alter the benthic flora and fauna communities, and some are killed (Larsson et al., 1985; Diaz and Rosenberg 2008). Hypoxia caused by eutrophication is of global concern (MA 2005; Diaz and Rosenberg 2008), and has increased in the Baltic Sea, especially in the coastal zones (Conley et al. 2011). Figure 1 shows a global map with areas of hypoxic systems, including the Baltic Sea (Diaz and Rosenberg 2008). Low oxygen conditions in the bottom water stimulate benthic phosphorus release (Viktorsson et al. 2013), raising phosphorus concentrations in the water column (Conley et al. 2002) and thereby reinforcing the effects of eutrophication (Vahtera et al. 2007). The latter are also reinforced in the Baltic Sea by the strong and permanent halocline, and the seasonal thermoclines in spring and summer, restricting the mixing of the water masses. The sources of nutrient loadings to the coastal zones are mostly run-off from land and benthic remineralization in shallow areas (Tett et al. 2003). Hence, all land pollutants enter the open sea via the coastal zones, making them particularly vulnerable to eutrophication as dilution often is slow, due to restricted water exchange (Tett et al. 2003).
Since the effects of eutrophication occur on different scales and in different ecosystems, studies of the pelagic ecosystems are important as they respond strongly both to terrestrial and atmospheric changes and are linked to deep layer processes, such as processes in the bottom-substrate. The mitigation and reduction of the anthropogenic pressures and undesirable perturbations in the Baltic Sea are in their nature of international concern, and common policies and agreements are required for this large region.

**Directives and International Polices**

The consequences of the pressures on the Baltic Sea are strong, undesirable perturbations, and several international agreements, directives and common policies aim to reduce the effects on this sensitive ecosystem. The first response to the increased anthropogenic impact on the sea was with the first establishment of a convention, in 1974 between seven coastal states, the Helsinki Convention on the Protection of the Marine Environment of the Baltic Sea Area (HELCOM 1974). The first common polices to reduce the anthropogenic nutrient input within Europe were established in 1991 with the European Council's Urban Wastewater Treatment Directive (UWWTD) (EEC 1991a) and the Nitrates Directive (EEC 1991b). In 1992 the Helsinki convention was extended to all bordering states as well as the European Community (HELCOM 1992), bringing more countries together. Eight years later, in 2000 the main European directive for water quality was created and was in the following years implemented within all member states: the European Commission's Water Framework Directive (WFD) (European Commission 2000). Today, most monitoring programmes for water quality within the European Union are linked to the requirements within the WFD to regularly monitor all inland, transitional and coastal waters, and improve the health of those waters that do not meet the targets of good ecological status.

HELCOM has developed a special plan for the Baltic Sea to enhance and develop the improvements of the environment. Hence, the Baltic Sea Action Plan (BSAP) was established in 2007 (HELCOM 2007). In 2008, a second water directive from the European Commission, the Marine Strategy Framework Directive (MSFD) (European Commission 2008), was decided. The formation and implementation of the MSFD aim of achieving good environmental status in a ecosystem-based approach, have made all waters, including the open sea, within Europe to be monitored and managed. Sweden’s Parliament has adopted 16 Environmental Objectives with the overall responsibility from the Swedish Government (Swedish EPA 2015). Objectives number 7 “Zero Eutrophication” and number 10 “A Balanced Marine Environment, Flourishing Coastal Areas and Archipelagos” are also relevant for this thesis but not further studied. Outside the Baltic Sea region and the
European Union the same problems are acknowledged, and programs have been developed to manage the seas, e.g. the OPSAR convention and US EPA (OECD 1982; OSPAR Commission 1992; US EPA 1996; OSPAR Commission 2008). By identifying the environmental problems concerning our common water quality at high political agendas, a framework based on international legal agreements has been established. This enforces joint monitoring and management strategies for human disturbed waters.

Water Quality Monitoring

Monitoring of the water quality is not new and the features of the sea have been studied for centuries. For example, the water transparency has been measured since 1866 (Secchi 1866; Lewis et al. 1988), ocean temperature since 1870 (hadobs.metoffice.com), salinity profiles since 1958 (Ingleby and Huddleston 2007; hadobs.metoffice.com) and chlorophyll since 1954 (www.nodc.noaa.gov), and in the Baltic Sea in general since 1980 (www.smhi.se/k-data/marine_environmental_data.html) and specifically in Himmerfjärden bay since the 70s (Elmgren and Larsson 1997). However, as we now are living in the Anthropocene (Crutzen 2002), causing multiple pressures on our closest environments and over the whole Earth, there is even a more immediate need to follow and study the changes in the ecosystems. Monitoring water quality for inland and coastal waters is a requirement for many governments and the private sector. These requirements include identifying long-term trends and understanding emerging problems over large areas that contain numerous water bodies – all to be done in near real-time.

The relevant parameters, in this thesis, for water quality monitoring can be found in the following legislations and guidelines, valid for the Baltic Sea;

- The Water Framework Directive 2000/60/EC, Annex V; Description of which elements that need to be monitored regularly for the assessment of the correct classification of the ecological status (European Commission 2000).


Several indicators are defined as important to monitor and assess the ecological status of the water bodies within the WFD and the environmental status within the MSFD for the achievement of the goals. For the WFD the goal is to achieve good ecological status of all water bodies (including marine waters up to one nautical mile from the shore) by 2015 and for the MSFD to achieve good environmental status in Europe’s marine waters by 2020. Also within the BSAP monitoring indicators are required to achieve a Baltic Sea in good environmental status by 2021 and the overall goal to have the Baltic Sea unaffected by eutrophication. Below, the monitoring indicators relevant for this thesis, and also mentioned within in the EU directives, are listed and described.

**Phytoplankton biomass**

Phytoplankton biomass is one of the water quality parameters to be measured for the classification of water bodies within the WFD (European Commission 2000), and the chlorophyll-a concentration is commonly used as a proxy for the standing stock of phytoplankton (Morel 1980; Ferreira et al. 2011).

Within the assessment for the WFD in Sweden, the monitoring of chlorophyll-a in each water body should be carried out at least three times under the period June to August and the data from at least three years within a six-year period shall be used (HaV 2015). Within the MSFD in descriptor 5.2 the chlorophyll concentration within the water body should be monitored to measure direct effects of nutrient enrichment according to the guidance in the WFD. Within the BSAP the monitoring program shall account for “events (e.g. toxic algal blooms) of importance for human health, recreational values or other economically important sectors” (HELCOM 2014). The ecological objective (in the BSAP) to have natural levels of algal blooms is evaluated using the chlorophyll-a concentration as an indicator. Hence, the chlorophyll-a concentration shall be monitored with a sampling frequency of more than 12 times per year (monthly but with weekly sampling in the vegetative period). Sweden shall sample a subset of 19 stations (with a sampling frequency minimum 12 times per year) for chlorophyll and 5 stations (2 coastal and 3 open sea) with high sampling frequency (20-30 times per year and weekly during the vegetative period). Chlorophyll-a is studied in papers I, II and V, as a proxy for phytoplankton biomass.

**Secchi depth**

According to HELCOM (2007), the water clarity is a reflection of eutrophication via the changes in phytoplankton biomass and other small organic particles. However, water clarity is also affected by changes in the amount of
other coloured substances that are related or most often unrelated to eutrophication. The objective to have clear waters within the BSAP is evaluated by using summer Secchi depth values. Within the WFD, transparency is one of the quality elements for the classification of the ecological status within coastal waters associated with the chemical and physical-chemical elements that support the biological elements (European Commission 2000). Secchi depth is used as a proxy for transparency, and the Swedish requirement for assessment are monthly measurements between June to August within a 3-year period in accordance with the HELCOM Combine manual (HaV 2015). Within the MSFD in descriptor 5.2 the water transparency related to the increase in suspended algae should be monitored to measure the direct effects of nutrient enrichment according to the guidance of the WFD. For the monitoring program within the BSAP Sweden shall sample Secchi depth at 52 stations 1-2 times per year, at 19 stations with a sampling frequency of minimum 12 times per year, at 5 stations (2 coastal and 3 open sea) with high sampling frequency (20-30 times per year and weekly during the vegetative period). The Secchi depth is studied in papers I, III and V.

Additional optical parameters

For the background assessment and to be able to quantify the effects of anthropogenic activities within the Baltic Sea, all other measurements shall be done in order to be able to account for the annual cycles of hydrographical and hydro-chemical parameters. Hence, measurements of turbidity, humic matter and light attenuation are examples of other optical parameters required to be monitored within the BSAP and the MSFD (European Commission 2008; HELCOM 2014).

Vertical light attenuation between 400 and 700 nm is the same as the photosynthetically active radiation (PAR), and it is stated within the BSAP monitoring programme that it shall always be measured when primary production measurements are performed. It can be derived directly from PAR irradiance (400-700 nm) measurements at different depths, or inferred indirectly from Secchi depth measurements (HELCOM 2014).

Humic/Organic matter

Humic matter should be measured to account for the annual and seasonal cycles of the hydro-chemical parameters within the BSAP (HELCOM 2007). Hence, measurements are included in the Swedish BSAP monitoring program and should be sampled at a subset of 19 stations, with a minimum sampling frequency of 12 times per year. Also, as turbidity, is organic matter mentioned in the indicative list in Annex III of the MSFD under the category “pressures and impacts” (European Commission 2008). The member states
are obliged to have an initial assessment of the inputs of organic matter from e.g. sewers, aquacultures in marine environments and riverine inputs, and also the pressure of nutrient and organic matter enrichment. Furthermore, a monitoring program and respective target limits should be set up if needed, based on the initial assessment. In paper III, the coloured dissolved organic matter is used as a proxy for dissolved organic matter from e.g. river inputs.

**Turbidity**

For the initial assessment of every marine region or sub-region, turbidity is listed as one of the physical and chemical characteristics to measure (Annex III in the MSFD, European Commission 2008). This initial assessment shall be used to determine good environmental status, based on the parameters in the indicative list. Hence, measurements of turbidity should be included in the monitoring programmes. Furthermore, shall the turbidity be measured in order to correct for possible error in e.g. precise analysis of phosphate and nitrite within the HELCOM COMBINE manual (HELCOM 2014). Turbidity may be used as an indicator/proxy for suspended particulate matter (paper IV).

**Bio-Optical Components**

In this study, bio-optics is defined as the study of the interaction between living organisms, dissolved and suspended constituents with the light in natural waters. Bio-optical components influence the absorption and scattering processes within the underwater light field. Water itself interacts with light, as it absorbs and scatters light. The other three main bio-optical components in water are phytoplankton, suspended particulate matter, and coloured dissolved organic matter. For remote sensing, knowledge of the bio-optical constituents is an important factor. Below are descriptions of each of them.

**Water**

Pure water is blue due to its light absorption at different wavelengths, characterized by very low absorption in the blue and green parts of the visible spectra and increasing in the yellow to higher absorption in the red and near-infrared with a very strong absorption in the infrared parts of the spectrum (Kirk 2011) (Figure 3). The blue colour of water is more easily seen in oceanic and coastal waters than in the small amount contained in a drinking glass. If water molecules did not absorb the light energy from the sun and convert it into heat the whole climate on earth would look different (Doerffer 2010). The scattering process of water molecules is wavelength dependent and have a high scattering in all directions (Kirk 2011).
Figure 3 Graph over the absorption and scattering spectra in the visible wavelengths for the different bio-optical components. The solid lines represent absorption (right y-axis) and the dashed lines scattering (left y-axis). Where $b_{(w)}$, $b^*(\text{phyto})$ and $b^*(\text{tripton})$ are the backscatter of water, specific backscatter of phytoplankton and tripton, (i.e. SPM) and $a_{(w)}$, $a^*(\text{phyto})$, $a_{(\text{tripton})}$ and $a_{(\text{CDOM})}$ are the absorption of water, specific absorption of phytoplankton, tripton and CDOM. A detailed description of the absorption and scattering properties of the optical components are given in Appendix I. The spectral absorption and scattering coefficients are based on a simulation in BI-OPTI (Hoogenboom, 1996).

Phytoplankton

According to Jeffrey and Vesk (1997) 75% of the global chlorophyll turnover occurs in oceans, lakes and rivers, whereas only 25% occurs on land by terrestrial plants. The absorption of light by phytoplankton (such as algae and photosynthetic cyanobacteria) is carried out by their photosynthetic pigments prior photosynthesis. The main pigments involved in photosynthesis are chlorophylls, carotenoids and phycobilin proteins. Since phytoplankton pigments are optically active, their absorption properties can be measured using spectrophotometry. The light spectrum of chloroplasts is affected by the protein complexes (e.g. carotenoids- and phycobilin pigments, and light-harvesting complexes), which they bind to and associate with. The role of these complexes is to capture the energy of the light photons and transfer it into chemical energy for growth (Jeffrey and Vesk 1997). Different algae contain different combinations of photosynthetic pigments, which lead to differences in the absorption of light at different wavelengths. Therefore, algae and cyanobacteria species can be distinguished from each other spectrophotometrically, by characteristic absorption curves. Today the knowledge of the absorption of light by phytoplankton is largely due to several studies of laboratory cultures. The absorption spectrum of chlorophyll-a
changes with the total amount, the photosynthetic pigments and the composition of species that are present in the water. A typical absorption spectrum of chlorophyll is characterized by two peaks, one larger around wavelength 440 nm and one smaller around 664 nm (Figure 3). Although we know a lot about the optical properties of phytoplankton there is still a lack of knowledge about the light absorption properties by phytoplankton in natural waters (Kirk 2011).

**Coloured Dissolved Organic Matter, CDOM**

The largest component of dissolved organic carbon (DOC) is coloured dissolved organic matter, CDOM (also known as humic substances, yellow substance, gilvin or Gelbstoff). This is a complex group of compounds that arise from the microbial decomposition of organic matter. CDOM varies in size from dissolved compounds to large aggregations of visible size and is chemically classified into three main fractions based on solubility characteristics (Kirk 1994).

- **Humin** is non-dissolvable material
- **Humic acids** are alkali-soluble acids that precipitate on acidification
- **Fulvic acids** are the smallest humic materials that remain in solution

CDOM is a small molecule that has a chromophoric response. The chromophore is the part of the molecule that absorbs, transmits or reflects certain wavelengths of visible light and therefore is responsible for its colour. These molecules contain electrons that occupy larger regions of space (molecular orbitals) and are not strongly fixed in covalent bonds between particular pairs of atoms so that they may be associated with several atoms. Electrons can absorb light and the reflectance of the remaining transmitted light gives rise to the observed yellow to brow colour of the solution. Due to this characteristic and high concentrations some water bodies are yellow-brown and for this reason the Baltic Sea has its characteristic optical colour (Kirk 1994). A typical absorption coefficient of humic substances is very high in the blue end of the visible spectrum, decreasing steadily with higher wavelength towards the red generating a logarithmic spectral slope (Figure 3). In the ultraviolet region the absorption is even higher. The absorption coefficient of CDOM, $g(\lambda)$, is usually measured at 440 nm (Kirk 2011), since it corresponds approximately to the mid-point of the maximum photosynthetic peak by chlorophyll-a pigment in the blue. The absorption in the blue is used to derive the sum of phytoplankton, CDOM and non-algal particle absorption. MERIS has a band at 442.5 (blue) nm to capture the chlorophyll maximum and one at 412.5 (violet) to distinguish the contribution from CDOM and non-algal particles (Table 1). The scattering of CDOM is negligible.
Suspended Particulate Matter, SPM

Suspended particulate matter (SPM) refers to all particulate substances in the water, including plankton and humic matter. The non-planktonic part of SPM is made up of particulate humic material, originating from soils or decomposed algae, and mineral particles from soils or sediments. Shallow waters can contain large amounts of suspended material derived from resuspension of sediments or from soil erosion in the catchment. Inorganic suspended particulate matter scatters to a very large extent while organic SPM mostly absorbs light (Figure 3). The absorption spectrum by SPM also decreases logarithmically from the blue to the red end of the light spectrum and is very similar but not as smooth as the exponential absorption spectra of CDOM. The slopes of SPM absorption spectra are usually less steep (Figure 3) (Kirk 2011). SPM is also referred to as Total Suspended Matter (TSM) (Doerffer 2002).

Remote Sensing, Light and Bio-Optics

Remote sensing means that data of an object or phenomena is received and analysed from a large physical distance without any physical contact. Generally it refers to Earth and atmosphere observations and is usually performed with sensors placed on an aeroplane or satellite. Remote sensing can be either passive or active, where passive remote sensing makes use of and registers the electromagnetic radiation from the Sun, whereas self-emitted radiation is used in active remote sensing (e.g. radar applications). Ocean colour and aquatic remote sensing, as used in this thesis (paper I, II and IV), is when the radiation from the Sun is reflected from the water, via the atmosphere or sky, to a sensor (the instrument receiving the radiation signal). The sensors used can be either conventional cameras for visible or near infrared (NIR) light or, as in this thesis, multi-spectral radiometers that register other types of wavelength.

In 1978, satellite research of the sea surface started with the launch of the Coastal and Zone Colour Scanner (CZCS) (operating time: 1978-1986), on the National Aeronautics and Space Administration (NASA) satellite Nimbus-7, making ocean colour remote sensing a relatively recent research field. Using the results from CZCS, NASA could show that it was possible to retrieve measurements of temperature, sea surface roughness and topography from the spectral reflectance (i.e. colour) from space. Many other ocean colour missions have been launched since then with constant improvements to the sensors due to feedback loops of both the research community and end-users. The most widely used satellite sensors for ocean colour applications have been the NASA satellites “Sea-viewing Wide Field of View Sen-
sor” (SeaWiFS) (operating time: 1997-2010), ‘Moderate Resolution Imaging Spectroradiometer’ (MODIS) Aqua/Terra (operating time: 2002- respectively 2000-) and the European Space Agency (ESA) satellite sensor “MEedium Resolution Imaging Spectrometer” (MERIS).

The satellite data used in this thesis (paper I, II and IV) has all been derived from the multi-spectral spectrometer MERIS, which was situated on board the satellite platform ENVISAT (operating time: 2002-2012). Without the synoptic data and the high temporal resolution provided by Earth observation satellite missions several global processes in the oceans could not have been observed. For example, the use of satellite data for monitoring applications has provided us with a completely new perspective on aquatic ecosystems and we have gained significant understanding of global ocean systems and the dynamics within. The spatial and temporal extent of algae blooms and accurate sea surface temperature measurements (Platt and Sathyendranath 2008) and periods of El Niño-La Niña (McClain 2009), are good examples of this.

**Distinctions Between Oceanic and Coastal Waters**

The conventional concept within the ocean colour research of a division of the oceanic waters into two categories, case 1 and case 2 waters, was first introduced by Morel and Prieur (1977). The classification of case 1 waters is when only the optical properties (the absorption and scattering of visible light) of water itself and phytoplankton determines the colour of the water. It means that the rather small contribution from other components (such as heterotrophic flagellates and bacteria as well as viruses) can be neglected. Hence, the optical characteristics of the water are a function of the phytoplankton concentrations. The classification of case 2 waters is logical when the colour of the water is also determined by the optical properties of CDOM and/or SPM. The optical components are treated separately as they can vary independently from each other. Also the bottom reflectance may have an influence on the water-leaving signal in shallow waters (Morel and Prieur 1977; IOCCG 2000). The Baltic Sea and many coastal areas are classified as case 2 waters, since the variations in the optical properties are dominated by factors other than phytoplankton. It has previously been found that CDOM is the most important optical component in the Baltic Sea, as it absorbs more light than phytoplankton and SPM, and therefore contributes most to the attenuation (Ferrari and Dowell 1998; Kratzer and Tett 2009). Hence, the applications of remote sensing and bio-optical data in the Baltic Sea and other case 2 waters are more complex. A schematic figure of the optical division is presented in Figure 4 from IOCCG (2000).
Figure 4 Ternary plot of case 1 and case 2 waters. Generally the Baltic Sea would be placed somewhere at the mid left side, quite low since it contains high loads of yellow substances (CDOM), phytoplankton and quite little suspended materials (SPM). It is classified as case 2 waters. Figure reprinted from IOCCG (2000).

The Light path in Water and Air

The reflectance signal from water that is detected by satellites (the signal to noise ratio) is 10% in case 1 waters, whereas less than 1% (only 0.4%) of the top of atmosphere (TOA) signal in CDOM dominated case 2 waters, like the Baltic Sea, (IOOCG 2010). Hence, 90-99.6% of the light is not reflected back into space (IOCCG 2010). What has happened on the way?

The light that reaches the satellite sensor, e.g. MERIS, is the water-leaving radiance ($L_w$) or radiance at the top of atmosphere. The photons have travelled from the Sun through the atmosphere, and some have been absorbed and scattered on the way before entering the water at the sea surface. At the surface certain proportion of the light is directly backscattered into the atmosphere (called sun glint if it appears on the image or in the view of vision) and the rest enters the water. In the water the light photons interact with the four main different bio-optical components: water itself, phytoplankton, suspended particulate matter, and coloured dissolved organic matter. After the interactions with the components in the water the light is backscattered up through the sea surface, entering the atmosphere again, and once more interacting with the aerosols before reaching the satellite sensor. For a schematic overview see Figure 5. The information from MERIS is then transferred, saved and archived. The characteristics of the long path the
light has travelled through are thus crucial to understand in order to correctly interpret and receive the information from the satellite.

The colour of the water and the light signal reaching the sensor are defined by the properties and concentrations of the components present within the water column and the water itself as well as the air molecules and aerosols in the atmosphere. Hence, the final signal carrying the information about the sea is affected by the incident sunlight (the downwelling irradiance, \( E_d \)) that reaches the sea surface, the atmosphere, pure water (by absorption and scattering) and the absorption and scattering properties of the in water constituents (chlorophyll-a, SPM and CDOM). The top-of-atmosphere signal detected by MERIS has to be atmospherically corrected (i.e. corrected for absorption and scattering of the aerosols and air molecules) and is then converted to remote sensing reflectance (see detailed description below). By processing the remote sensing reflectance, ocean colour data products from the satellites are received. Examples of those are concentrations of chlorophyll pigments, SPM and CDOM absorption. The reflectance itself at different wavelength is also one of the main products as many algorithms use it as an input, e.g. the turbidity algorithm developed in paper IV.

Inherent optical properties (IOPs) are independent of the changes in the radiance distribution (angular distribution and the incident light field), they depend only upon the medium, e.g. the absorption and scattering coefficient of pure water, chlorophyll, SPM and CDOM (Prieur and Sathyendranath 1981; IOCCG 2006). Apparent optical properties (AOPs) depend both on the medium (the IOPs) and the light field within the medium, i.e. the ambient light field and the angular distribution (Kirk 2011). Examples of AOPs are irradiance, radiance and remote sensing radiance. The theory of inherent and apparent optical properties is explained more detailed in Appendix I.
Figure 5 A schematic illustration of the factors influencing the water-leaving radiance (detected by the remote sensor, e.g. MERIS), the remote sensing reflectance and the retrieval of the water quality monitoring products. It changes with the effects of water surface roughness, scattering and absorption in the atmosphere, scattering and absorption by water, scattering by SPM (Suspended Particulate Matter), absorption and scattering of phytoplankton, absorption by CDOM (Coloured dissolved Organic Matter) and also with depth by sometimes effects of bottom reflectance or absorption and reflectance from macroalgae. A more detailed explanation of the processes involved in this illustration is given in Appendix I.
SCIENTIFIC METHODS

Study Areas
The area of investigation for this thesis is the Baltic Sea. It consists of optically complex waters (i.e. optical case 2 waters), with high levels of CDOM absorption, as well as strong influence from both chlorophyll-a and coastal SPM. In paper I and II the Himmerfjärden bay, situated in northwestern Baltic proper, was used as a study case of how remote sensing and bio-optical methods can be used in the coastal zones. In paper III, a coastal region in the Bothnian Sea as well as several sub-areas within the Baltic proper were included to conduct a comparative study. In paper IV, Himmerfjärden bay was used as an example for the development and application of the SPM and turbidity model. In paper V, the Skagerrak area was included, providing data for Secchi depth studies in three different Baltic Sea regions. The regions investigated are presented in the map over the Baltic Sea area (Figure 2), detailed descriptions of the study area maps over in situ sampling locations can be found in each paper. The areas of investigation were chosen according to the available research facilities, scientific collaborations and monitoring data. For the Himmerfjärden area with the Askö laboratory as a base, the aquatic remote sensing group at Stockholm University has collected a substantial database for bio-optical research and validation of satellite data. The research facilities used were the Askö laboratory at the Baltic Sea centre in the Baltic Proper, the Umeå marine sciences centre at Umeå University in the Bothnian Sea, and the Oceanographic unit at the Swedish Meteorological and Hydrological Institute (SMHI) in the Skagerrak.

Field Data
All field data in this thesis has been collected and analysed accordingly to standard scientific methods. Metadata, such as for example wind direction, visibility, air pressure, cloud cover, wave characteristics and water temperature have been collected accordingly to the SeaWiFS and MERIS validation protocols, (Mueller and Austin 1995; Doerffer 2002) for match-up data by the remote sensing group at Stockholm University. Detailed descriptions of sampling, laboratorial and chemical analyses can be found in the method parts for the respective papers.
Satellite Data

As mentioned before the satellite sensor used in this thesis (paper I, II and IV) is the multispectral spectrometer MERIS on ENVISAT. ENVISAT stopped communicating in spring 2012 (two days before our scheduled field campaign!). MERIS was the first ocean colour sensor especially adapted to coastal zones. During 10 years MERIS provided global data every 2-3 days. The time series from MERIS are unique, as it provides very high quality images of ocean colour for open oceans and coastal areas with a ground spatial resolution of 300m x 300m in all spectral bands (Doerffer et al. 1999). Other ocean colour satellites usually only provides data in 1 km resolution and are therefore mostly restricted to open sea applications. An exception is NASA’s MODIS which has a restricted number of bands with 250 m and 500 m resolution and therefore, to some extent, can also be used for coastal applications. When measuring the reflectance the bandwidth is important for the accuracy, where narrower and more spectral bands improves the accuracy. In order to derive the diffuse attenuation of light, $K_d(490)$, chlorophyll-a concentration, SPM concentrations and CDOM from reflectance data the bands in MERIS were carefully chosen (Doerffer et al. 1999). The narrow bandwidth over a large spectrum, the high resolution and the choice of specific spectral bands for ocean colour measurements are the main features that make MERIS especially suited for studies of coastal as well as inland waters. In Table 1 MERIS 15 spectral bands and their applications are presented (between 390 and 1040 nm), of which nine are in the visible and six in the near infra-red spectra (ESA 2011). When processing satellite data the most critical procedure is the atmospheric correction, i.e. the correction of the absorption and scattering by aerosols in the atmosphere. Furthermore, high quality ocean colour data requires having pixels with information of only the water reflectance. Hence, different types of flags addressing anomalies in the reflectance spectra are used to select the valid pixels. Examples for specific flags are cloud, haze, sun glint, low viewing angle, land and algae blooms. The satellite data used in this thesis was processed by Christian Vinterhav and Susanne Kratzer at Stockholm University and Petra Philipson, Brockmann Geomatics Sweden AB, for paper I, by Brockmann Consult GmbH Germany and Petra Philipson, Brockmann Geomatics Sweden AB within the ESA project Marcoast-2 in paper II, and the data for paper IV was provided by CoastColour and processed by Jose M. Betrán-Abaunza at Stockholm University. The detailed description of the procedures and data sources is found under the method sections of all papers.
Table 1. MERIS 15 Spectral Bands and their applications adopted from ESA (2011).

<table>
<thead>
<tr>
<th>Band Index</th>
<th>Band Centre (nm)</th>
<th>Bandwidth (nm)</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>412.5</td>
<td>10</td>
<td>Yellow substance and detrital pigments</td>
</tr>
<tr>
<td>2</td>
<td>442.5</td>
<td>10</td>
<td>Chlorophyll absorption maximum</td>
</tr>
<tr>
<td>3</td>
<td>490</td>
<td>10</td>
<td>Chlorophyll and other pigments</td>
</tr>
<tr>
<td>4</td>
<td>510</td>
<td>10</td>
<td>Suspended sediment, red tides</td>
</tr>
<tr>
<td>5</td>
<td>560</td>
<td>10</td>
<td>Chlorophyll absorption minimum</td>
</tr>
<tr>
<td>6</td>
<td>620</td>
<td>10</td>
<td>Suspended sediment</td>
</tr>
<tr>
<td>7</td>
<td>665</td>
<td>10</td>
<td>Chlorophyll absorption, Chl fluorescence reference</td>
</tr>
<tr>
<td>8</td>
<td>681.25</td>
<td>7.5</td>
<td>Chlorophyll fluorescence peak</td>
</tr>
<tr>
<td>9</td>
<td>708.75</td>
<td>10</td>
<td>Chlorophyll fluorescence reference, atmosphere corrections</td>
</tr>
<tr>
<td>10</td>
<td>753.75</td>
<td>7.5</td>
<td>Vegetation, clouds</td>
</tr>
<tr>
<td>11</td>
<td>760.625</td>
<td>3.75</td>
<td>O₂ R-branch absorption band</td>
</tr>
<tr>
<td>12</td>
<td>778.75</td>
<td>15</td>
<td>Atmospheric corrections</td>
</tr>
<tr>
<td>13</td>
<td>865</td>
<td>20</td>
<td>Vegetation, water vapour reference</td>
</tr>
<tr>
<td>14</td>
<td>885</td>
<td>10</td>
<td>Atmospheric corrections</td>
</tr>
<tr>
<td>15</td>
<td>900</td>
<td>10</td>
<td>Water vapour, land</td>
</tr>
</tbody>
</table>
CENTRAL FINDINGS AND DISCUSSION

All five papers within this thesis contribute, in different ways, to improved monitoring of the coastal zone. Below are the main findings for each parameter described and discussed with references to the papers contributing to the insights. The results and the development of the operational satellite system and the conclusions within the Marine policy paper (paper I) are the opening for this thesis. The results of paper I give a well-illustrated summary of the incorporation of bio-optics and remote sensing within integrated coastal zone management for the Baltic Sea. In paper I, the main environmental issue for the study site, Himmerfjärden bay, was identified to be eutrophication (Franzén et al. 2011; paper I). Hence, in the latter papers of this thesis the use of different bio-optical parameters for water quality assessment and remote sensing as an additional tool for monitoring and management have been further developed and evaluated scientifically.

Conceptual Model

In paper I, two conceptual models were developed. The first for evaluation of how bio-optical parameters and ocean colour remote sensing can be used within monitoring and integrated coastal zone management and the second as part of a physical-biological model by providing input data and assessment of output data. The first model is shown below (Figure 6) with an extension for how the other studies of bio-optical measurements and remote sensing (paper II-V) within this thesis are linked to the conceptual model. Furthermore, it shows where the different bio-optical parameters can contribute in general to the assessment of water quality and identification of pressures within coastal zone management.

Chlorophyll-a

In paper I the chlorophyll-a concentration was identified as one of the main indicators to monitor the Himmerjärden bay, with the response eutrophication linked to anthropogenic nitrogen input. Monitoring of chlorophyll-a is included in most monitoring programmes as phytoplankton biomass is an important factor for pelagic and benthic ecosystems. Phytoplankton responds
quickly to several changes in the environment, such as light conditions and nutrients. Algal blooms can be problematic and raise cascade effects on the ecosystems. Hence, the chlorophyll-a concentration is one of the main indicators for eutrophication and by regular monitoring of the reductions and actions taken to improve the water quality the effects can be evaluated. Therefore, a lot of efforts are put into chlorophyll-a as water quality indicator and also regarding the composition of phytoplankton communities. Furthermore, the retrieval of chlorophyll-a from satellite reflectance measurements are also developed (Kratzer and Vinterhav 2010; Matthews 2011 and Beltrán-Abaunza et al. 2014). In paper II, chlorophyll retrieved from MERIS reflectance was evaluated as an additional monitoring tool for chlorophyll-a assessment in coastal areas compared with conventional in situ monitoring data from ships. The amount of chlorophyll observations was increased by 125-176% by adding satellite data. This increase in data showed that both the temporal and spatial coverage of the phytoplankton dynamics could be improved, although this study area is sampled in situ rather frequently when compared to other sites. The increased temporal and spatial coverage of satellite data improves the assessments and evaluations of algal blooms. Moreover, the correlations between both match-up data (0-3 days difference) and monthly means were high (r=0.9 and r=0.76), with a lower bias for the monthly means. Chlorophyll-a data from remote sensing can also be used for the validation of eutrophication models (paper I). The effect of chlorophyll-a

Figure 6 Conceptual model modified from paper I on how remote sensing and bi-ooptical studies can be used within monitoring and management. An extension of the model with references to the papers in this thesis is shown outside the black box. Reprinted with the permission from Elsevier.
concentration, along with other optical parameters, on another indicator for eutrophication, Secchi depth, was evaluated in paper V. The results from this study are described under the section about Secchi depth.

**Coloured Dissolved Organic Matter**

In paper III the Öre Estuary in the Gulf of Bothnia was compared with coastal gradients in the Baltic Proper. The relationship between the optical properties of the CDOM pools and the empirical relationships to DOC, salinity, and Secchi depth was found to be different for the two regions. The results indicate more freshwater influence onto the CDOM pool in the Gulf of Bothnia with higher allochthonous material. Another main result found was a partial decoupling between CDOM and DOC, where the proportion of DOC related to CDOM absorption was larger in the Gulf of Bothnia. The information of the seasonal variations, the local relationships to salinity, found in paper III, contribute to the understanding of the annual cycles of the hydro-chemical parameters within the BSAP (HELCOM 2014) and as input data in bio- or hydro-chemical models of nutrients and primary production. Furthermore, the changes in CDOM absorption are important to monitor for climate change investigations, as future scenarios project increased loadings of land-runoff, caused by increased precipitations (Meier et al. 2012a; Meier et al. 2012b; paper III). Retrieving CDOM absorption correctly from remote sensing in optical case 2 waters, such as the Baltic Sea, is a challenge due to the very low signal-to-noise ratio. CDOM is systematically underestimated in Baltic Sea waters, but can be corrected for by local corrections factors (Beltrán-Abaunza et al. 2014). Hence, the ranges and the optical relationships in paper III can contribute to the development of improved remote sensing algorithms (i.e. inverse modelling) for CDOM and chlorophyll-a, especially in the more CDOM-rich northern parts. Furthermore, studies of in situ sampled CDOM absorption and the optical relationships are important for chlorophyll-a and Secchi depth algorithm developments (paper II, III and V), as remote sensing reflectance is strongly affected by CDOM in the blue.

**Turbidity and Suspended Particulate Material**

Turbidity measurements indicate the amount of particles in the water and are an easy to measure and a cost-effective method to evaluate the seasonal and spatial dynamics of water quality (paper IV). Turbidity is used as a proxy for SPM. Changes in turbidity affect the transparency of the water and therefore also the ecosystems (Kirk 2011). A model to predict SPM concentrations based on in situ turbidity measurements was developed in paper IV, and was
found to be robust with a strongly predictive power. The *in situ* model was implemented into a satellite algorithm to retrieve SPM from remote sensing reflectance and turbidity. The bias of the SPM retrieval decreased from about 11% from the standard satellite processor to less than -5% and the relative error was reduced with about 7%. The improved algorithm also enhanced the patterns of the spatial variability in the satellite images.

Monitoring of water quality by measurements of turbidity and SPM is important for understanding coastal processes, and turbidity is listed as a mandatory parameter in the MSFD. The use of inorganic SPM as an indicator for coastal processes has been evaluated in Kratzer and Tett (2009) and Kyryliuk (2014). Turbidity and SPM also reflect other processes, such as resuspension of sediments and are also highly correlated to chlorophyll-a and Secchi depth (Davies-Colley and Smith 2001; Devlin et al. 2008; Devlin et al. 2011; Capuzzo et al. 2015). In paper V the effect of inorganic SPM to changes in Secchi depth and implications for eutrophication assessment is evaluated. The results from paper V are further discussed under the Secchi depth section. As a response to the demands in the MSFD, the Finish Environmental Agency (SYKE) includes almost daily satellite retrieved turbidity maps (250 m resolution) in their operational system processed with a local algorithm for MODIS and also previously MERIS (SYKE 2015a). Hence, the use of turbidity measurements within monitoring programmes would add information about the hydro-chemical cycles to be assessed within the MSFD.

Secchi Depth

Secchi depth is a key indicator both within the WFD and the HELCOM Baltic Sea Action Plan (European Commission 2000; HELCOM 2007) and transparency is one of the monitoring elements within the MSFD (European Commission 2008). In paper I the main indicator chosen to assess changes in water quality due to eutrophication was Secchi depth. Secchi depth was used as the direct link between both ecology (i.e. in the developed ecological model) and socially, as a measure of the social economy value for the residents and tourists (Franzén et al. 2011; Paper I). Furthermore, Secchi depth may also be a link between ecological models and ocean colour satellite data, as it can be directly derived from remote sensing reflectance, and it can also be used as an input for light conditions in physical-biological models. Similar to the diffuse attenuation coefficient $K_d(490)$ Secchi depth can be used as a parameter for light forcing within models as it is inversely related to $K_d(490)$. There are Secchi depth algorithms for satellite measurements in the Baltic Sea (Kratzer et al. 2003; Pierson et al. 2008), and they have recently been developed and improved for the whole Baltic Sea region by ap-
plying a generalised linear model to predict the inverse Secchi depth as a function of $K_d(490)$ by Stock (2015). Hence, the possibility to routinely measure satellite derived Secchi depth for monitoring of temporal and spatial changes and for management by incorporating satellite data in water quality assessments and management decisions are on the increase. However, as all optical constituents determine the Secchi depth, the latter is a complex and not always straightforward indicator (paper V). The results in this thesis show that the slopes for the relationships between Secchi depth and CDOM absorption varies, with steeper slopes in the Baltic Proper (paper III). The difference might be caused by the fresher terrestrial material associated with higher CDOM absorption in the Bothnian Sea, thus absorbing more of the light (paper III). Many management actions to reduce chlorophyll-a concentrations are also usually seen as a way to improve the Secchi depth. In paper V, empirical models for Secchi depth were developed, based on data from different optical regions and using chlorophyll-a and SPM concentration and CDOM absorption as predicting variables. It was found that the effects of the predicting variables to the variations in Secchi depth were not the same in the different local empirical models. The empirical models were based on the seasonal differences in the Bothnian Sea and different relationships among the prediction variables for both the Baltic Proper and the Skagerrak. In the Bothnian Sea the variations in Secchi depth were mostly explained by inorganic SPM and CDOM and only to a minor extent by chlorophyll-a. All three components together had a large influence in the Baltic Proper, with a stronger influence of inorganic SPM when compared to the other areas. The main contribution to the variations in the Secchi depth in the Skagerrak was due to CDOM, followed by chlorophyll-a, whereas inorganic SPM had little or no influence at all and chlorophyll-a concentration a pronounced influence. The Secchi depths were recalculated based on the empirical models by setting the chlorophyll-a values to the threshold for the reference value, or at the threshold value between moderate and good ecological/environmental status for each water body or region. The results showed that decreases in only chlorophyll concentrations, even down to the reference conditions, were not enough to reach the good ecological/environmental status of Secchi depth for each water body or region. Hence, our results show that using Secchi depth as an only indicator for changes in chlorophyll-a is not applicable in any of the investigated water types.

Remote Sensing and Bio-Optical Monitoring

Successful ecosystem based management of the water quality in the Baltic Sea requires effective, good and reliable monitoring methods. Regular monitoring programmes can to a certain extent fulfil the requisites for water quality monitoring with regards to legislation, although the environmental
changes are difficult to monitor. Most field and laboratory measurements are expensive to conduct and are usually restricted in temporal and spatial coverage (Kratzer and Tett 2009; Kratzer et al., 2011, papers I, II, and IV). Satellite measurements can increase both the temporal and spatial resolution with high accuracy of water quality indicators (e.g. Brockmann et al. 2004; Andrefouet et al. 2008; Platt and Sathyendranath 2008; papers I, II, IV). Thus, monitoring by remote sensing can improve data collection to meet the demands by directives and legislation (Gohin et al. 2008; Bresciani et al. 2011; Ferreira et al. 2011; Novoa et al. 2012; papers I and II). In the COMBINE manual, for the Baltic Sea Action Plan, satellite imagery is stated as supporting tool for monitoring the spatial distribution of phytoplankton biomass in the surface layer, and especially for surface accumulations of cyanobacteria (HELCOM 2014). There are some good examples of the use of remote sensing as an addition to in situ monitoring within the WFD, e.g. the studies by Chen et al. (2004; 2007b). Both Gohin et al. (2008) and Novoa et al. (2012) use chlorophyll-a derived from remote sensing for the assessment of water quality classes. The study by Novoa et al. (2012) was also highlighted by the European Commission (2012). Moreover, in a very recent study Cristina et al. (2015) was using MERIS data in the context of the MSFD. An operational satellite service at the Finish Environmental Agency delivers images of chlorophyll-a, turbidity and sea surface temperature on an almost daily basis for monitoring support (SYKE 2015a). The operational service developed in paper I provided high-quality satellite data of chlorophyll-a and SPM concentrations, CDOM absorption and Secchi depth. The data was easily accessible and could be directly accessed by the end users via a standard web browser through a GIS-based map service. The stakeholders and end users were strongly involved in the setting up of the service and gave valuable input. There are several other operational services for satellite data available in different European regions monitoring the water quality in e.g. the North Sea or lakes and marine systems based in the Netherlands, Belgium, Switzerland, Germany and Denmark. Earth observation missions provide data that transcends national boundaries and covers whole water basins, which makes it possible to follow the changes in whole regions at the same time. For example, both the Swedish Hydrological and Meteorological Institute and the Finish Environmental Agency provide forecasts of algal blooms and surface accumulations in the Baltic Sea during the summer months (Figure 7) (SMHI 2015; SYKE 2015b). Furthermore, the long-time satellite record for cyanobacteria blooms in the Baltic Sea has been evaluated recently by Kahru and Elmgren (2014). Operational remote sensing monitoring of both chlorophyll-a and SPM concentrations, turbidity and Secchi depth would be a helpful input for the assessment of good ecological and good environmental status within the European Commission’s water directives (papers I, II, IV).
In situ monitoring of bio-optical parameters, such as turbidity, is an easy and cost-effective way to assess hydro-chemical and biological changes in the system, as required by the Marine Strategy Framework Directive (European Commission 2008; paper IV). As mentioned before, it can also be retrieved accurately from remote sensing data. In situ data is needed for the development of algorithms, based on forward and inverse modelling, and for validation of satellite measurements. The same can be said about the assessment of humic substances by CDOM absorption of fluorescence measurements. Incorporating CDOM measurements to a higher extent within monitoring programs, both from remote sensing and in situ measurements, would improve the evaluation of hydro-chemical climate change effects as well as ecosystem changes (Andersson et al. 2015; paper III). Paper V re-evaluates Secchi depth as a direct indicator for chlorophyll changes caused by eutrophication, showing the need for more optical measurements within monitoring programmes.

Limitations for the retrieval of satellite data in the Baltic Sea are cloud cover (IOCCG 2000) and low azimuth angle of the sun during the winter months in high latitudes. Despite the regular cloud cover satellite data can provide information about bloom events at seasonal and annual scales, but may be limited in a highly variable environment with rapid changes (Frolov et al., 2013). Field sampling can provide detailed information about e.g. depth profiles on small spatial scales, whereas satellites provide large spatial scale patterns of the top layer. Therefore, a combination of in situ and satellite data is the best approach. Restrictions in the spatial resolution of the satellite sensors limits the data availability close to the coast (i.e. monitoring of the coastal zones), as the water pixels may get blended with the signal from land.
in addition to bottom reflectance within shallow areas. Data gaps between missions hamper real-time services and this is recognized within the remote sensing community (IOCCG 2008). Reducing the data gaps is a high priority for the Space Agencies and users, and the upcoming series of satellites within the Copernicus mission (via the Sentinel satellites) (Donlon et al. 2012) from the European Space Agency is a clear commitment towards reaching long-term satellite-based Earth Observation monitoring programs.

Image-based information is easily available and understandable and therefore a very powerful tool within management and for decision-making. The interpretations of satellite images without expert explanations should be used with caution, as special training and high processing skills are needed for an efficient and correct use of satellite data. Hence, the evaluation of satellite data may be limited for the general user. Therefore, close collaborations of researchers with end-users and stakeholders are of highest priority for the implementation of satellite data within monitoring and management. Dissemination of the progress and results to stakeholders and end-users is an important factor for the successful development of ocean colour and bio-optical products (paper I).

Studies of local relationships and differences in the inherent optical properties of water bodies are essential for the development and improvement of ocean colour algorithms. Thus, fulfilling the need for gathering bio-optical in situ data and addressing the uncertainties in their retrieval by remote sensing is a priority within the field.
The results from papers I, II and IV show that water quality products from bio-optical and remote sensing methods can be derived with high accuracy and be used to complement conventional in situ ship-based monitoring. In paper I the operational satellite service provided high-resolution water quality images of Secchi depth, chlorophyll-a and SPM concentration and CDOM absorption, delivered to end-users. The agreement between the monitoring methods compared in paper II showed that satellite retrieved chlorophyll-a concentrations can be used as a complementary method. The temporal resolution was shown in paper II to be increased if satellite measurements were to be used within monitoring programmes. The increase in observations would be more important for areas rarely sampled or for optical parameters not measured on a regularly basis, such as turbidity, SPM, CDOM and light attenuation. Satellite measurements also provide a more holistic view ecological systems. For example, the derived products from ocean colour satellite sensors can provide a basis for better decision making for coastal management by choosing investigation sites with contrasting water quality, taking local gradients into account and evaluating the existing monitoring locations. Spatial and temporal information increases, e.g. light attenuation maps show the dynamics of the physical conditions for algal growth (paper I). The increased spatial resolution is also shown in the time series in paper II, where the start, the development and the decline of a summer bloom was followed. Moreover, the coastal influence and the spring bloom development could also clearly be seen in the images. Comparison of the spatial dynamics of the SPM in paper IV shows improved accuracy and precision compared to the standard product from MERIS. With the new algorithm, coastal SPM could be more easily distinguished from SPM associated to algae.

The bio-optical and satellite methods developed and evaluated in this thesis are highly relevant for monitoring the ecological status of the water bodies within the European Union’s Water Framework Directive, to assess the environmental status of regions and sub regions for the European Union’s Marine Strategy Framework Directive and for HELCOM’s Baltic Sea Action Plan. The results are important for the Baltic Sea area, but also generally for other seas and international water management treaties (e.g. OSPAR). Using and developing bio-optical data and remote sensing can contribute to an improved capacity to assess and predict the changing status and trends relat-
ed to hydro-chemical cycles, eutrophication and climate change. For example, monitoring of CDOM absorption and SPM concentration can indicate changes in the terrestrial run-off due to e.g. climate change (paper III). The strong relationship found between turbidity and the concentrations of suspended particulate material in paper IV shows that increased turbidity measurements within monitoring programmes are a valuable water quality parameter. Satellite derived chlorophyll-a concentrations and Secchi depth could be used to a higher extent than today for the assessment of the ecological status within directives and legislation. In fact, the Swedish water authorities did use the satellite products based on the operational system in paper I, provided by Petra Philipsson (Brockmann Geomatics Sweden AB), for the latest WFD assessment of the ecological status for Swedish coastal waters. The satellite products were used as second choice data when *in situ* data was not available and the satellite-derived indicators were then used as expert judgment for the water body classification. This is a big step forward for the work of all researchers and experts working with coastal ocean colour applications.

It is important that the respective indicators for the assessment of water quality provide correct and relevant information. In paper V we could show that the variability of the optical indicator Secchi depth was largely determined by the other two optical factors (CDOM absorption and SPM concentrations) rather than by the chlorophyll-a concentration alone. Empirical models were applied on management scenarios for water bodies by reducing the chlorophyll-a concentrations to the target levels to reach the criteria for good ecological/environmental status. The results show that even when the chlorophyll-a concentration was low enough, the target level for Secchi depth still could not be reached in many of the water bodies studied due to a large background level of CDOM absorption and/or inorganic SPM concentrations in the coastal zone, presumably not related to eutrophication. Hence, the maximum values of the Secchi depth are also determined by CDOM and inorganic SPM. Detailed information about all three bio-optical constituents is important for understanding of the changes in the underwater light field and for developing remote sensing algorithms, as shown in all papers.

With this work I want to contribute to the development of bio-optical and remote sensing as indicators for ecosystem health and water quality monitoring. The results will also be applicable to the Earth Observation missions from the European Space Agency; Copernicus and the next generation of ocean color sensors; the Ocean Land Colour Instrument (OLCI) to be launched on Sentinel-3A in autumn 2015 and to be followed by Sentinel-3B. The design of OLCI will largely be based on MERIS and will have the same spatial and similar spectral resolution, especially adapted for ocean colour applications.
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Inherent Optical Properties, IOPs

Absorption of light in marine ecosystems depends on the optical properties of the water itself, concentrations of CDOM and the photosynthetic biota (phytoplankton, cyanobacteria and macrophytes) and the non-living particulate matter (Prieur and Sathyendranath 1981). Also living non photosynthetic organisms such as zooplankton affect the absorption and are included within the suspended component, but their concentrations are much lower than that of phytoplankton. Absorption and scattering are strongly wavelength dependent. Hence, different concentrations and characteristics of the water constituents alter the light in the water column differently. If, for example, there are high levels of CDOM more light is absorbed closer to the surface and thus the photic depth decreases. The absorption of light is dependent on the concentrations of all optical components present in the water. Therefore the total absorption coefficient, \( a(\lambda) \), can be defined as the sum of the different absorption coefficients of the different components present in the water, as well as the absorption coefficient of the water itself:

\[
a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_d(\lambda) + a_{CDOM}(\lambda) \tag{Kirk 2011}
\]

Where \( a_w(\lambda) \) is the absorption coefficient by water, \( a_{ph}(\lambda) \) is the absorption coefficient for photosynthetic pigments, \( a_d(\lambda) \) is the absorption coefficient for detrital and suspended material (SPM) and \( a_{CDOM}(\lambda) \) is the absorption coefficient for CDOM. The unit for the absorption coefficient, \( a(\lambda) \), is usually expressed as per meter; m\(^{-1}\).

Particle scattering of light photons generally does not remove light; it increases the path length and changes the directions of the photons, which are still available for photosynthesis after scattering (Kirk 2011). In sea water the scattering processes are mostly caused by water itself, sea salt and particles. Particle scattering is divided into two types; inelastic and elastic, where inelastic scattering changes the light energy and elastic scattering does not change the energy of the photons. A very small proportion of the photons are scattered inelastically by water molecules, and those photons appear in the scattered light as emission bands in other wavelengths than the excitation wavebands. This is called Raman scattering, which is caused by oxygen-
hydrogen (O-H) vibrational stretching in the water molecules, and is wavelength dependent. This scattering by water molecules usually does not change the wavelength (energy) of the light photon being scattered, and Raman scattering was found to be the same in sea water as in pure water (Kirk 2011).

The specific absorption and scattering coefficients of chlorophyll-a and SPM; $a^*_{chl-a}(\lambda)$ and $a^*_{d}(\lambda)$; $b^*_{chl-a}(\lambda)$ and $b^*_{d}(\lambda)$, are denoted with a star (*) and are the absorption or scattering at a specific wavelength ($\lambda$) divided by the chlorophyll-a or SPM concentration respectively. The specific absorption of CDOM, $a^*_{CDOM}(\lambda)$, is the absorption of CDOM at a specific wavelength.

Volume Scattering Function (VSF) describes the scattering of the incident light as a function of scattering angle for a given medium per unit path length. Since the light is scattered in all possible directions it needs to be accounted for when estimating the scattering of light in the water by remote sensing. Hence, the total scattering coefficient, $b(\lambda)$, is the integration of the VSF over all solid angles and is measured as scattering unit m$^{-1}$. The total scattering coefficient, $b(\lambda)$, can be divided into the forward scattering coefficient, $b_f(\lambda)$, and the backward scattering coefficient, $b_b(\lambda)$:

$$b(\lambda) = b_f(\lambda) + b_b(\lambda)$$

(Kirk 2011)

where $b_f(\lambda)$ relates to the light being scattered in a forward direction from the light beam and $b_b(\lambda)$ relates to the part of the light that is scattered back into the opposite direction from the light beam. The backward scattering coefficient is also simply called backscattering coefficient. The backscattered light is the light that penetrates the sea surface and is eventually detected by ocean colour sensors. The backscattering coefficient is defined as the integral of the VSF over all backward directions, and the forward scattering coefficient is the integral of the VSF in all the forward directions; $x>90^\circ$ or $x<90^\circ$, respectively (IOCCG 2000).

Phytoplankton and large particles mostly scatter the light forward and just a little backwards. Inorganic material usually causes low absorption but high backscatter. The scattering by water molecules is wavelength dependent and has a high scattering over all angles, and seawater scatters about 30% more than pure water due to the salts (Kirk 2011). Due to higher productivity of phytoplankton, resuspension of sediments, input of terrestrial particulate material from river run-off, the scattering coefficient values are higher for inland and estuarine waters than for the open sea (Kirk 2011). For the Baltic Sea this pattern has been found in (Kratzer and Tett 2009), where the suspended material decreased from the coast towards open waters.
**Attenuance** is the fraction of the radiant flux that is lost due to scattering and absorption in a collimated beam of light and is measured as the beam attenuation coefficient, \( c(\lambda) \). It is in other words the sum of the total coefficient for absorption, \( a(\lambda) \), and scattering, \( b(\lambda) \), measured as reduced flux \( m^{-1} \) by:

\[
c(\lambda) = a(\lambda) + b(\lambda)\]  

(Kirk 2011)

**Apparent Optical Properties, AOPs**

Apparent optical properties (AOPs) are the detectable changes in e.g. reflectance and irradiance, which are affected by changes in the radiance distribution.

**Radiance** is the radiant flux coming from a point of the sea surface in a particular direction. The radiance, \( L(\theta, \phi) \), is a measure of the flux per unit area and per unit solid angle, and describes how the light field is dependent on how the fluxes vary as a function of direction. \( L(\theta, \phi) \) is the radiance in the direction defined by the zenith angle, \( \theta \), and the azimuth angle \( \phi \). The various irradiances can then be obtained by suitable integrations of \( L \) over the appropriate angles. This is e.g. the water-leaving radiance (\( L_w \)) coming from the water towards the sensor, i.e. the part of the sun light that has penetrated into the water, interacted with water and the constituents within before it is scattered back through the surface, leaving the water and travelling through the atmosphere before reaching the sensor (IOOCG 2010).

**Irradiance** is defined as the flux per unit surface area, i.e. the flux received by a flat collector divided by the surface area of the collector. **Upwelling irradiance**, \( E_u(\lambda, z) \), is the flux of light in an upward direction at a specific wavelength (\( \lambda \)) and a specific of depth (\( z \)). It is the light energy coming from the water that is transmitted upwards. **Downwelling irradiance**, \( E_d(\lambda, z) \), is the light flux in all the downwards directions at a specific wavelength (\( \lambda \)) and a specific depth (\( z \)). It is the light energy coming from the water that is transmitted downwards.

**Reflectance**, \( R \), is the dimensionless spectral variation at the sea surface and is wavelength dependent. Reflectance can also be named with the term albedo. At any depth, \( z \), the reflectance, \( R \), is defined as:

\[
R(\lambda, z) = \frac{E_u(\lambda, z)}{E_d(\lambda, z)}
\]

The downwelling irradiance, \( E_d \), is approximately reduced exponentially with depth: \( E_d(\lambda, z) = E_d(\lambda, 0) e^{-K_d z} \). \( E_d(0) \) is the value of the downward irradiance just below the surface and \( E_d(z) \) at depth \( z \) (IOOCG 2010).
When measuring the reflectance from remote sensing one has to take into account that the sensor only detects the reflectance from a narrow field of view in a certain angle, and only measures a small fraction of the total upwelling flux, and thus does not receive all the water-leaving irradiance.

**Remote sensing reflectance,** $R_{RS}(\theta, \phi, \lambda, \theta)$ is closely related to the reflectance $R(\lambda, z)$ at the sea surface and to the upwelling radiance, $L(\theta, \phi)$, (at a certain zenith angle, $\theta$, and azimuth angle $\phi$) instead of the upwelling irradiance, $E_u(\lambda, z)$, and is defined as:

$$R_{RS}(\theta, \phi, \lambda, 0) = \frac{E_u(\theta, \phi, \lambda, 0)}{E_d(\lambda, 0)}$$

The remote sensing reflectance is calculated at the depth, $z = 0$ (at the surface or just below). The light that reaches the sensor on MERIS and on other remote sensing instruments comes from a point of the sea surface in a particular direction and is called the “water-leaving radiance” or just the “reflectance”. This is the radiance coming from the water towards the sensor, i.e. the light that has penetrated into the water and has been affected by the optical properties before it leaves the water and reaches the sensor.

In shallow waters, light that has reached the sea bottom can also be reflected and thus influence the ocean colour signal (IOCCG 2000). Hence, the *bottom reflectance* is influenced by the water clarity and depth, as well as the bottom type e.g. sand, rock or macroalgae.

**Photosynthetically active radiation (PAR)** is the term for the spectral range of the solar radiation that photosynthetic organisms can make use of for gaining energy during photosynthesis. The range is the same as the visible light to the human eyes, between 400 and 700 nm. The depth range of the PAR penetration i.e. the difference between the PAR value at the surface $\text{PAR}(0)$ and at a certain depth $\text{PAR}(z)$ can give us valuable information about the depth where there is enough light for photosynthesis. The slope of the PAR attenuation, $K_a(\text{PAR})$, is determined by the linear slope of the log-transformed PAR as a function of depth ($z$). The Euphotic depth is defined as the depth at which 1 % of the downwelling light available for photosynthesis (PAR) is reached. The measured water depth by optical remote sensors on satellites is roughly about half the Euphotic depth (PAR 50%), which corresponds approximately to the Secchi depth (Aas et al. 2014).

**The diffuse attenuation coefficient,** $K_d(\lambda)$, describes the decrease of the light attenuation as a function of depth and wavelength, having an exponential decrease. The slope of the $K_d(\lambda)$ attenuation, is determined by the linear slope of the log-transformed attenuation at a specific wavelength as a function of depth ($z$). Hence, it is a measure of the gradual loss in light intensity,
often measured at 490 nm, $K_d(490)$. $K_d(\lambda)$ defines the rate of decrease of the downwelling irradiance with depth:

$$K_d(\lambda) = \frac{1}{E_d(\lambda)} \cdot \frac{\Delta E_d(\lambda)}{\Delta Z}$$

$K_d(490)$ is related to Secchi depth, as both variables are a measure of the extinction of light in the water column. The inverted Secchi depth can be retrieved with good accuracy from satellites by using reflectance band ratios $K_d(490)$ algorithms (Kratzer et al., 2003; Kratzer et al., 2008; Alikas et al. 2015). $K_d(490)$ is also correlated to the Photosynthetic Active Radiation (PAR) diffuse attenuation, $K_d$(PAR), and can thus be derived from remote sensing, providing a measure of the light energy available for photosynthesis (Kratzer et al. 2008; Pierson et al. 2008). $K_d$ is often used as a proxy for the water clarity and as an input to compute primary production as a function of light availabilities at certain depths (IOCCG 2000; paper I).

**Modelling Remote Sensing Reflectance and Water Quality Properties**

The remote sensing reflectance ($R_{RS}$) is the information used in ocean colour remote sensing. Since the signal has interacted with the water and the constituents within, the water leaving reflectance looks different depending on the concentrations of the bio-optical components, such as chlorophyll-a, CDOM and SPM. The remote sensing reflectance can then be expressed as a function of the concentrations of the various substances present in the water column. In (Figure 8) some examples of $R_{RS}$ from different types of waters are displayed (IOCCG 2000). The dependence and difference of the reflectance signal is clearly seen for different concentrations of bio-optical components. The signal is for example stronger with higher SPM concentrations.

There are two ways of modelling in ocean optics

- Forward model
- Inverse model

Forward models predict the remote sensing spectral reflectance at the top-of-atmosphere based on a quantitative description of the reflection, scattering and absorption properties of the optical components both in air and water (Kirk 1994; Kratzer 2000; Zaneveld et al. 2005) (Figure 9). The concentrations and the properties of the optical parameters are relatively easy to measure *in situ*. 
Inverse modelling works the other way around, determining the concentrations of the in-water constituents from the reflectance detected by the satellite (Figure 9). In order to solve inverse models the exact definitions of the radiometric quantities and the inherent optical properties (i.e. the scattering and absorption of both aerosols and water constituents) need to be known, as well as the apparent optical properties, in order to describe the characteristics of the light attenuation. All these parameters must be accounted for with their physical relationships and solved by mathematical calculations and modelling (IOCCG 2006; Kirk 1994; Zaneveld et al. 2005). The inverse approach is much more difficult to solve than the forward approach, as it is done by radiative transfer theory. Zanevald et al. (2005) claims that “This is a problem for which there is no exact solution, so various approximations must always be made”.

**Figure 8** Graph showing different reflectance spectra depending on the water constituents. (a) waters with very high SPM and CDOM concentrations, (b) high SPM and CDOM concentrations, (c) moderate SPM and CDOM with some phytoplankton, (d) clear water, (e) waters with moderate chlorophyll and SPM concentrations, (f) waters with moderate chlorophyll concentration. Figure modified to gray scale and reprinted from IOCCG (2000).
The solutions for the inverse model are usually made by semi-analytical approaches or neural network solutions among others, while purely empirical relationships are most often only valid for the same or (optically) very similar waters, as those they were developed for (IOCCG 2006). Knowledge and studies in bio-optics is therefore essential to further develop both inverse and forward approaches, to be able to interpret remote sensing images and retrieve water quality products correctly.

Morel and Prieur (1977) described the relationship between reflectance ratio, \( R \), the backscattering coefficient and the absorption coefficient. This relation is also valid for \( R_{RS} \) at the surface (IOCCG 2006).

\[
R_{RS} (0^-) = \frac{L_n (0^-)}{E_d (0^-)} = F_R \frac{b_b (z)}{a(z)}
\]

where \( R_{RS}(0^-) \) is the remote sensing reflectance just below the surface, with units of sr-1. The RRS is proportional to the backscattering coefficient and inversely proportional to the absorption coefficient. The factor \( F_R \) (sr-1) is dependent on the radiance distribution and the volume scattering function (Morel and Prieur 1977; Zaneveld et al. 2005). This relation was simplified in Morel and Prieur (1977) for case 1 waters with a value of \( F_R = 0.33 \):

\[
R_{RS} (0^-) = 0.33 \frac{b_b (z)}{a (z)}
\]
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