Water Quality and Optical Properties of Swedish Lakes and Coastal Waters in Relation to Remote Sensing

BY

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Abstract


Semi-analytical models for remote sensing of water quality parameters need to be parameterized with specific inherent optical properties. In this thesis, data on specific inherent optical properties of Swedish lakes and coastal waters is presented. Also, the problems of measuring in situ spectral backscattering are addressed. It is shown how measured specific inherent optical properties are used to parameterize semi-analytical bio-optical models. The models are then used to produce large synthetic data sets based on the distribution of water quality parameters, and from these data sets, band ratio or single band ratio algorithms for remote estimation of water quality parameters are constructed. A similar model was also used to calculate under water PAR from measured water quality parameters.

The specific inherent optical properties of Swedish lakes and coastal waters are very similar to earlier reported data from the oceanic environment. However, different relations of the water quality parameters will affect the inherent optical properties absorption and backscattering. The absorption spectra are dominated by yellow substance with terrestrial origin. Phytoplankton absorption is low, and account in general only for about 10 % of the total absorption in regions where phytoplankton pigments are active. The spectral backscattering is dominated by suspended particulate inorganic matter. Phytoplankton backscattering is almost negligible, except in cases where the phytoplankton community is dominated by highly scattering cyanobacteria. Experiences from remote sensing campaigns and modeling shows that remote chlorophyll estimation is most effective at longer wavelengths, where the absorption of yellow substance is low. However, modeling also predicts that large uncertainties have to be expected in the estimation of chlorophyll, both from variation in the specific phytoplankton absorption and from influences of other optically active water quality parameters.

Key words: Water quality, inherent optical properties, remote sensing, bio-optical models.

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PREFACE

This thesis is a summary of studies on optical properties of Swedish lakes and coastal waters and remote sensing of lakes. The studies are presented in the papers denoted below. In the text, the papers are referred to by their roman numbers (e.g. Paper I). The work was carried out at the Department of Limnology, Evolutionary Biology Center, Uppsala University, Sweden.


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CONTENTS

Abstract 2
Preface 3
Contents 4
Introduction 5
  A brief history 5
Definitions and the concept of remote sensing 6
Inherent and Apparent Optical Properties 8
  Relations between Inherent Optical Properties and Water Quality in Swedish Lakes and Coastal Waters 10
Methods 11
Different approaches to remote sensing of freshwaters 13
Summary of the Papers 14
  Paper I 14
  Paper II 15
  Paper III 16
  Paper IV 17
  Paper V 17
  Paper VI 18
  Paper VII 19
General Discussion 19
Conclusions 22
Summary in Swedish 22
Acknowledgements 24
References 24
INTRODUCTION

Remote sensing of natural waters has many practical applications, but its use requires overcoming many delicate problems. The intention with this work was to clarify how water quality can affect the inherent optical properties of Swedish lake and coastal waters and how in turn the inherent optical properties will determine the possibilities of using remote sensing as a tool for the assessment of water quality. Below follows a brief description of how the field has developed over the last decades and some definitions that can help to set this work into a broader context.

A brief history

Optical remote sensing of oceanic waters was developed as a science in the seventies and eighties by workers like Gordon (Gordon, Brown et al. 1975; Gordon, Brown et al. 1988), Morel (Morel and Prieur 1977), Sathyendranath (Sathyendranath, Lazzara et al. 1987) and their associates. A driving force was the development of satellite technology, which in 1978 led to the launch of the Nimbus 7 satellite carrying the Coastal Zone Color Scanner (CZCS). This was the first optical satellite instrument designed especially for remote sensing of oceans and its main focus was the spatial distribution of chlorophyll (ocean color). The CZCS was designed as a proof-of-concept experiment and only scheduled to work for one year, but continued to live on until 1986 when it eventually ceased to function. The collected data is still in use and has greatly contributed to the knowledge of how chlorophyll is distributed over the oceans and provided a general proof of the potential of remote sensing of oceans. Today, the SeaWiFS (Sea-viewing Wide Field-of-view Sensor) on the SeaStar satellite has replaced CZCS as the dominant source of remote sensing data of the oceans. One reason for the early success of the CZCS was the combination of traditional remote sensing techniques and the use of theoretical aquatic optical models. Aquatic optics had been an independent science from the middle of this century with early work by (Jerlov 1951; Jerlov 1976) and later extensive theoretical work by Preisendorfer (summarized in Preisendorfer 1976) and his co-worker Mobley (i.e. Mobley 1994).

Remote sensing of lakes has developed in parallel to that of the oceans but has had a somewhat more difficult start as no specially-designed satellite sensors were available which in turn lead to a slower integration of remote sensing with studies of aquatic optics (see below). (Dekker 1993) also partly related this somewhat slower development to the fact that freshwater science is less organized than oceanography. Despite this, early studies were performed using the MSS (Multispectral Scanner) and the TM (Thematic Mapper) sensors onboard the Landsat satellites although they were primarily designed for terrestrial applications. Already in 1974, (Bukata, Harris et al. 1974) assessed chlorophyll concentration in Lake Ontario, Canada from Landsat data. Almost two decades later, Dekker and co-workers (Dekker, Malthus et al. 1991) concluded after using optical modeling together with satellite data that the Landsat systems not could be used to discriminate between chlorophyll concentration and suspended matter with general algorithms. The earlier success was obtained either locally or through fortuitous relationships between the optical properties of the water. In the mid nineties, the focus on satellites was widened as airborne multispectral sensors, more suitable for remote sensing of freshwaters, become commercial available. At about the same time, optical field equipment for oceanographic and limnological use became available, leading to an insight that the use of optical models (Gordon, Brown et al. 1975; Morel and Prieur 1977; Morel 1980; Prieur and Sathyendranath 1981; Gordon, Brown et al.
1988; Sathyendranath, Prieur et al. 1989) was applicable even to freshwaters (Bukata, Jerome et al. 1979; Kirk 1981; Kirk 1984; Gallie and Murtha 1992; Dekker 1993; Jupp, Kirk et al. 1994; Pierson 1998; Pierson 1999). In 1993, Arnold Dekker published his Ph.D.-thesis “Detection of optical water quality parameters for eutrophic waters by high resolution remote sensing.” In this thesis, he addressed many of the main issues in both optical modeling and airborne multispectral remote sensing of lakes, and showed how algorithms derived from modeling could be used on remote sensing data. However, today, there is an apparent lack of in-water optical data from freshwaters, and we rely mainly on data from the oceans. One reason for this is that the concentrations and the relationships between the optically active substances in freshwaters can in some cases demand a slightly different approach to the measurements of optical properties (Davies-Colley and Vant 1987; Tassan and Ferrari 1995; Strömbeck 2001).

The remote sensing of Swedish natural waters began in the early 1970:ies when data from the Landsat 1 (ERTS-1) earth resource satellite become available to the scientific community. Studies included estimations of turbidity and phytoplankton but used mainly qualitative methods (Svensson 1973; Svensson, Hellldén et al. 1975; Örström 1976; Hellldén and Åkersten 1977 in Lindell 1980). Later, Lindell and co-workers made transect measurements in Lake Mälaren of chlorophyll (fluorescence) and transmissivity using the ATOS III system (Lindell 1979), which then were related to Landsat satellite imagery by regression analysis. They also presented satellite-based maps of water quality (Lindell 1980; Lindell 1981; Lindell, Steinvall et al. 1985; Lindell, Karlsson et al. 1986). During these studies, it became evident that the success of satellite remote sensing of freshwaters by regression analysis would be limited because of the low spectral and radiometric resolution of the Landsat systems and its poor radiometric calibration. In 1996, an airborne GERIS imaging spectrometer was flown over Lake Erken during a cyanobacteria bloom, but no field measurements were made and the overall quality of the data was low (Östlund 1999). In 1997 a second trial was made when the CASI instrument was flown over Lake Erken, Lake Mälaren and the Archipelago of Stockholm in the SALMON project. At this time, extensive field measurements were made, which were also followed by campaigns aimed at measuring inherent and apparent optical properties in a wide range of Swedish lakes and coastal waters.

The results presented in this thesis are essentially based on this latter work from 1997 to present (2000).

DEFINITIONS AND THE CONCEPT OF REMOTE SENSING

In this work, remote sensing is defined as the passive measurement of electromagnetic radiation of wavelengths between 400 and 750 nm. This corresponds to what we call visible light, ranging from violet (400 nm) over blue, green and yellow to red (700 nm). The reasons why we are restricted to this wavelength interval are simple. The shorter limit is set up by the fact that the intensity of solar radiation below 400 nm is very low, and that organic matter in lake water strongly absorbs violet light. The longer limit is also to some extent set up by the intensity of solar radiation, but the main reason in this case is that the water itself is a strong absorber of red and near infrared light. This means that very little natural light can penetrate water outside the wavelength band of 400 to 750 nm, and consequently, we have no direct need for making optical measurements outside this range.

Remote sensing is carried out from different types of platforms. The platforms commonly used are satellite and aircraft although boats or buoys often are used for more experimental and research oriented activities. The sensors used are commonly referred to as radiometers. A
radiometer records incoming electromagnetic radiation in certain channels (wavelength bands). If the radiometer can record a more or less continuous spectra over all wavelengths it is usually called hyperspectral or a spectroradiometer. Radiometers designed for continuous recording of spectra are called scanners and the recorded data can be used to compose an image. As a rule of thumb, satellites carry scanners with limited number of channels, while aircraft mounted scanners can be hyperspectral. Shipborne sensors are usually non-scanning hyperspectral and sensors mounted on buoys are typically non-scanning and designed to match the channels of a corresponding satellite scanner.

The light measured from above a waterbody is a function of the inherent optical properties of the water and other factors such as the reflection from the water surface, the solar spectrum, the elevation of the sun and the transmissivity of the atmosphere. The data measured by the remote sensor is thus the upwelling radiance passing through the water surface but with some important effects added. These include mainly the surface reflection from the water body and path radiance of the atmosphere, i.e. radiation that is scattered by atmospheric particles in a way that it reaches the remote sensor. Typically, only 10% of the radiance reaching a satellite remote sensor results from reflectance within the water body itself (Kirk 1994). To extract this fraction from the larger atmospheric signal, several techniques of atmospheric corrections exist. Some of these techniques are discussed and used in the papers of this thesis, but the details of the huge field of atmospheric correction is left to other more initiated writers.

Remote sensing of freshwaters can be considered to be useful only for estimations of water quality parameters in the upper most part of the water column. 90% of the light reflected from a waterbody originates from within the depth that can be calculated as $1 / K_d$ (Kirk 1994, see below). In this work, the clearest water body Lake Vättern has an average lowest $K_d$-value of 0.18 $\text{m}^{-1}$ at around 555 nm. That means that most reflected light comes from 0 to 5.6 m. Considering that Lake Vättern is a very clear lake for being in Sweden, this depth interval will in most other lakes be much smaller and consequently there are no practical problems with influences of bottom reflection. However, the dimictic nature of most Swedish lakes will make remote sensing estimations in many cases applicable to whole epilimnion, as this layer often is well mixed by wind and wave action.

The satellite sensors used for remote sensing of oceans are inappropriate when applied to freshwater for two mains reasons; firstly the spatial resolution is often too low. The SeaWiFS sensor and the MODIS (Moderate Resolution Imaging Spectroradiometer) aboard the Terra satellite both have a spatial resolution of approximately 1 km. This is too low for most Swedish lakes and archipelago waters, which are either relatively small or have complicated morphology. Therefore, in many cases, influences by land will make satellite remote sensing of lakes impossible. Secondly, their spectral resolution is not adapted for freshwater use. Generally speaking, ocean water can be stated to be optically dominated by phytoplankton, while freshwaters are dominated by suspended organic and inorganic matter and dissolved humic substances. However, new sensors are being developed, and the remote sensing community are now waiting for the MERIS sensor (Medium Resolution Imaging Spectrometer) carried by ENVISAT. MERIS will have a spatial resolution of about 300 meters and a set of bands suitable for freshwaters and will thus be the first satellite sensor of immediate use for remote sensing of lakes.

To my knowledge, no operational remote sensing system for routinely monitoring of lakes exist today and the main reason for this is the lack of ideal satellite sensors for lake applications. Instead we have mainly relied on experimental campaigns using airborne sensors like e.g. the CASI (Compact Airborne Spectrographic Imager), ROSIS (Reflective Optics System Imaging Spectrometer), DAIS (Digital Airborne Imaging Spectrometer), AISA (Airborne Imaging Spectrometer for different Applications) or GERIS (Geophysical and
Environmental Research Imaging Spectrometer) sensors. The use of airborne instruments do indeed give very valuable opportunities to test optical lake models. The spatial resolution can in practice be reduced a few meters, and the radiometric calibration of the instrument can be checked and compared to e.g. in situ instruments. However, these are still not suitable for operational use. The main reason, except for technical ones (see e.g. Östlund 1999) is that such experiments demand complicated logistics in order to perform simultaneous sampling and measurements during periods of good weather. Undoubtedly, airborne systems will be very useful if we can rely fully on optical models, and not on simultaneous sampling and measurements.

**INHERENT AND APPARENT OPTICAL PROPERTIES**

When light penetrates a water body, it will either be absorbed or scattered. Eventually, all light will be absorbed except for that scattered in a way that it can leave the waterbody through the surface. The processes of absorption and scattering can be quantified and expressed as the fraction of light absorbed or scattered from a parallel light beam passing through a very short (actually infinitesimally small) layer of media (Kirk 1994). First we make use of the intermediate term absorbance, A:

\[ A = \Phi_a / \Phi_0 \]

where \( \Phi_0 \) is the incident light flux in the parallel beam and \( \Phi_a \) is the light flux absorbed by the medium. Then we arrive at the absorption coefficient \( a \) by

\[ a = \Delta A / \Delta r \] \hspace{1cm} \text{eq. 1} \]

where \( \Delta r \) is the thickness of the medium. The scattering coefficient \( b \) is defined analogously to the absorption coefficient. Both are wavelength dependent (\( \lambda \)) and expressed in the unit of \( \text{m}^{-1} \). \( a \) and \( b \) can be added together to form \( c \);

\[ c(\lambda) = a(\lambda) + b(\lambda) \] \hspace{1cm} \text{eq. 2} \]

where \( c \) is the attenuation coefficient. These three optical properties are usually called inherent optical properties (from hereon called IOP:s) since they only are functions of the waterbody itself, and not of the incoming light. There is also a fourth IOP; the volume scattering function \( \beta(\Phi) \), which describes more in detail in which directions the light is scattered. The in situ volume scattering function is very hard to measure, and only a few measurements are today in use, of which a series of measurements reported by Petzold (1972) stand out as the most reliable (Maffione and Dana 1997). The volume scattering function is only briefly discussed in this work, although it is of profound value in all aquatic optics. A fifth IOP:s that can be derived from the volume scattering function or from the scattering coefficient is the backscattering coefficient \( b_b \), i.e. the fraction of the incoming light that is scattered back towards the incident beam at angles less than 90°. Based on the volume scattering functions reported by Petzold (1972) backscattering equals 1.9 to 4.4 % of the total scattering depending on the type of water.
A central term in aquatic optics and remote sensing is the reflectance of the water. In this case reflectance means the reflection caused by the waterbody itself and not reflectance caused by the surface (surface reflectance). The most common reflectances are defined as:

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

\( R \) is called the irradiance reflectance, and \( E \) is the irradiance through a horizontal plane weighted by the cosine of its incoming angle to the normal. The indices \( u \) and \( d \) means upwelling and downwelling respectively. Radiance reflectance (\( R_r \)) is defined as:

\[ R_r(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} \]  

where \( L_u \) is the upwelling radiance and \( E_d \) is the downwelling irradiance. Briefly explained, radiance is light measured in a narrow angle using e.g. a lens. Irradiance on the contrary is light measured from all directions striking a horizontal plane from either an upward or downward direction. In remotes sensing, radiance reflectance is the desired parameter, since it is the reflectance that is measurable by a remote sensor. Radiance reflectance is an example of apparent optical properties (AOP:s). These properties change not only with the constituents of the water but also with the nature of the incoming light.

The IOP:s and the AOP:s has been linked to each other through mathematical Monte Carlo simulations (Kirk 1984);

\[ R = (0.975 - 0.629 \mu_0) \frac{b_b}{a} \]  

where \( \mu_0 \) is the cosine of the solar zenith angle just under the surface. This formula is based on the volume scattering function measured by Petzold (1972) in the turbid ocean waters of San Diego Harbor, USA where \( b_b \) equals 1.9 % of \( b \) and it is considered to be valid for many coastal and moderately turbid inland waters. Several similar expressions exist (e.g. Gordon, Brown et al. 1988) but the main point here is that it is theoretically possible to determine the IOP:s \( a \) and \( b \) from a reflectance spectra of a waterbody.

Another useful AOP is the vertical attenuation coefficient for downwelling irradiance \( K_d \), which describes the spectral attenuation of the sunlight in the water. This parameter is most easily estimated by measurements of the downwelling irradiance at two known depths; \( z \) and \( z_0 \).

\[ K_d(\lambda) = -\frac{\Delta \ln E_d(\lambda, z, z_0)}{\Delta z} \]  

where \( \Delta \ln E_d \) is the change in the natural logarithm of \( E_d \) and \( \Delta z \) is the depth interval. If the measurements are made right under the surface and at the depth where the irradiance has diminished to 1 % of the value right under the surface, we get the average vertical attenuation coefficient for downwelling irradiance within the euphotic zone, \( K_d(\text{av}) \). \( K_d(\text{av}) \) depends on the IOP:s \( a \) and \( b \), but also on the volume scattering function of the water, i.e. to what extent and in which directions scattering occurs. It also depends on the height of the sun, as low sun angles result in a longer distance for the light to travel to reach a given depth than do a high
sun angle. Using Monte Carlo simulations Kirk (1981) showed that the average Kd from the surface down the depth where 1 % of the incoming light remains could be calculated with the formula

\[ K_d(\lambda, av) = \frac{1}{\mu_0} \{ a(\lambda)^2 + [g_1 \mu_0 - g_2] a(\lambda) b(\lambda) \}^{1/2} \]  

where \( \mu_0 \) is the cosine of the solar zenith angle right under the surface and \( g_1 \) and \( g_2 \) are constants determined by the volume scattering function of the water. When it is assumed that the volume scattering function measured in the turbid ocean waters of San Diego Harbor, USA (Petzold 1972; Kirk 1994) is representative for the waters in this work, one obtains the values of 0.425 and 0.19 for \( g_1 \) and \( g_2 \) respectively. When \( K_d(\lambda, av) \) is known, the downwelling irradiance \( E_d(\lambda) \) can be estimated at any depth within a water body by the equation

\[ E_d(\lambda, z) = E_d(\lambda, z_0) e^{-K_d(\lambda, av)z} \]  

Relations between Inherent Optical Properties and Water Quality in Swedish Lakes and Coastal Waters

The IOP:s are dependent on the different optically active substances in the water and follow Beer’s law. That means that they also are proportional to the concentrations of the different optically active substances. In this work, the total absorption and scattering spectra of the waters were assumed to be influenced by the following constituents:

\[ a(\lambda) = a_{ys}(\lambda) + a_{ph}(\lambda) + a_d(\lambda) + a_w(\lambda) \]  

\[ b(\lambda) = b_{SPIM}(\lambda) + b_{ph}(\lambda) + b_w(\lambda) \]  

\( ys \) means here dissolved yellow substance (also called CDOM, DOC, gelbstoff, gilvin, aquatic humus etc.), \( ph \) means phytoplankton, \( d \) detrital material, \( SPIM \) means suspended particulate inorganic matter and \( w \) means the pure water itself. These two formulas are not unique for this work, but they are very useful for describing the inherent optical properties of Swedish lake and coastal waters. Compared to most ocean waters, the yellow substance absorption in freshwaters is much higher and usually also dominates the absorption spectra at shorter wavelengths. The reason for this is that the yellow substance in freshwaters to a great extent comes from the surrounding terrestrial environment, and enters the water body through inlets and groundwater inflows. In many ocean waters, the yellow substance is mainly attributable to the phytoplankton as derivative products, and consequently of lower concentration. The terrestrial influence can also be seen in the absorption of the detrital material. This material is to some extent derivatives of phytoplankton, but comes probably also from inflows and from resuspension of sediments. The effect can also be seen in the scattering spectra; suspended particulate inorganic matter from inlets and resuspended sediments dominates the scattering, while that associated with phytoplankton play a minor role.

The optically active substances contribute to both the absorption and scattering coefficients. A common way to quantify this contribution is to use specific inherent optical properties.
These explain how much absorption and scattering a certain concentration of a substance contribute with. Ignoring the wavelength dependency, the equations above then become

\[ a = a_{ys} + C_{Chl} a_{ph}^{*} + C_{SPOM} a_{d}^{*} + a_{w} \]  
\[ b = C_{SPIM} b_{SPIM}^{*} + C_{Chl} b_{ph}^{*} + b_{w} \]

where \( C_{Chl} \) is the chlorophyll \( a + \) phaeophytin a concentration in \( \mu g/l \), \( C_{SPOM} \) and \( C_{SPIM} \) concentrations of suspended particulate organic and inorganic matter respectively in \( mg/l \), and the star (*) indicates that the parameters are specific and related to one concentration unit of the corresponding substances. The absorption of yellow substance is normally not made specific, but used as a parameter itself, and the absorption and scattering due to pure water can be found tabulated (Smith and Baker 1981). A third equally important equation can be set up for the backscattering coefficient:

\[ b_{b} = C_{SPIM} b_{SPIM}^{*} + C_{Chl} b_{ph}^{*} + b_{bw} \]

**METHODS**

Below follows a description of the main field and laboratory measurements used in this work. The methods were chosen from several criteria: they should be consistent with methods commonly used in oceanography, but also with standard methods used by Swedish water quality laboratories. It was also important that the methods were applicable in field under simple conditions, e.g. in small boats etc. and also as a part of other routine measurements.

The measurements were made as a combination of in situ and laboratory measurements. For the in situ measurements, a HOBI Labs HydroScat-6 \( b_{v} \)-meter (Maffione and Dana 1997) and a WET Labs C-Star \( c \)-meter were used. These instruments were mounted on a frame, together with a depth and a temperature sensor. The frame was lowered slowly through the water column and down to approximately 15 meters (if allowed by the water depth), and all instruments were logged continuously, resulting in depth profiles with a resolution typically less than 10 centimeters. Water for the analyses was sampled using either a standard water sampler or a pump system. The water was if possible stored in dark and cold until analyzed.

For measurements of yellow substance \( a_{ys}(\lambda) \), the water was filtered in the field through Whatman GF/F filters or in the case of Lake Vättern; Millipore 0.2 \( \mu m \) membrane filters (Kirk 1976). After arrival to the lab, the absorption of the samples was measured spectrophotometrically (400 and 750 nm) in 10 cm-cells with pure water as a reference was and at room temperature. The use of GF/F-filters can be discussed as they are not the standard for use in yellow substance measurements in oceanography. One main reason for using the GF/F filters was that GF/F filters were used for measurements of the particulate absorption, so that material passing through filters would be included the measured total absorption spectra. Also, absorbance of GF/F filtered water is a standard parameter measured in many water quality programs in Sweden.

After the measurements, scattering correction was performed according to Bricaud et al. (1981):

\[ a_{ys}(\lambda) = a_{ys}^{'}(\lambda) - a_{ys}^{'}(750) \frac{750}{\lambda} \]  

\[ eq. 14 \]
where $a_{ys}$ is the measured yellow substance. The second term is a correction for the scattering error, based on the assumption that any value measured at 750 nm is attributable to scattering, and that the spectral dependency of the scattering is $\lambda^{-1}$. Bricaud and co-workers concluded that any apparent absorption at 700 nm of GF/C filtered sea water mainly was an effect of scattering, and suggested from calculations that a $\lambda^{-1}$ dependency was suitable for making an approximate scattering correction. Davies-Colley and Vant (1987) later used the same correction for freshwater samples, but used 740 as the reference wavelength instead of 700 nm. In this work we instead choose to use 750 nm.

The phytoplankton absorption $a\text{ph}(\lambda)$ and detrital absorption $a\text{d}(\lambda)$ was measured spectrophotometrically (400-750 nm) with the Whatman GF/F filter pad technique (Yentsch 1962; Mitchell 1990) using the formulas of by Cleveland and Weideman (1993). The “depigmentation” and discrimination between phytoplankton and detrital absorption was performed with sodium-hypochloride according to Tassan and Ferrari (1995). The advantage of this latter method is that the depigmentation can be done immediately in the field directly in the bottles.

The total backscattering was measured at six wavelength bands centered on 442, 470, 510, 589, 620 and 671 nm ($\lambda_{1-6}$) with the HOBI Labs Hydroscat-6 backscattering sensor (Maffione and Dana 1997). The measurements of the HS-6 are sensitive to high attenuation in the water, and therefore a correction method for this was developed. This method involves among other things separate measurements of the beam attenuation at 660 nm and estimation of phytoplankton scattering, backscattering and attenuation from the chlorophyll concentration $C_{Chl}$ (Strömbeck 2001).

The total beam attenuation at 660 nm $c(660)$ was measured with a WET Labs C-Star c-meter (25 cm pathlength). All c-meters are subjected to scattering errors as it is practically impossible to make a detector with an acceptance angle approaching zero. The measurements were therefore corrected for scattering according to the method by Bricaud and co-workers (1995):

$$c(660) \approx 1.075 \, c'(660) - 0.075 \, a_w(660) \quad \text{eq. 15}$$

where $c'(660)$ is the measured beam attenuation at 660 nm and $a_w(660)$ is the absorption of pure water at 660 nm. Bricaud and co-workers used a Sea-Tech 25 cm pathlength c-meter (transmissometer) with an acceptance angle of 0.9°, which is about equal to the Wet Labs c-meter with an acceptance angle of 0.85° (Kitchen pers. comm.) used in this work.

Beside the measurements described above, additional measurements of the water quality were made. For chlorophyll concentrations, $C_{Chl}$, 0.5 to 3.0 liters of water was filtered through Whatman GF/F-filters, and the chlorophyll $a$ + pheophytin $a$ concentration was measured spectrophotometrically on ethanol extracts of the filters according to the ISO 10260 standard method (ISO 1992). The concentration of suspended matter $C_{SPM}$ was measured gravimetrically after filtration of 0.3 to 4.0 liters of water through pre-weighed and pre-combusted Whatman GF/F-filters, and the inorganic fraction $C_{SPIM}$ was measured after combustion in 550 °C for 3 hours. The organic fraction $C_{SPOM}$ was determined by subtraction of $C_{SPIM}$ from $C_{SPM}$. In brackish waters, the filters were rinsed with approximately 300 ml of distilled water after the filtration in order to remove the effects of salt in the filters. The detection limit of this method was estimated to 0.1-0.25 mg/l depending of the amount of filtered water.
DIFFERENT APPROACHES TO REMOTE SENSING OF FRESHWATERS

The papers that this work is based on describe very well the development of the bio-optical group at the University of Uppsala in general. It can also be seen as a compact series of articles describing the general trends in remote sensing of freshwaters. Remote sensing of freshwaters can basically be made through two different approaches or through a combination of the two; empirically or semi-analytically. Traditionally in the empirical approach, remote sensing data is related by regression analysis to lake truth measurements of water quality parameters, usually chlorophyll or suspended particulate matter. This approach needs extensive field work and logistics since samples have to be collected from the water body simultaneously or near simultaneously with the overflight of the sensor. In practice, this is more or less impossible and in reality the researchers are left with only a few lake truth points. However, the advantage of this approach is that even though few parameters are measured, it still can be very accurate during one campaign in a limited area (e.g. one lake). Parameters not measured include atmospheric effects, surface reflection, effects of different sun angles, differences in the inherent optical properties of the studied water body, and absolute calibration of the sensor. The disadvantages are obvious, since when all or a selection of these parameters are not considered, the derived algorithms can not be expected to be of a general validity, but only applicable the studied water body. The empirical approach is therefore not recommended for developing algorithms for operational remote sensing (monitoring) of freshwaters.

In the semi-analytically approach, an in-water optical model is used to interpret the remote sensing data. These models are based on equations similar to equations 4 and 9-13 described above and use the inherent optical properties or concentrations of different optically active substances as input, and give estimates of radiance reflectance as the output. They can also be used in the reverse way, i.e. to determine the concentrations of the optically active water quality parameters from a spectrum of radiance reflectance (Jupp, Kirk et al. 1994; Keller, Keller et al. 1998; Pierson 1998). This is usually called inverse modeling or simply inversion. The great advantage with these models is that they can be calibrated against field data collected independently from the remote sensing campaigns, and consequently the need for lake truth measurements is reduced. Semi-analytical models have been proven to be suitable for interpreting remote sensing measurements of lakes if their parameterization, i.e. how the water quality parameters are related to the inherent optical properties, is performed with care. However, inverse modeling with a fully spectral semi-analytical model is usually very slow, and not yet realistic for large remote sensing dataset. Instead the models can be used in their forward direction to produce large synthetic data sets of radiance reflectance resulting from different combinations of water quality parameters, that in turn are used to construct statistical algorithms for interpretation of the remote sensing data. The drawbacks of the semi-analytical approach are also obvious. No model is better than its parameterization, which can be quite a demanding task. The relations between water quality parameters and inherent optical properties are known to be remarkably stable both spatially and temporary, but the existing differences will of course affect the model output. Also, the methods for measuring the inherent optical properties will affect these relations. Thirdly, the equations of radiance reflectance that the models are based on themselves (e.g. equation 5) are based on computer simulations which indeed seem to be good enough to produce realistic results, but care must be taken when choosing which model to use. As a fourth factor I’d like to mention use of the models to produce synthetic datasets. The resulting algorithms will to some extent
depend of the distribution of the water quality data they are based on. Finally, the overall accuracy of aquatic remote sensing measurements is to a great extent affected by the accuracy of the atmospheric correction. As mentioned above, the signal reflected from the water body can be as low as 10% of signal detected by the remote sensor.

**SUMMARY OF THE PAPERS**

The papers that this work is based on describes very well the development of the bio-optical group at the University of Uppsala in general. It can also be seen as a compact series of articles describing the general trends in remote sensing of freshwaters. The work involves both the empirical and the semi-analytical approach to remote sensing of lakes, but the main task was to study the relations between the inherent optical properties and water quality parameters, and how these can affect calculated radiance reflectance. This was done by using a bio-optical semi-analytical model (Pierson 1998). The fieldwork was done in several Swedish natural waters: Lake Erken, Lake Mälaren and the Archipelago of Stockholm (brackish). Later, the two largest lakes of Sweden, Lakes Vänern and Vättern, were incorporated in the study.

**Paper I**


In this paper, we took the empirical approach to estimate mainly the surface chlorophyll concentration during a cyanobacterial bloom in Lake Erken, Central Sweden from CASI and Landsat TM data. Several steps were taken to make the work robust against factors that otherwise would reduce the general validity of the empirical approach. The remote sensing data were geometrically and atmospherically corrected. A large amount of lake truth data points was obtained by using a flow through system measuring chlorophyll fluorescence (fig. 1) and beam attenuation, which was calibrated against point measurements of chlorophyll concentration and concentrations of suspended particulate matter. Finally, maps of surface chlorophyll were produced, based on regression analyses between the lake truth data and selected spectral bands in the remote sensing data.

![Figure 1. Field data and corrected CASI reflectance (705 nm). (Östlund, Flink et al. 2001)](image-url)
My contribution to this work was the development and set-up of the *in situ* flow-through system, logistics and sampling, co-ordination of the analyses, data handling and calibration of the data from the flow-through system. I also contributed to the discussion concerning time differences and influences by other substances than chlorophyll on the regression.

**Paper II**


Here we used historical long-term water quality data from the three largest lakes in Sweden (Lakes Vänern, Vättern and Mälaren) to study the performance of the new MERIS satellite sensor. From the long-term data frequency distributions were derived and used to create large synthetic datasets with random but yet possible combinations of the parameters chlorophyll, yellow substance absorption and suspended particulate inorganic matter. A bio-optical model, mainly parameterized by field data from Lake Mälaren in 1997, was then used to estimate the inherent optical properties absorption and backscattering and finally the spectral radiance reflectance of the water bodies. The resulting spectra of radiance reflectance were divided into 10 nm bands and regression coefficients were calculated between all possible band ratios and chlorophyll, yellow substance absorption and suspended particulate inorganic matter. The suggested MERIS band or band ratio algorithms (fig. 2) are based on these regression
analyses, but interpolated to wider bands of this sensor. The paper demonstrates the use of bio-optical modeling as a rapid screening tool for evaluation of preliminary remote sensing algorithms.

In this paper, I was responsible for the field analyses and for calculation of the relations between the water quality parameters and the absorption and backscattering coefficients. I was also involved in the general discussion about the algorithm development.

**Paper III**


In this paper, we used preliminary relations between water quality parameters and absorption and backscattering coefficients derived from field measurements to study how the variability in those relations could affect a remote sensing algorithm. The study was focused on Lake Mälaren in 1997, and the apparent covariation of the optically active substances in Lake Mälaren during the period of study was used to create a large synthetic dataset which drove a bio-optical model in order to estimate spectra of radiance reflectance. Variations in the specific inherent optical properties based on field measurements were also induced in the model. Prediction intervals were calculated for the band ratio 700-710 / 678-685 nm as a function of the chlorophyll concentration. From this work, we concluded that variations in suspended particulate inorganic matter can cause large errors in the estimation of chlorophyll (fig. 3). It also became clear that we need more studies of the relations between chlorophyll and phytoplankton absorption and backscattering in order to obtain more accurate estimates of chlorophyll using semi-analytical model derived algorithms.

As the principal author, I was responsible for all material in this paper.

![Figure 3](image.png)

*Figure 3. Prediction intervals for remote estimation of chlorophyll. (Strömbeck and Pierson 2001)*
Paper IV

This work dealt with attenuation correction methods of the commercially available HydroScat-6 backscattering sensor manufactured by HOBI Labs, CA, USA. Depending on the water type, the sensor needs appropriate correction, and HOBI Labs have supplied two different corrections: one simple correction that seems to perform well under many oceanic conditions, and one that uses additional water quality measurements and that can be used in more turbid waters. In more attenuating freshwaters, both of these methods will fail to correct the instrument for attenuation errors. I presented two new methods that perform better than the previous methods, but also demands more additional data (fig. 4). One was a simple extension of the second method by HOBI Labs, and the other was a more complex method based on independent measurements of absorption and beam attenuation coefficients. The latter method was based on sound assumptions about the absorption and scattering of freshwaters, and will thus provide the base of an accurate correction of the instrument in any type of water.
I am the single author of this paper and of course responsible for the whole content.

![Figure 4. Backscattering spectra corrected with different methods](image)

Paper V

In this work I presented a summary of the relations between water quality parameters and inherent optical properties (i.e. specific inherent optical properties) that I’ve measured in Swedish lakes and coastal waters during 1997-2000. These include absorption related to chlorophyll, detrital material and yellow substance and total backscattering. I also described other parameters derived from correction methods or modeling in conjunction with the measurements such as backscattering related to suspended particulate inorganic matter, the
total backscattering efficiency and the backscattering efficiency inorganic matter, beam attenuation and the vertical attenuation coefficient. Typical spectra can be seen in figure 5. I am the single author of this paper and of course responsible for the whole content.

Figure 5. Typical absorption and backscattering spectra of Swedish lakes and coastal waters.

Paper VI


Figure 6. Remotely estimated (CASI) and ground truth chlorophyll concentrations.

In this paper we used a simple bio-optical model similar to the ones used in Paper II and III to estimate the optically active substances from CASI data recorded over Lake Mälaren, Sweden. The model was parameterized with the specific inherent optical properties from Eastern Lake Mälaren that were described in Paper V, and a large record of measured water quality parameters (spanning over more than 25 years) was used to produce a synthetic dataset from which remote sensing algorithms then were derived. The CASI data was atmospherically corrected by the 6S model. From these data, maps showing the distribution
of chlorophyll, suspended particulate inorganic matter and yellow substance were created. The maps were validated against continuous field data of chlorophyll (fig. 6) and suspended inorganic matter measured with the same equipment described in Paper I.

I was responsible for the development and set-up of the *in situ* flow-through system, logistics and sampling, co-ordination of the analyses, data handling and calibration of the data from the flow-through system. I also supplied the relations between the water quality parameters and the inherent optical properties and took part in the general discussions concerning the paper.

**Paper VII**


In this paper, the vertical attenuation coefficient of PAR (photosynthetically active radiation) was calculated from water quality parameters using the specific inherent optical properties derived in Paper V. A number of profiles of the downwelling quantum irradiance in the PAR region were measured in different lakes and used for validation of the model (fig. 7). The paper shows that general relationships between water quality parameters and inherent optical properties can be used successfully for e.g. subsequent studies of phytoplankton primary production.

![Figure 7. Modeled versus measured Kd(PAR, q).](image)

I’m responsible for the relations between the water quality parameters and the inherent optical properties, the simple atmospheric model and the calculations of the vertical attenuation coefficient.

**GENERAL DISCUSSION**

From Paper I, we concluded that it is perfectly possible to estimate water quality by the empirical approach if there is enough lake truth data. However, the resulting algorithms might be site-specific. This is very likely the case with the algorithms used in Lake Erken. Despite the fact that steps were taken for reducing such factors that would make the algorithms environment-dependent (e.g. atmospheric correction), several other factors affected the general validity. These included in this case the type of phytoplankton. During the time of the Lake Erken experiment, the phytoplankton community was totally dominated by the
blooming colonial cyanobacteria *Gloeotrichia echinulata*. These colonies are very buoyant and accumulate close to the surface during calm conditions. If the wind increases, the colonies are rapidly mixed into the epilimnic water. This will of course affect any remote sensing algorithm for chlorophyll estimation that does not take the vertical distribution of the phytoplankton into account. The colonies are probably also very efficient light scatterers because of the gas-vacuoles (see e.g. Ganf, Oliver et al. 1989). Figure 1 shows the relation between measured chlorophyll and the reflectance at around 705 nm. This wavelength has been recommended as a reference wavelength for chlorophyll algorithms (Dekker 1993; Pierson and Strömbeck 2000) as phytoplankton absorption is very low at 705 nm. Here we had an apparent influence of phytoplankton at this wavelength, which probably was due to increased scattering. Paper III also illustrates well the effects of scattering on remote sensing algorithms for chlorophyll estimation. When phytoplankton backscattering is high in relation to backscattering by inorganic particles, great variation can be expected in the radiance reflectance ratio 705 / 676 nm. As the concentration of inorganic particles increase, the inorganic backscattering will rapidly start to dominate the total backscattering, and the variation in the radiance reflectance ratio 705 / 676 nm as a function of chlorophyll will decrease. In Lake Erken, the presumably high backscattering of the *Gloeotrichia echinulata* colonies in combination with the relatively low concentrations of suspended inorganic particles will thus probably account for some of the variations in the relationship between the measured chlorophyll and the reflectance that can be seen in figure 1. A third factor is the time difference between the recording of the remote sensing data and the sampling. In Lake Erken, the *Gloeotrichia echinulata* concentration was very patchy and partly moving with the wind, a factor that undoubtedly affected the radiance reflectance.

In paper VI the semi-analytical approach was taken to estimate water quality parameters from the same type of CASI data as in Paper I, but from a different lake. A simple bio-optical model was parameterized by the field data presented in Paper V, and a large synthetic dataset based on a long term water quality record was produced. The dataset was then input in the bio-optical model, the resulting spectral radiance reflectance was calculated for each combination of input parameters and used to construct band or band ratio remote sensing algorithms for the different water quality parameters. In this case, the extensive lake truth measurements were only used for validation of the algorithms. The advantages of this approach were described above, and Paper VI can serve as an example of how the semi-analytical approach is used in practice. However, the results in Paper VI were not totally satisfying, which reminds us about the importance of having a well parameterized bio-optical model.

Paper III showed how variations in the specific inherent optical properties themselves and the combinations of the different water quality parameters affected a band ratio algorithm for chlorophyll estimation. However, the data used in Paper III suffered from quality problems, mainly concerning the backscattering spectra. In the preliminary method used to correct the measured backscattering, a phytoplankton backscattering efficiency of 1 % was used. This was probably too high; in the subsequent work chosen values were 0.5 or 0.1 %. The overestimation of the phytoplankton backscattering also affected the spectral shape of the inorganic backscattering. The field data that were reported in the paper suggested that the response of the band ratio as a function of chlorophyll was greater in reality than in the prediction of the model. Also, the large spread in the band ratio that were induced by the variability in the inherent optical properties and by the distribution of the optically active substances could not be seen in the field data.

The effects of different parameterization of a bio-optical model can also be seen by comparing the results in Paper II with those of Paper VI. Also in paper II (as in paper VI) long
term data was used to construct band ratio algorithms for three different lakes. However, the parameterization of the bio-optical model in paper II was based on field measurements from Lake Mälaren only. The parameterization in Paper VI was based on a more extensive and more local dataset (Eastern Lake Mälaren) collected over a longer time period. If we compare the algorithms recommended in Paper II with those in Paper VI, we will see that the band ratio algorithms for chlorophyll and yellow substance estimation are very similar despite differences in the parameterization of the phytoplankton and yellow substance absorption, while the single band algorithm for suspended particulate inorganic matter differs greatly. Subsequently, very different results would be obtained if those algorithms were applied on the same remote sensing data set, although the spatial relations essentially would stay the same. The main reason for these differences was the value of the inorganic specific backscattering (\( b_{\text{bb}} * (442) \) or \( b_{\text{SPIM}} * (442) \)). This was given the values 0.057 and 0.037 m\(^2\) g\(^{-1}\) respectively, i.e. they differed almost by a factor of 2. Also, different values were used of the exponent \( n (B_{\text{bb}}) \) that determines the spectral shape. A smaller value of \( n \) resulted in a relatively higher backscattering at long wavelengths. The higher value of the specific inorganic backscattering used in Paper II was mainly the result of using an early version of the method for attenuation correction of the in situ backscattering sensor, in which scattering played a more important role.

With this knowledge, the obvious way to increase the precision of the bio-optical models is increased measurements of inherent optical properties. In paper V, which in many ways is the core of this work, my efforts so far within this area are summarized. We seem to have enough knowledge of the phytoplankton absorption coefficient. The reported data was remarkably similar to data reported for ocean waters. We may also have enough data of the backscattering by suspended particulate inorganic matter. The reported data for the inorganic backscattering was in almost total agreement with earlier reported data from different freshwaters, although relatively large variations could be seen. However, the techniques for measuring absorption and backscattering coefficients are based on many assumptions which may lead to errors. The influence of e.g. yellow substance absorption on band ratio algorithms for chlorophyll remote estimation is well known (Dekker 1993; Pierson and Strömbeck 2000). We also know quite well the general shape of the yellow substance absorption spectra, but better parameterization of the bio-optical model would probably be achieved by better understanding how scattering by sub-micrometer particles affect the yellow substance measurements. We need more information about the phytoplankton backscattering. Phytoplankton are recognized as rather unimportant backscatterers in ocean waters, but might be of significant importance in freshwaters dominated by cyanobacteria (see Paper I). There is also very little or no data available from the community of aquatic optics of the scattering phase functions of freshwaters.

Some of the problems of measuring backscattering in highly absorbing and scattering waters were addressed in Paper IV. In this paper, a model for correction of backscattering measurements was presented. The model was a direct result of the poor performance of the in situ backscattering sensor in the strongly absorbing freshwaters encountered in this work. The correction method is of general validity, but it can also be replaced by making complimentary measurement with modern in situ instruments, such as spectral absorption and attenuation meters. However, since the model was based on sound assumptions of the spectral behavior of absorption and scattering, it can also be used in a full spectral mode. In this way, it becomes a valuable tool to study how different water quality parameters affect the measured backscattering.

The overall quality of the measurement of the specific inherent optical properties can be seen in Paper VII, where an underwater PAR model based on average specific inherent optical
properties was validated against independent PAR-measurements. Paper VII can also serve as a bridge between this work and more traditional limnology such as spatial and temporal studies of primary production or physiological studies of e.g. visibility.

**CONCLUSIONS**

In this work I presented extensive measurements of the specific inherent optical properties of Swedish lakes and coastal waters. The overall quality of the measurements was good and their variability was surprisingly small. They can therefore be considered to be generally valid for a vast range of lakes and coastal waters. The specific inherent optical properties has been and will be used in semi-analytical bio-optical models. Such models use water quality parameters for calculation of the spectral inherent optical properties absorption and backscattering, and output spectral radiance reflectance of the water body. The precision of the models depends mainly on the parameterization, i.e. the quality of the specific inherent optical properties. Semi-analytical bio-optical models are very useful for interpretation of remote sensing data. Similar models are also useful for other applications, e.g. for corrections of *in situ* optical measurements and estimations of the under water irradiance from water quality parameters. One strong point with the models is that they can be used in conjunction with long term records of water quality parameters to create remote sensing algorithms. The algorithms will then be based on realistic distributions of the water quality parameters.

Although we now have extensive data on the specific inherent optical properties from our field work, we lack important data on phytoplankton scattering and backscattering. These parameters will affect the correction of the *in situ* measured backscattering, and will also influence remote sensing algorithms derived from modeling. Therefore it will be necessary to expand the measurements of scattering in Swedish freshwaters. It is desirable to know in more detail how phytoplankton and suspended particulate inorganic matter contribute to scattering and backscattering. Another factor affecting the remote sensing algorithms is the yellow substance absorption. It is thus necessary to use more accurate methods to measure spectral shapes of yellow substance absorption, and also to estimate the influences of scattering on the measurements.

The use of bio-optical models for remote sensing seems very promising, although we still are on an experimental level. Increased precision in the estimation of chlorophyll concentration can be reached by increased knowledge about the phytoplankton scattering. It is especially desirable to know more about the behavior of cyanobacteria. Increased precision of the models can probably also be obtained by more extensive validation against field measurements of radiance reflectance. Such experiments will undoubtedly provide us with valuable information that can be used in the more general bio-optical models.

**SUMMARY IN SWEDISH**

Fjärranalys av vattenkvalitet i sjöar är fortfarande i sin linda, eftersom vi ännu inte har några lämpliga satelliter. De satelliter som är konstruerade för att kunna mäta klorofyllhalter i världshaven, t.ex. SeaWiFS (SeaStar), har en spatial upplösning större än en kilometer, vilket är allt för stort för de flesta svenska sjöar. Inom en snar framtid kommer vi dock få tillgång till MERIS-instrumentet, vilket kommer att ha en spatial upplösning på c:a 300 m. Således kan vi förvänta oss en snabb framtid av fjärranalysen av sjöar.

Fjärranalys av vattenkvalitet i sjöar kan bedrivas enligt två olika principer; den empiriska och den halvanalytiska (semi-analytical). I den empiriska metoden används regressionstekniker för att korrelera t.ex. okorrigerad satellitdata mot klorofyllhalten i sjöar. Denna metod kan vara mycket framgångsrik vid enstaka tillfällen och inom begränsade områden, men den ger inte samband som är universella, eftersom man ofta inte tar någon hänsyn till atmosfäriska effekter, ytreffektion, vattnets optiska egenskaper etc. I den halvanalytiska metoden används man sig istället av modeller som beräknar vattnets optiska egenskaper och reflektion utifrån koncentrationerna av de optiskt aktiva ämnen.

Denna avhandling består av sju artiklar, och mitt arbete har i första hand gått ut på att mäta och modellera inherent optical properties (IOP:s) i Svenska sjöar och kustområden. Dessa optiska egenskaper beror enbart på de olika optiskt aktiva ämnen i vattnet, och jag har därför relaterat dem till halterna av DOC (eller yellow substance, mätt i m⁻¹), klorofyll och organiska och organiska partiklar. I arbetet har även ingått utvecklandet av en korrektionsmetod för mätningar av bakåtspridning i sjöar med ett kommersiellt instrument utvecklat för klart havsvatten. Bakåtspridningen påverkar både reflektionens styrka och spektrala form och är således helt central i halvanalytiska modeller.

De mätta sambanden har använts i halvanalytiska modeller för att bestämma vilka våglängdsområden hos vattnets reflektion som är lämpliga att använda för fjärranalys av de olika optiskt aktiva ämnen. Modellerna har även körts med data från långa tidsserier för att simulera hur reflektionen har varierat med tiden. Simuleringar har sedan i sin tur använts för att konstruera beräkningsalgoritmer för fjärranalys av de olika optiskt aktiva ämnen, bestående av ett eller två våglängdsintervall. I ett delarbete tillämpades denna metod på multispektral data (flera våglängdsintervall) mätt med det flygburna CASI-instrument över östra delen av Mälaren. I ett annat arbete användes den tidigare nämnda empiriska metoden för att uppskatta koncentrationen och utbredningen av cyanobakterier (blågröna alger) i sjön Erken.

Som en sista del i arbetet tillkom utvecklandet av en modell som bygger på mätningsresultaten av IOP:s och som använder koncentrationer av de olika optiskt aktiva ämnen för att beräkna det ljus som finns tillgängligt för algers och växtplanktonrens fotosyntes i sjöar. Detta arbetet visar att IOP:s i Svenska sjöar och kustområden är väldigt lika de som tidigare rapporterats från havsområden, men att de skiljer sig åt i proportionerna. Vanligtvis är de också större än i haven. Erfarenheterna från fjärranalysexperimenten visar att den halvanalytiska metoden är mycket lovande, men att den kräver fler och bättre mätningar av IOP:s och deras förhållande till vattnens optiskt aktiva ämnen. Detta gäller speciellt
växtplanktons påverkan på spridning och bakåtspridning, och den spektrala formen på absorptionsspektrumen hos DOC.

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