MERIS, MODIS and ETM+ Channel Configurations in the Estimation of Lake Water Quality from Subsurface Reflectance Using Semi-analytical and Empirical Algorithms

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Abstract

We studied the estimation of lake water quality from measured subsurface reflectances in order to find out the potential of the channel configurations of three satellite instruments (MERIS, MODIS and ETM\textsuperscript{+}). The semi-analytical method was based on the inversion of a bio-optical reflectance model and the empirical method on using channel ratios or single channels. The dataset, consisting of data from 11 lakes located in Finland, has a wide range of water quality: the sum of chlorophyll a and phaeophytin a (CChl-a) ranging from 0.8 to 72 \(\mu\text{g} \ \text{l}^{-1}\), total suspended solids (CTSS) from 0.4 to 24 mg l\textsuperscript{-1} and the absorption coefficient of CDOM at 400 nm (\(a_{\text{dom}}(400)\)) from 0.4 to 14 m\textsuperscript{-1}. The results from the inversion method indicate that MODIS and MERIS have nearly optimum channel configurations for the estimation of CTSS and \(a_{\text{dom}}(400)\) in the lakes we studied. The analyses of the empirical algorithms suggest that MERIS has optimum channels for water quality estimations. The estimation accuracy of CChl-a and CTSS by the inversion method was about the same for the two estimation methods, but in case of \(a_{\text{dom}}(400)\) the empirical algorithms were clearly better than the inversion method. \(a_{\text{dom}}(400)\) was estimated using ETM\textsuperscript{+} channels with about the same accuracy as by MERIS and MODIS channels.

Key words: reflectance, water quality, inversion, channel ratios, lakes, remote sensing

1. Introduction

Interpretation of water quality from remote sensing data is often based on empirical algorithms where water quality variables are estimated from the reflectance at one wavelength or from ratios between reflectances measured at two wavelengths. Empirical estimation methods can be divided into purely empirical and semi-empirical algorithms. Semi-empirical algorithms rest on the knowledge on how the optical properties of optically active variables affect the reflectance at the applied wavelengths. Chlorophyll \(a\), for example, can be estimated with the blue/green reflectance ratio in the case...
of oceans (O'Reilly et al., 1998) and with NIR/red ratio (Gitelson et al., 2002; NIR=near-infrared) in lakes. Both algorithms utilize the absorption maximums of phytoplankton located at about 440 and 675 nm.

Empirical methods have particularly proved applicable to clear ocean waters, but in lakes and coastal waters the estimation of one water quality variable is often disturbed by other optically active substances (OAS). One way to solve this problem in these ‘case 2’ waters is to use interpretation methods that are based on bio-optical modeling. Such models calculate the reflectance from the specific inherent optical properties (SIOPs) and from the concentrations of optically active substances. Estimation of water quality using bio-optical reflectance modelling is usually based on the inversion of the applied model. The inversion method has been used in coastal and ocean applications (see e.g. Doerffer & Fischer, 1993; Garver & Siegel, 1997; Schiller and Doerffer, 1999; Maritorena et al., 2000; Lee and Carder, 2004) as well as in lake applications (e.g. Bukata et al., 1981, Gege, 1998; Kutser et al., 2001; Pierson and Strömbeck, 2001). The problem of increased computing time due to pixel-by-pixel inversion of hyperspectral satellite images has been solved by the use of neural networks (e.g. Schiller and Doerffer, 1999) and by matrix inversion (Hoge and Lyon, 1996; Hoogenboom et al., 1999b). Gons (1999) used a combination of bio-optical modeling and a channel ratio in the estimation of chlorophyll-a in eutrophic lakes. The advantages of using bio-optical modeling in the interpretation are 1) all channels of the remote sensing instrument are utilized and 2) regional, seasonal and water type differences in the SIOPs can be considered in the interpretation.

The aim of this paper was to investigate the suitability of the channel configurations of three satellite instruments for the estimation of OAS concentrations of lakes using the inversion method and empirical algorithms. The studied OAS consisted of chlorophyll a, total suspended solids and coloured dissolved organic matter (CDOM). The analyses were based on the measured subsurface reflectance spectra from which reflectances were constructed for each satellite instrument channel. The channel configurations included in the study consisted of two ocean color instruments (ENVISAT MERIS, TERRA/AQUA MODIS) together with LANDSAT ETM+. MODIS and MERIS are multispectral instruments having similar channel configuration in the VIS(visible)-NIR range of the spectrum with the exception that MERIS has channels at 620 and 705 nm, which are not found in MODIS. ETM+ has three wide channels in VIS. Although ETM+ was designed for land applications it has also been used in water quality studies of lakes (e.g. Kloiber et al., 2002, Vincenta et al., 2004) and coastal waters (e.g. Lavery et al., 1993) due to its good spatial resolution (30 m). Many of the published water quality algorithm studies of lakes have focused on one estimation method or on one lake type only. For our study we selected 11 lakes, displaying a range of varying lake type (oligotrophic – eutrophic, humic). The semi-analytical bio-optical reflectance model needed in inversion was first parametrized using SIOP's measured in the field and laboratory.
2. Material and methods

2.1 Description of lakes

Optical and limnological measurements were carried out in 1997 and 1998 at 14 stations representing 11 lakes located in southern and northern Finland (Table 1). Five of the stations were surveyed both in May and in July-August. Each lake had one measurement station with the exception of Lake Norvajärvi and Lake Pääjärvi, each of which had two stations, and of Lake Lohjanjärvi, where there were three stations in May and four stations in August. The reflectance spectra of 12 stations were used in model testing and in the estimation of OAS. The remaining reflectance spectra were not accepted for further analyses due to noise caused by waves or large variations in incoming solar radiation. However, the SIOPs of all stations were utilized in the parametrization of the reflectance model. The OAS concentrations and optical properties of the stations are presented in Table 2.

Table 1. Main characteristics of the lakes studied. Number of stations and measurement months are also given. Each lake was sampled at one station with the exception of Lohjanjärvi (4 stations), Pääjärvi (2 stations) and Norvajärvi (2 stations). Oligo = oligotrophic, Meso = mesotrophic, Eu = eutrophic, S. Finland = southern Finland, N. Finland = northern Finland.

<table>
<thead>
<tr>
<th>Lake</th>
<th>Short name</th>
<th>Region</th>
<th>Coordinates</th>
<th>Area km²</th>
<th>$z_{\max}$ m</th>
<th>Lake type</th>
<th>Month</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enäjärvi, Vihti</td>
<td>Ena</td>
<td>S. Finland</td>
<td>60°20'N 24°23'E</td>
<td>5</td>
<td>3.4</td>
<td>Eu</td>
<td>Aug.</td>
</tr>
<tr>
<td>Lohjanjärvi</td>
<td>Loh</td>
<td>S. Finland</td>
<td>60°15'N 23°55'E</td>
<td>94</td>
<td>12.6</td>
<td>Meso-Eu</td>
<td>May, Aug.</td>
</tr>
<tr>
<td>Vesijärvi, Lahti</td>
<td>Ves</td>
<td>S. Finland</td>
<td>61°02'N 25°37'E</td>
<td>111</td>
<td>41</td>
<td>Meso</td>
<td>Aug.</td>
</tr>
<tr>
<td>Puujärvi</td>
<td>Puu</td>
<td>S. Finland</td>
<td>60°15'N 23°45'E</td>
<td>7</td>
<td>21</td>
<td>Oligo</td>
<td>May, Aug.</td>
</tr>
<tr>
<td>Keravanjärvi</td>
<td>Ker</td>
<td>S. Finland</td>
<td>60°37'N 25°5'E</td>
<td>1</td>
<td>2.2</td>
<td>Humic</td>
<td>May</td>
</tr>
<tr>
<td>Vasikkajärvi</td>
<td>Vas</td>
<td>N. Finland</td>
<td>67° 7'N 26° 5'E</td>
<td>0.3</td>
<td>17</td>
<td>Oligo</td>
<td>July</td>
</tr>
<tr>
<td>Norvajärvi</td>
<td>Nor</td>
<td>N. Finland</td>
<td>66°37’N 25°47'E</td>
<td>11</td>
<td>15</td>
<td>Oligo</td>
<td>July</td>
</tr>
<tr>
<td>Pöyliöjärvi</td>
<td>Pöy</td>
<td>N. Finland</td>
<td>66°27’N 25°48'E</td>
<td>1.3</td>
<td>8</td>
<td>Humic</td>
<td>July</td>
</tr>
<tr>
<td>Sonkajärvi</td>
<td>Son</td>
<td>N. Finland</td>
<td>66°37’N 25°14'E</td>
<td>3.2</td>
<td>11</td>
<td>Humic</td>
<td>July</td>
</tr>
<tr>
<td>Sierijärvi</td>
<td>Sie</td>
<td>N. Finland</td>
<td>66°28’N 25°57'E</td>
<td>4</td>
<td>2.5</td>
<td>Eu</td>
<td>July</td>
</tr>
</tbody>
</table>

The lakes were classified (Table 1) according to OECD (1982) based on the maximum chlorophyll $a$ concentration (values measured in July-August in this study):

- oligotrophic ($C_{\text{Chl-a}}(\text{max}) \leq 8 \, \mu g \, l^{-1}$)
- mesotrophic ($8 \, \mu g \, l^{-1} < C_{\text{Chl-a}}(\text{max}) \leq 25 \, \mu g \, l^{-1}$)
- eutrophic ($C_{\text{Chl-a}}(\text{max}) > 25 \, \mu g \, l^{-1}$)

Humic lakes, characterized by the high concentration of CDOM and the relatively low concentration of total suspended solids and chlorophyll $a$, were separated from the rest of the lakes ($a_{\text{cdom}(400)} \geq 4.0 \, \text{m}^{-1}$ and $C_{\text{Chl-a}}(\text{max}) < 8 \, \mu g \, l^{-1}$).
Table 2. The concentrations of OAS, Secchi depth, $K_d$(PAR), $a_{tot}(412)$ and $b_{tot}(555)$ of the stations. $a_{tot}(412)$ and $b_{tot}(555)$ were measured with ac-9 and are presented without pure water.

<table>
<thead>
<tr>
<th>Station</th>
<th>Month</th>
<th>C_{TSS} , \text{mg l}^{-1}</th>
<th>C_{Chl-a} , \mu\text{g l}^{-1}</th>
<th>a_{cdom}(400) , \text{m}^{-1}</th>
<th>Secchi , \text{m}</th>
<th>K_d$(PAR) , \text{m}^{-1}</th>
<th>$a_{tot}(412) , \text{m}^{-1}</th>
<th>$b_{tot}(555) , \text{m}^{-1}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Puu-m*</td>
<td>May</td>
<td>1.9</td>
<td>4.5</td>
<td>2.1</td>
<td>3.9</td>
<td>1.1</td>
<td>2.0</td>
<td>1.2</td>
</tr>
<tr>
<td>Loh1-a*</td>
<td>Aug.</td>
<td>15.5</td>
<td>55</td>
<td>5.3</td>
<td>0.8</td>
<td>3.8</td>
<td>6.2</td>
<td>6.6</td>
</tr>
<tr>
<td>Loh2-a*</td>
<td>Aug.</td>
<td>4.6</td>
<td>13.5</td>
<td>3.8</td>
<td>1.5</td>
<td>1.9</td>
<td>3.6</td>
<td>2.6</td>
</tr>
<tr>
<td>Loh3-a*</td>
<td>Aug.</td>
<td>5.9</td>
<td>10.5</td>
<td>3.9</td>
<td>1.9</td>
<td>2.0</td>
<td>3.5</td>
<td>2.5</td>
</tr>
<tr>
<td>Loh4-a*</td>
<td>Aug.</td>
<td>3.0</td>
<td>11.5</td>
<td>3.3</td>
<td>2.9</td>
<td>1.</td>
<td>3.1</td>
<td>1.9</td>
</tr>
<tr>
<td>Ena-a*</td>
<td>Aug.</td>
<td>10</td>
<td>37</td>
<td>1.9</td>
<td>1.1</td>
<td>2.8</td>
<td>3.7</td>
<td>7.9</td>
</tr>
<tr>
<td>Nor1-a*</td>
<td>Aug.</td>
<td>0.8</td>
<td>3.5</td>
<td>3.1</td>
<td>4.0</td>
<td>1.5</td>
<td>2.9</td>
<td>1.0</td>
</tr>
<tr>
<td>Nor2-a*</td>
<td>Aug.</td>
<td>1.1</td>
<td>3.3</td>
<td>3.6</td>
<td>3.3</td>
<td>1.5</td>
<td>2.9</td>
<td>0.9</td>
</tr>
<tr>
<td>Sie-a*</td>
<td>Aug.</td>
<td>19.6</td>
<td>73</td>
<td>18.2</td>
<td>0.4</td>
<td>7.8</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sin-a*</td>
<td>Aug.</td>
<td>1.7</td>
<td>5.7</td>
<td>13.0</td>
<td>2.2</td>
<td>3.9</td>
<td>10.6</td>
<td>1.7</td>
</tr>
<tr>
<td>Poy-a*</td>
<td>Aug.</td>
<td>1.0</td>
<td>7.6</td>
<td>10.0</td>
<td>2.5</td>
<td>3.0</td>
<td>8.4</td>
<td>1.2</td>
</tr>
<tr>
<td>Vas-a*</td>
<td>Aug.</td>
<td>0.4</td>
<td>0.8</td>
<td>0.3</td>
<td>11.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.3</td>
</tr>
<tr>
<td>Loh1-m</td>
<td>May</td>
<td>17</td>
<td>9.7</td>
<td>9.2</td>
<td>0.8</td>
<td>-</td>
<td>7.5</td>
<td>8.1</td>
</tr>
<tr>
<td>Loh2-m</td>
<td>May</td>
<td>10</td>
<td>7.2</td>
<td>5.4</td>
<td>1.1</td>
<td>-</td>
<td>5.2</td>
<td>4.5</td>
</tr>
<tr>
<td>Loh3-m</td>
<td>May</td>
<td>7.8</td>
<td>4.2</td>
<td>4.8</td>
<td>1.2</td>
<td>-</td>
<td>4.5</td>
<td>3.6</td>
</tr>
<tr>
<td>Ker-m</td>
<td>May</td>
<td>4.4</td>
<td>8.8</td>
<td>14.3</td>
<td>1.4</td>
<td>-</td>
<td>12.5</td>
<td>2.8</td>
</tr>
<tr>
<td>Puu-a</td>
<td>Aug.</td>
<td>1.7</td>
<td>1.3</td>
<td>1.3</td>
<td>7.0</td>
<td>0.8</td>
<td>1.2</td>
<td>0.9</td>
</tr>
<tr>
<td>Ves-a</td>
<td>Aug.</td>
<td>2</td>
<td>11.5</td>
<td>1.4</td>
<td>2.8</td>
<td>-</td>
<td>1.7</td>
<td>2.1</td>
</tr>
<tr>
<td>Paa1-a</td>
<td>Aug.</td>
<td>2.1</td>
<td>5.5</td>
<td>7.4</td>
<td>2.7</td>
<td>-</td>
<td>6.1</td>
<td>1.4</td>
</tr>
<tr>
<td>Paa2-a</td>
<td>Aug.</td>
<td>1.6</td>
<td>6.8</td>
<td>7.2</td>
<td>2.7</td>
<td>2.7</td>
<td>6.2</td>
<td>1.4</td>
</tr>
</tbody>
</table>

* Stations used for testing the bio-optical reflectance model and the water quality algorithms. All stations were utilized in model parametrization.

2.2 Limnological and optical measurements

Water samples were taken from depths of 0–0.4 and 0.8–1.2 m. In the subsequent analyses the average concentrations of these two depths were used. Water quality determinations of the samples were made in the water laboratories of the Regional Environment Centres of Uusimaa and of Lapland. Concentration of total suspended solids ($C_{TSS}$) was measured using gravimetric determination of the matter removed by a filter ($EN \, 872$, Nuclepore polycarbonate 0.4 µm filter). Concentration of the sum of chlorophyll $a$ and phaeophytin $a$ ($C_{Chl-a}$) was determined with a spectrophotometer after their extraction using hot ethanol ($ISO \, 10260$, GF/C filter). The absorption spectra (380–800 nm) of CDOM were measured with a spectrophotometer (5 cm long cuvette) from a sample filtered through a Nuclepore polycarbonate 0.4 µm filter. The absorption measurements were corrected for residual scattering (due to small particles not retained by the filter) by subtracting absorption at 750 nm from the measured values in 400–750 nm ($Gallie$, 1994). The absorption coefficient at 400 nm ($a_{cdom}(400)$) was used as a measure of CDOM concentration. Phytoplankton species and phytoplankton biomass were determined by microscopic counting.
The optical measurements conducted from a boat consisted of upwelling and downwelling irradiances (Li1800UW underwater spectrometer, LI-COR Corporation), and total absorption and attenuation coefficients (ac-9 absorption/attenuation meter, WET Labs Inc.). Downwelling and upwelling spectral irradiance (300–850 nm with a step of 2 nm) were measured at depths of 0.5, 1, 2 and 3 m. The Li18000UW was kept away (about 1.5 m) from the boat by a boom. To measure the upwelling irradiance, the Li1800UW instrument was turned around with the detector facing downward. The long integration period (40 s) resulted in noisy irradiance spectra, particularly in windy conditions. To remove this intensity variation due to wave focusing, the spectra were smoothed by the Butterworth recursive filter method. Variation in the global radiation (i.e. direct solar plus diffuse sky radiation) between upwelling and downwelling irradiance measurements may result in erroneous reflectance. Because of this, the underwater irradiances were corrected by the ratio between the average incident irradiance above the water surface during one measurement series (duration about 30 minutes) and the incident irradiance corresponding to the time of each underwater spectrum measurement (Herlevi, 2002). The incident irradiance (400–1100 nm) above the water surface was recorded with a Li200SA sensor.

The underwater reflectances (\(R\)) were calculated by dividing the upwelling irradiance (\(E_u\)) by the downwelling irradiance (\(E_d\)) at each depth:

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

In the subsequent analyses we mainly used reflectances measured at the depth of 0.5 m.

The diffuse attenuation coefficient \(K_d\) was calculated from downwelling irradiances \(E_d\) measured by the Li1800UW underwater spectrometer at the depths of 0.5 and 1.0 m:

\[
K_d(z, \lambda) = \frac{1}{z_2 - z_1} \ln \left[ \frac{E_d (z_2, \lambda)}{E_d (z_1, \lambda)} \right]
\]  (2)

where \(z\) is water depth. \(K_d(PAR)\) was obtained by calculating the mean \(K_d\) of the 400-700 nm region and it ranged between 0.6 and 7.8 m\(^{-1}\) (Table 2).

The wavelengths used in the ac-9 absorption/attenuation meter were 412, 440, 488, 510, 532, 555, 650, 676 and 715 nm. The measurements were performed as depth profiles of the whole water column by lowering the instrument at a steady speed from the boat. Typically, three profiles were measured at each station. In the further analyses of the data, we used the average values of the measurements taken from 0–2 m. The obtained values were corrected for temperature and scattering according to the ac-9 manual (WET Labs, 1995). The total scattering coefficient was obtained as the difference between the corrected attenuation and absorption coefficient.
2.3 Structure of the bio-optical model

Calculation of irradiance reflectance just beneath the water surface, \( R(0-,\lambda) \), is based on the following equation (Gordon et al., 1975 and simplified by Jerlov, 1976):

\[
R (0-,\lambda) = C \frac{b_{b,Tot}(\lambda)}{a_{Tot}(\lambda) + b_{b,Tot}(\lambda)}
\]

where \( b_{b,Tot}(\lambda) \) is the total backscattering coefficient and \( a_{Tot}(\lambda) \) is the total absorption coefficient. \( C \) depends mainly on the illumination and viewing geometry. Here \( C \) was estimated by the equation presented by Kirk (1984):

\[
C = -0.629\mu_0 + 0.975
\]

where \( \mu_0 \) is the cosine of the solar zenith angle in the water. The model simulates reflectance in the 400-750 nm range with a step of 2 nm. Utilizing Beer’s law \( a_{Tot}(\lambda) \) and \( b_{b,Tot}(\lambda) \) in Eq. (3) are obtained by summing up the absorption and backscattering coefficients of the optically active substances in the water.

Similar bio-optical reflectance models to the one described here have been widely used in lake water quality studies (e.g. Bukata et al., 1981; Dekker, 1993; Hoogenboom et al., 1998a; Kondratyev et al., 1998; Podznyakov et al., 1998; Pierson and Strömbeck, 2000). The main differences between the models are the number of the optically active substances included and the numerical values of the specific inherent optical properties. We assumed four optically active components in the model: phytoplankton, tripton, colored dissolved organic matter and pure water. Tripton is non-living particulate matter and it mainly consists of detritus and inorganic particles. Total backscattering was calculated without considering phytoplankton and tripton backscattering separately.

The total spectral absorption coefficient is described by:

\[
a_{Tot}(\lambda) = a_w(\lambda) + a_{cdom}(\lambda) + a_{ph}(\lambda) + a_{tri}(\lambda)
\]

where \( a_w(\lambda) \) is the absorption coefficient of pure water (Buiteveld, 1994), \( a_{ph}(\lambda) \) is the absorption coefficient of phytoplankton, \( a_{cdom}(\lambda) \) is the absorption coefficient of CDOM and \( a_{tri}(\lambda) \) is the specific absorption coefficient of tripton.

Absorption by CDOM is calculated by assuming an exponential increase with a decreasing wavelength (Bricaud et al., 1981):

\[
a_{cdom}(\lambda) = a_{cdom}(400) e^{-S_{CDOM}(\lambda-400)}
\]

where \( a_{cdom}(400) \) is the absorption coefficient of CDOM at 400 nm and \( S_{CDOM} \) is the slope factor.

Absorption by phytoplankton, \( a_{ph}(\lambda) \), is calculated by:

\[
a_{ph}(\lambda) = a_{ph}^*(\lambda) C_{Chl-a}
\]
where \( a^* \text{Ph}(\lambda) \) is the Chl-a specific absorption coefficient of phytoplankton.

Absorption by tripton, \( a_{\text{Tri}}(\lambda) \), is expressed as:

\[
a_{\text{Tri}}(\lambda) = a^*_{\text{TSS}}(\lambda) C_{\text{TSS}}
\]

where \( a^*_{\text{TSS}}(\lambda) \) is the specific absorption of bleached total suspended solids and \( C_{\text{TSS}} \) is the concentration of TSS. Here we define absorption by tripton using \( C_{\text{TSS}} \), because tripton concentration measurements were not available. \( a^*_{\text{TSS}}(\lambda) \) is described analogous to the calculation of \( a_{\text{dom}}(\lambda) \) (Roesler et al., 1989):

\[
a^*_{\text{TSS}}(\lambda) = a^*_{\text{TSS}}(400) e^{-S_{\text{Tri}}(400)}
\]

where \( a^*_{\text{TSS}}(400) \) is the specific absorption of bleached total suspended solids at 400 nm and \( S_{\text{Tri}} \) is the slope factor of tripton absorption.

The total backscattering coefficient \( b_{\text{Tri},\text{Tot}}(\lambda) \) is described by:

\[
b_{\text{Tri},\text{Tot}}(\lambda) = b_{\text{Tri}}(\lambda) + b_{\text{Tri}}^* C_{\text{TSS}}
\]

where \( b_{\text{Tri}}(\lambda) \) is the backscattering coefficient of pure water (Buiteveld, 1994), and \( b_{\text{TSS}}^* \) is the specific scattering coefficient of TSS. The backscattering probability of pure water, \( b_{\text{Tri}} \), was set at 0.5 (Sathyendranath et al., 1989). \( b_{\text{TSS}}^* \) is the backscattering probability of TSS.

We assumed that the specific scattering coefficient of TSS \( b^*_{\text{TSS}}(\lambda) \) can be described by a power function:

\[
b^*_{\text{TSS}}(\lambda) = b^*_{\text{TSS}}(555) \left( \frac{555}{\lambda} \right)^{n_b}
\]

where \( b^*_{\text{TSS}}(555) \) is the specific scattering coefficient of TSS at 555 nm and \( n_b \) is the scattering exponent.

### 2.4 Estimation of model coefficients

Our aim was to develop a reflectance model applicable for the lake types typical to Finland. The most important monitoring period during ice-free conditions in Finland is July–August. This because of the phytoplankton biomass, the occurrence of cyanobacteria and the low oxygen concentrations in the hypolimnion. Therefore, we mainly used the SIOPs from July-August in the model parametrization. The SIOPs in spring can be different from those in the period July-August due to distinct phytoplankton species and material discharge from the watershed during spring flooding.

The Chl-a specific absorption coefficient of phytoplankton, \( a^*_{\text{Ph}} \) in Eq. (7), was calculated using the power function originally presented by Bricaud et al. (1995):

\[
a^*_{\text{Ph}}(\lambda) = A(\lambda) C_{\text{Chl}}^{-B(\lambda)}
\]
where $A(\lambda)$ and $B(\lambda)$ are positive empirical coefficients. Bricaud et al. (1995) published the average coefficients based on ocean data. Here $A(\lambda)$ and $B(\lambda)$ were obtained from a study of Ylöstalo et al. (2005) carried out in 2000 and 2002 at 10 Finnish lakes. Three of the lakes and five of the station in our study were the same as in Ylöstalo et al. (2005). According to Eq. (12) $a^*_{ph}$ decreases from oligotrophic to eutrophic waters. This is due to the package effect and the possible systematic changes between species composition/pigmentation and trophic level (Bricaud et al., 1995). The specific absorption coefficient of bleached total suspended solids ($a^*_{TSS(400)}$) and the slope factor of tripton absorption ($S_{Tri}$) were also taken from the study by Ylöstalo et al. (2005).

The slope factor $S_{cdom}$ was estimated by fitting Eq. (6) to the measured $a_{cdom(\lambda)}$ (18 spectra, wavelength range used in the optimization was 400-750 nm). Two lakes were excluded from the optimization: Lake Sierijärvi (high scattering in the long wavelength region because of ineffective filtering) and Lake Vasikkajärvi (noisy absorption spectrum arising from a cuvette that was too short for this clear water lake). The $S_{cdom}$ obtained through optimization was 0.0150 nm$^{-1}$. The variation of $S_{cdom}$ in different lakes/stations was small (standard deviation = 0.000902 or 5.8% of the mean, min = 0.0136 nm$^{-1}$, max = 0.0175 nm$^{-1}$).

The specific scattering coefficient, $b^*_{TSS(555)}$, and the scattering exponent, $n_b$, were estimated from the ac-9 measurements. The specific scattering coefficient ($b^*_{TSS(\lambda)}$) was calculated for the nine ac-9 wavelengths by:

$$b^*_{TSS(\lambda)} = \frac{b_{Tot}(\lambda) - b_a(\lambda)}{C_{TSS}}$$  \hspace{1cm} (13)

where $b_{Tot}(\lambda)$ is the total scattering measured with the ac-9. The mean value of the $b^*_{TSS(555)}$ was 0.811 l m$^{-1}$ mg$^{-1}$ (mean of August without Sie-a and Puu-a, n=13, the name abbreviations are explained in Table 1 and Table 2) and the scattering coefficient $n_b$ obtained through optimization against the measured $b^*_{TSS(\lambda)}$ was 0.70 (August without Sie-a, n=14). Sie-a was excluded from the estimations because of the non-linearity in the ac-9 measurements. The reliable measurement of a and b with ac-9 in this very eutrophic lake would require a shorter optical pathlength than the 25 cm used in our study (ac-9 is available also with 10 cm pathlength, WET Labs, 1995). In waters with high $c$ the 25 cm pathlength results in poor resolution and unreliable a and b.

In addition, the backscattering ratios are needed for the calculation of $b_{b,Tot}$ (Eq. 10). The backscattering probability of TSS ($b_{TSS}$) was estimated by fitting the modeled reflectance spectrum (Eq. 3) with the 12 reflectance spectrum measured with the LI-1800UW. The 400–448 nm range was not included in the analyses, because of the difficulties in measuring the low irradiance levels and possible instrument self-shading in the blue end of the spectrum. We assumed the backscattering ratios to be constant over the whole wavelength range. All the optimized coefficients ($S_{cdom}$, $n_b$, $b_{TSS}$) were determined with least-squared method using the Nelder-Mead simplex search technique (Nelder and Mead, 1965).
2.5 Estimation of water quality

The applicability of the channel configurations of MERIS, MODIS (1 km data) and ETM+ for the estimation of OAS were tested using the inversion technique and the empirical algorithms. For these experiments reflectances were averaged for the satellite instrument channels (Table 3). The wavelength range used in the inversion and empirical methods was 450-750 nm. For this reason the MODIS channel 8 (743–753 nm) and the MERIS channel 10 (750–757.5 nm) were replaced by 744–750 nm. Channel 2 (438–448 nm) of MERIS and MODIS was replaced by 450–460 nm. In addition, we examined whether the use of the full reflectance spectrum (450–750 nm with a step of 2 nm) improved the estimation accuracy of OAS. Before the empirical analyses using the full spectrum the 10 nm moving averages were calculated for every R(λ).

Table 3. Channels of ETM+, MODIS (1 km data) and MERIS satellite instruments in the 400-760 nm range. The same channels (except MODIS and MERIS channel 1) were used in the OAS estimations.

<table>
<thead>
<tr>
<th>Channel number</th>
<th>Wavelength range nm</th>
<th>ETM+</th>
<th>MODIS</th>
<th>MERIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>450-520</td>
<td>405-420</td>
<td></td>
<td>407.5-417.5</td>
</tr>
<tr>
<td>2</td>
<td>530-610</td>
<td>438-448 (this study: 450-460)</td>
<td></td>
<td>437.5-447.5 (this study: 450-460)</td>
</tr>
<tr>
<td>3</td>
<td>630-690</td>
<td>483-493</td>
<td></td>
<td>485-495</td>
</tr>
<tr>
<td>4</td>
<td>526-536</td>
<td></td>
<td>505-515</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>546-556</td>
<td></td>
<td>555-565</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>662-672</td>
<td></td>
<td>615-625</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>673-683</td>
<td></td>
<td>660-670</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>743-753 (this study: 743-750)</td>
<td></td>
<td>677.5-685</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td></td>
<td></td>
<td>700-710</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td></td>
<td></td>
<td>750-757.5 (this study: 743-750)</td>
<td></td>
</tr>
</tbody>
</table>

The applied inversion method is based on the maximum likelihood method assuming that the forward (reflectance) modeling error is normally distributed. Following this, the maximum likelihood estimate for multiple variables is obtained by searching the maximum value of a multi-dimensional Gaussian conditional probability density distribution. When the modeling errors of different channels are assumed to be independent from each other, the obtained constrained minimization problem for the joint estimation of C_{TSS}, C_{Chl-a} and a_{cdom}(400) is:

\[
\min_{TSS, Chl-a, a_{400}} \sum_{i=1}^{n} \frac{1}{2\sigma_i^2} (R_{i,\text{sim}} - R_{i,\text{mea}})^2
\]

with respect to constraints: \(0.2 \leq C_{TSS} \leq 25 \text{ mg l}^{-1}\), \(0.2 \leq C_{Chl-a} \leq 100 \text{ \mu g l}^{-1}\) and \(0.2 \leq a_{cdom}(400) \leq 25 \text{ m}^{-1}\)
where $\sigma_i$ is the standard deviation of statistical reflectance modeling error for channel $i$. $R_{i,\text{sim}}$ and $R_{i,\text{mea}}$ are the simulated and measured reflectances for channel $i$, respectively. $\sigma_i$ is estimated using the root mean squared error (rmse), which is calculated from the residual errors between the measured and simulated reflectances (Eq. 16). The simulated reflectances for the 12 stations were obtained using measured $C_{\text{TSS}}$, $C_{\text{Chl-a}}$ and $a_{\text{cdom}(400)}$ as model input. In practice, each inverse variance term, $\sigma_i^{-2}$, weights each channel according to its estimated modeling accuracy. Eq. (14) can be used with any spectral channel configuration or using averaged channels. However, the minimum number of channels ($n$) has to be as high as the number of estimated variables in order to avoid an ill-posed inversion problem.

The best empirical algorithms were identified by calculating correlations of $C_{\text{TSS}}$, $C_{\text{Chl-a}}$ and $a_{\text{cdom}(400)}$ with all $R(\lambda)$ (450–750 nm with a step of 2 nm) and all possible ratios of two $R(\lambda)$. The general formulation of the empirical algorithms was:

$$C_i = aX + b \quad (15)$$

where $C_i$ is the concentration of variable $i$, $a$ and $b$ are empirical parameters and $X$ is an independent variable (reflectance of a single channel or reflectance ratio of two channels).

The accuracy characteristics of the model and OAS algorithms were defined by $R^2$ and root mean squared error (rmse), which is defined as:

$$\text{rmse} = \sqrt{\frac{1}{N-p} \sum_{i=1}^{N} (\hat{Y}_i - Y_i)^2} \quad (16)$$

where $\hat{Y}_i$ is the estimated value and $Y_i$ is the measured value. $p=0$ in calculating the residual error of the optimization problem (Eq. 14) and in calculating rmse of the inversion estimates, and $p=2$ for the empirical algorithms. The relative rmse ($\%$) was calculated from the rmse and the measured average value.

3. Results

3.1 Bio-optical reflectance model

The simulated (Eq. 5) and measured (ac-9) $a_{\text{tot}}$ are presented in Fig. 1. At three Lohjanjärvi stations (Loh1-a, Loh2-a, Loh3-a), the simulated $a_{\text{tot}}$ is slightly higher than the measured $a_{\text{tot}}$. The specific backscattering coefficient at 555 nm ($b_{\text{b,TSS}(555)} = b_{\text{TSS}} \cdot b_{\text{TSS}(555)}$) was estimated by optimizing the backscattering probability ($b_{\text{TSS}}$) of the reflectance model. This resulted in $b_{\text{TSS}}=0.0131$, corresponding to $b_{\text{b,TSS}} (555)$ of 0.0106 l m$^{-1}$ mg$^{-1}$. The model coefficients are summarized in Table 4. The simulated and measured reflectances for the 12 stations are shown in Fig. 2. The biggest discrepancies were in the eutrophic lakes (Sie-a, Ena-a, Loh1-a).
Fig. 1. Simulated (—) and measured (o, with ac-9) total absorption coefficients ($a_{\text{tot}}$) without the contribution of pure water. The measured $a_{\text{tot}}$ of Sie-a station were not included due to the non-linearity of the ac-9 measurements. The scale of the x-axis varies by station.

Fig. 2. Measured (——) and simulated (—) $R(\lambda)$ of 12 stations. $R^2 = 0.921$, rmse = 24.8%.
Table 4. The coefficients of the reflectance model.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Symbol</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorption coefficient of pure water</td>
<td>$a_w(\lambda)$</td>
<td>see the reference</td>
<td>Buiteveld (1994)</td>
</tr>
<tr>
<td>Specific absorption of phytoplankton</td>
<td>$a_{ph}(\lambda)$</td>
<td>see the reference</td>
<td>Ylöstalo et al. (2005)</td>
</tr>
<tr>
<td>Slope factor of CDOM absorption</td>
<td>$S_{CDOM}$</td>
<td>0.0150 nm$^{-1}$</td>
<td>18 stations of this study</td>
</tr>
<tr>
<td>Specific absorption of bleached TSS at 400 nm</td>
<td>$a_{TSS(400)}$</td>
<td>0.13 l m$^{-1}$mg$^{-1}$</td>
<td>Ylöstalo et al. (2005)</td>
</tr>
<tr>
<td>Slope factor of tripton absorption</td>
<td>$S_{n_t}$</td>
<td>0.012 nm$^{-1}$</td>
<td>Ylöstalo et al. (2005)</td>
</tr>
<tr>
<td>Specific scattering of TSS at 555 nm</td>
<td>$b_{TSS(555)}$</td>
<td>0.811 l m$^{-1}$mg$^{-1}$</td>
<td>13 stations of this study</td>
</tr>
<tr>
<td>Scattering exponent of TSS</td>
<td>$n_b$</td>
<td>0.705</td>
<td>14 stations of this study</td>
</tr>
<tr>
<td>Scattering coefficient of pure water</td>
<td>$b_w(\lambda)$</td>
<td>see the reference</td>
<td>Buiteveld (1994)</td>
</tr>
<tr>
<td>Backscattering probability of pure water</td>
<td>$b_{p_w}$</td>
<td>0.5</td>
<td>Sathyendranath et al. 1989</td>
</tr>
<tr>
<td>Backscattering probability of TSS</td>
<td>$b_{p_{TSS}}$</td>
<td>0.0131</td>
<td>12 stations of this study</td>
</tr>
</tbody>
</table>

3.2 Estimation of water quality

The weight term $(1/2\sigma_t^2)$ in the constrained minimization problem of the inversion method (Eq. 14) was obtained by calculating the rmse($\lambda$) between the measured and simulated $R(\lambda)$ (Fig. 3). The rmse was highest at 560, 630 and 700 nm, mainly due to the discrepancies in the measured and simulated $R$ in the mesotrophic and eutrophic stations.

![Fig. 3. rmse between the measured and simulated $R(\lambda)$.](image-url)

The statistical accuracy characteristics of the inversion based water quality estimates are presented in Table 5. The results were examined mainly by using the rmse, which in our dataset was more sensitive to the accuracy differences than $R^2$. The results from the MERIS and MODIS inversions were very similar (Fig. 4). In the case of $C_{TSS}$ and $a_{cdom(400)}$ the rmse was slightly lower for MERIS than for MODIS. Both MERIS and MODIS inversions overestimated the highest $a_{cdom(400)}$ (Sie-a). In case of $C_{Chl-a}$ the high concentrations were estimated accurately, but at the low concentrations the correlation was low. The estimation accuracies with the MERIS and MODIS inversions
were almost as good as in the inversion that used the whole reflectance spectrum with a 2 nm step (Fig. 5). The three highest values of $C_{\text{TSS}}$ and $C_{\text{Chl-a}}$ were clearly underestimated in the ETM+ based inversion (Fig. 4), but $C_{\text{TSS}}$ below 10 mg l$^{-1}$ were in general estimated accurately. The best overall results with ETM+ inversion were obtained for $a_{\text{cdom}}(400)$ that yielded a rmse only slightly lower than in case of MERIS and MODIS.

Fig. 4. Measured and estimated OAS with the inversion method using MERIS channels 2-10 (a-c), MODIS channels 2-8 (d-f) and ETM+ channels 1-3 (g-i).

In the empirical algorithm study, the correlation between $C_{\text{TSS}}$ and $R(\lambda)$ increased with longer wavelengths (until the 700–730 nm region). The best correlation was obtained with MERIS channel 700-710 nm (rmse=18.1%, $R^2=0.978$, Fig. 6, Table 6). In case of MODIS, the channel at 747 nm yielded the highest correlation with $C_{\text{TSS}}$ (rmse=22%, $R^2=0.968$). The correlation of the ETM+ channel 630-690 nm with $C_{\text{TSS}}$ was lower than in case of the mentioned MERIS and MODIS channels. The best correlation of $C_{\text{Chl-a}}$ was obtained with the MERIS channel ratio $R_{705}/R_{665}$ (rmse=27%, $R^2=0.958$). The MODIS channel ratio $R_{747}/R_{667}$ yielded clearly lower correlations (rmse=41%, $R^2=0.904$). In case of ETM+, $C_{\text{Chl-a}}$ could be approximately estimated with the same empirical algorithm as $C_{\text{TSS}}$ (based on the 630-690 nm channel, Fig. 6(h)), which can be explained by the strong correlation ($R^2 = 0.98$, $n=12$) between $C_{\text{Chl-a}}$ and $C_{\text{TSS}}$. Several channel ratios between reflectance in the 620-730 nm range and $R$ in the 445-600 nm range yielded high correlations with $a_{\text{cdom}}(400)$. The ratio between $R$ centered in the 660–667 nm and $R$ centered in the 485–490 nm resulted in the lowest rmse (13–16%, Fig. 6, Table 6) for all three channel configurations.
Fig. 5. Measured and estimated OAS with the inversion method using the whole spectrum (450-750 nm).

Table 5. Statistical accuracy characteristics of the inversion based estimates. The correlations are shown in Figs. 4 and 5.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Channel configuration</th>
<th>$R^2$</th>
<th>rmse%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{TSS}$</td>
<td>Full spectrum</td>
<td>0.974</td>
<td>20.7</td>
</tr>
<tr>
<td></td>
<td>MERIS</td>
<td>0.973</td>
<td>19.8</td>
</tr>
<tr>
<td></td>
<td>MODIS</td>
<td>0.966</td>
<td>25.0</td>
</tr>
<tr>
<td></td>
<td>ETM+</td>
<td>0.967</td>
<td>58.8</td>
</tr>
<tr>
<td>$C_{Chl-a}$</td>
<td>Full spectrum</td>
<td>0.980</td>
<td>25.0</td>
</tr>
<tr>
<td></td>
<td>MERIS</td>
<td>0.943</td>
<td>29.1</td>
</tr>
<tr>
<td></td>
<td>MODIS</td>
<td>0.903</td>
<td>37.3</td>
</tr>
<tr>
<td></td>
<td>ETM+</td>
<td>0.659</td>
<td>105.6</td>
</tr>
<tr>
<td>$a_{cdom}(400)$</td>
<td>Full spectrum</td>
<td>0.964</td>
<td>28.8</td>
</tr>
<tr>
<td></td>
<td>MERIS</td>
<td>0.968</td>
<td>34.0</td>
</tr>
<tr>
<td></td>
<td>MODIS</td>
<td>0.975</td>
<td>31.6</td>
</tr>
<tr>
<td></td>
<td>ETM+</td>
<td>0.933</td>
<td>25.9</td>
</tr>
</tbody>
</table>

Table 6. Empirical algorithms with statistical accuracy characteristics. The correlations are shown in Fig. 6.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Channel configuration</th>
<th>Algorithm</th>
<th>$R^2$</th>
<th>rmse%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{TSS}$</td>
<td>MERIS</td>
<td>$C_{TSS} = 247 \ R_{700-710} - 0.506$</td>
<td>0.978</td>
<td>18.1</td>
</tr>
<tr>
<td></td>
<td>MODIS</td>
<td>$C_{TSS} = 811 \ R_{743-750} - 0.116$</td>
<td>0.968</td>
<td>21.8</td>
</tr>
<tr>
<td></td>
<td>ETM+</td>
<td>$C_{TSS} = 324 \ R_{630-690} - 2.08$</td>
<td>0.820</td>
<td>51.9</td>
</tr>
<tr>
<td>$C_{Chl-a}$</td>
<td>MERIS</td>
<td>$C_{Chl-a} = 76.7 \ R_{700-710}/R_{660-670} - 52.7$</td>
<td>0.958</td>
<td>26.7</td>
</tr>
<tr>
<td></td>
<td>MODIS</td>
<td>$C_{Chl-a} = 186 \ R_{743-750}/R_{662-672} - 27.6$</td>
<td>0.904</td>
<td>41.3</td>
</tr>
<tr>
<td></td>
<td>ETM+</td>
<td>$C_{Chl-a} = 1120 \ R_{630-690} - 7.30$</td>
<td>0.720</td>
<td>69.1</td>
</tr>
<tr>
<td>$a_{cdom}(400)$</td>
<td>MERIS</td>
<td>$a_{cdom}(400) = 2.96 \ R_{660-670}/R_{485-495} - 0.588$</td>
<td>0.979</td>
<td>14.2</td>
</tr>
<tr>
<td></td>
<td>MODIS</td>
<td>$a_{cdom}(400) = 2.94 \ R_{662-672}/R_{483-493} - 0.659$</td>
<td>0.980</td>
<td>13.6</td>
</tr>
<tr>
<td></td>
<td>ETM+</td>
<td>$a_{cdom}(400) = 3.03 \ R_{630-690}/R_{450-520} - 1.19$</td>
<td>0.974</td>
<td>15.9</td>
</tr>
</tbody>
</table>
The analyses of all possible two channel ratios and single channels of the full reflectance spectrum (450–750 nm with a step of 2 nm) did not reveal any new $C_{\text{TSS}}$ and $C_{\text{CDOM}}$ algorithms that would have been more accurate than the best algorithms using the satellite instrument channels. With regard to $C_{\text{Chl-a}}$, the introduction of the 665–675 nm channel ($C_{\text{Chl-a}} = 65.3 \frac{R_{700-710}}{R_{665-675}} - 43.8$) resulted in slightly lower rmse (21.7%) than the use of MERIS channel ratio ($R_{700-710}/R_{660-670}$) (rmse=26.7%, Table 6).

4. Discussion

4.1 Reflectance model

This study provided extensive data for testing the bio-optical reflectance model, because of large differences in water quality between the lakes. Our objective was to construct a model that could be used as an interpretation tool in applying remote sensing techniques to Finnish lakes in the period July–August. The reflectances were calculated using the concentrations of OAS ($C_{\text{TSS}}$, $C_{\text{Chl-a}}$ and $a_{\text{cdom}(400)}$) at each station, while the SIOPs were assumed to be the same in all lakes (with the exception of $C_{\text{Chl-a}}$ dependent $a^{*}_{\text{ph}}$).

The ability of the bio-optical reflectance model to simulate the measured reflectance mainly depends on how well the SIOPs are known. The backscattering probability of TSS ($b_{pTSS}=0.0131$) was estimated here by calibrating the model against
measured reflectances. This value is close to the value reported for Dutch lakes (0.0157, Dekker 1993). The resulting $b^{*}_{b,TSS}$ (555) of 0.0106 l m$^{-1}$ mg$^{-1}$, calculated from the backscattering probability and the scattering coefficient, is also in agreement with other lake studies. In the Dutch Lake IJsselmeer, for example, the $b^{*}_{b,TSS}$ (550) was 0.011 l m$^{-1}$ mg$^{-1}$ (Hoogenboom et al., 1998a), and Heege and Fischer (2004), assuming wavelength independent backscattering, reported a specific backscattering coefficient of 0.0086 l m$^{-1}$ mg$^{-1}$ for Lake Constance, Germany.

The biggest discrepancies in the reflectance simulations were in the eutrophic lakes, namely Enäjärvi, Sierijärvi and at station Loh1-a of Lake Lohjanjärvi. (Fig. 2). This may be due to the fact that in eutrophic lakes the absorption and backscattering properties of phytoplankton have a strong impact on the reflectance. These properties can differ considerably depending on the dominating phytoplankton species, but they could not be taken into account in the model because the lake specific SIOPs of phytoplankton were not available. Here we used the average, $C_{Chl-a}$ dependent $a^{*}_{ph(\lambda)}$ (Eq. 12) of Finnish lakes in August conditions, although $a^{*}_{ph(\lambda)}$ can vary according to the species composition, the physiological state of phytoplankton and the prevailing light conditions. In the eutrophic lakes of this study the phytoplankton species composition was diverse. For example, in Lake Lohjanjärvi (Loh1-a) and in Lake Sierijärvi (Sie-a) the phytoplankton biomass was dominated by two cyanobacteria: Nostocales (83% of the biomass) and Chroococcales (72%), respectively. By contrast, in Lake Enäjärvi photoplankton was more heterogeneous: Dinophyta (28%), Chroococcales (24%), Nostocales (19%), and Chlorophyceae (19%).

Backscattering was here calculated without the separation of total particles into tripton and phytoplankton. The specific backscattering coefficient of phytoplankton can vary between phytoplankton species due to the variations in shape and in refractive index of phytoplankton cells. For example, cyanobacteria with gas-vacuoles have high scattering coefficients (Ganf et al., 1989). Unfortunately, however, direct measurements of scattering properties of phytoplankton are few. As a consequence, the estimation of backscattering properties of phytoplankton in bio-optical modeling of lakes (Dekker, 1993; Kutser, 1997; Strömbeck, 2001) has mainly been based on the research results of the ocean phytoplankton (e.g. Morel, 1980; Sathyendranath et al., 1989; Ahn et al., 1992).

The model seems to overestimate reflectance in the short wavelength region (400–450 nm). The measured reflectances in this region were not reliable in the lakes with high $a_{cdom}(400)$, because in the short wavelengths the upwelling and downwelling irradiances (due to strong absorption by CDOM) were low and their measurement accuracy was poor. In addition, the upwelling irradiance measurements were not corrected for the instrument self-shading. Self-shading leads to underestimation of the measured reflectance and it depends on the radius of the instrument, absorption coefficient, solar altitude, and on the ratio between diffuse and direct solar irradiance (Gordon and Ding 1992). The correction methods (Gordon and Ding, 1992; Zibordi and Ferrari, 1995) for instrument self-shading have been mainly developed for the ocean waters and they have not been tested in waters with high CDOM levels. The correction methods also
require knowledge on the ratio between diffuse and direct solar irradiance, which was not available for our field measurements. The error due to self-shading increases with increased absorption. Most of our study lakes have high CDOM concentrations and the biggest error is therefore expected in the blue region of the spectrum. This region (400–448 nm) was not included in the determination of $b_TSS$ and in the inversion calculations.

The slope factor of CDOM absorption used here (0.0150 m$^{-1}$) lies within the range that has been reported for lakes in Estonia and Finland (mean value 0.016-0.017, Sipelgas et al., 2003) and Sweden (mean value 0.015, Pierson and Strömbeck, 2001). The comparison of published $S_{CDOM}$ are, however, difficult because of differences in the wavelength range used in the estimation of $S_{CDOM}$, in the filter type (pore size) and in the method to correct spectrophotometric measurements for the residual scattering.

### 4.2 Inversion

In the inversion of full reflectance spectrum, $a_{cdom}(400)$ was overestimated at the most eutrophic station Sie-a (Fig. 5(c), measured $a_{cdom}(400) = 18.2$ m$^{-1}$). One explanation for this may be the exceptional $b_TSS(555)$ of Sie-a. Another reason could be the underestimation of the measured R at 450–500 nm arising from the low measurement accuracy of low irradiance levels. This was further confirmed by the use of the 500–750 nm region instead of 450–750 nm in the inversion, which decreased the $a_{cdom}(400)$ estimate from 22.8 m$^{-1}$ to 19.1 m$^{-1}$. In a study of error propagation on inversion of irradiance reflectance in Lake Constance, Gege (2002) concluded that the two most important sources of error in the estimation of $a_{cdom}(400)$ were $S_{CDOM}$ and $C_{TSS}$. The estimation $C_{TSS}$ was not critically effected by errors of other OAS, but was sensitive to the specific backscattering coefficient.

$C_{Chl-a}$ was estimated with a lower accuracy than $C_{TSS}$, and $a_{cdom}(400)$, particularly at low $C_{Chl-a}$ concentrations. This could be due to the fact that absorption by CDOM shadows the first absorption maximum (at 440 nm) of Chl-a and that the second absorption maximum (at 675 nm) is quite narrow. Also noise in the measured reflectance together with variation in the specific absorption and backscattering properties of phytoplankton can reduce the estimation accuracy of $C_{Chl-a}$. The low estimation accuracy of $C_{Chl-a}$ by inversion in 'case-2' waters has also been reported by Lahet et al. (2000) and Gege (2002). According to Gege (2002) $C_{Chl-a}$ estimation by inversion in Lake Constance was very sensitive to errors in $a_{cdom}(400)$ and $S_{cdom}$ and they must be known with an accuracy of a few percent if a $C_{Chl-a}$ error of 25% is required.

In our study the estimation accuracy of OAS by inversion is somewhat better than those obtained in similar lake studies with large variations in water quality (Kutser et al., 2001; Pierson and Strömbeck, 2001). However, the comparison to those two earlier studies is difficult, because the applied optimisation method and the possible weighting factors for different wavelengths were not described in detail.
4.3 Empirical algorithms

The best empirical \( C_{\text{TSS}} \) and \( C_{\text{Chl-a}} \) algorithms of our study are the same as those found in shipborne and airborne reflectance or radiance measurements in several lake regions (e.g. Millie et al., 1992; Dekker, 1993; Gitelson et al., 1993; Schalles et al., 1998; Kallio et al., 2001; Pierson and Strömbeck, 2001; Kallio et al., 2003). The widely used NIR/red- ratio (ratio of two channels at about 705 and 670 nm) in the \( C_{\text{Chl-a}} \) algorithm is based on the Chl-a related absorption maximum at about 675 nm. The 705 nm wavelength region is a good normalizing channel because absorption by other OAS is low and reflectance is mostly influenced by backscattering. For the same reason the reflectance in the 700-730 nm region is optimal for estimating the \( C_{\text{TSS}} \).

The best empirical \( a_{\text{cdom(400)}} \) algorithm (based on \( R_{662-672}/R_{483-493} \)) confirms the findings of Pierson and Strömbeck (2000). Based on the simulated water leaving radiance reflectances of three largest lakes in Sweden, Pierson and Strömbeck (2000) concluded that \( a_{\text{cdom(412)}} \) was best predicted by linear regression against a channel ratio of wavelength > 600 nm to a wavelength in the 400-580 nm range. In one of the lakes studied by Pierson and Strömbeck (2000), the use of the Chl-a absorption channel (660-680 nm) yielded higher correlations than the remaining wavelengths at >600 nm. In this algorithm reflection changes due CDOM absorption in the short wavelength region are normalized by changes in reflection not related to CDOM in the longer wavelengths. The 660-680 nm is the best region for normalization, and is probably due to the small variation in reflectance. The increase in reflectance due to increased backscattering by phytoplankton in this region is balanced by the decrease in reflectance due to phytoplankton absorption. Our study shows that even the wide channels of ETM+ (ratio \( R_{630-690}/R_{450-520} \)) yielded almost as low rmse as the narrow channels of MERIS and MODIS in the estimation of \( a_{\text{cdom(400)}} \). Kutser et al. (2004) used a ratio based on the channels 530–610 and 630–690 nm of satellite data (EO-1 ALI) in the regional estimation of CDOM in lakes. They did not use channel 1 (450–520 nm) in the algorithm, because of uncertainties in the atmospheric correction in the blue region of the spectrum. In our experiment the ratio \( R_{630-690}/R_{530-610} \) yielded a rmse of 44% (R²=0.80), but without the most eutrophic Lake Sierijärvi the rmse was as low as 14.4% (R²=0.98).

The strong correlation between OAS can lead to purely empirical algorithms that are not based on the optical properties of the OAS in question and therefore they may not be generally valid. Our dataset was characterized by a strong positive correlation between \( C_{\text{Chl-a}} \) and \( C_{\text{TSS}} \). Because of this correlation \( C_{\text{Chl-a}} \) could be approximately estimated with the same algorithm as \( C_{\text{TSS}} \) in case of the ETM+ channels. The rest of the best empirical algorithms of this study can be considered as semi-empirical, because they can be explained by the optical properties of OAS.

4.4 Comparison of the channel configurations

MERIS has the best channel configuration of the three tested satellite instruments for the estimation of OAS by the inversion and empirical algorithms in the studied
lakes. In the case of \( \text{C}_{\text{TSS}} \) and \( \text{C}_{\text{Chl-a}} \) the accuracy of MODIS was close to that of MERIS. The essential difference between MERIS and MODIS is that MERIS has the 705 nm channel, which improves the accuracy of the estimation of \( \text{C}_{\text{TSS}} \) and \( \text{C}_{\text{Chl-a}} \) particularly when using the empirical algorithms. The channel configuration of MERIS has one additional advantage as compared to MODIS. The 620 nm channel can namely be utilized in the estimation of the cyanobacteria pigment phycocyanin (Dekker, 1993; Simis et al., 2005).

The wide channels of ETM+ were less suitable for the estimation of \( \text{C}_{\text{TSS}} \) and \( \text{C}_{\text{Chl-a}} \) than the narrow channels of MODIS and MERIS. However, the low concentrations of \( \text{C}_{\text{TSS}} \) (< 7 mg l\(^{-1}\)) were estimated accurately using the ETM+ inversion. At some stations even the high \( \text{C}_{\text{TSS}} \) were estimated accurately with the empirical ETM+ algorithm based on the ETM+ channel 3 (630–690 nm). Reflectance in this wavelength region is influenced, for example, by the phytoplankton absorption, which probably causes large variation in the accuracy of the estimation of \( \text{C}_{\text{TSS}} \) in meso-eutrophic lakes. The exception in the channel configuration comparison was \( \text{a}_{\text{cdom}}(400) \), which was estimated by the empirical methods and inversion with about the same accuracy for all three instruments. Although the ETM+ channel configuration is designed for land applications, it seems to be suitable for the estimation of \( \text{a}_{\text{cdom}}(400) \) in the boreal lakes.

According to the results MERIS has optimum channels (490, 665 and 705 nm) for the OAS estimation by empirical methods, since the best algorithms using the full spectrum were in practice the same as in case of MERIS. In the inversion the use of the whole spectrum (450–750 nm, 151 channels) instead of the MERIS channels improved only slightly the estimation accuracy of OAS. It is obvious that the inversion method could be improved if the lake-specific SIOPs were available. The inversion method is also sensitive to the measurement accuracy of the whole reflectance spectrum; in our CDOM rich lakes the measurement of low reflectance at the blue end of the spectrum is problematic.

Our study shows the potential of different channel configurations for estimating OAS. When applying actual remote sensing data for OAS estimations, the overall results are additionally affected by atmospheric disturbance, surface reflectance and instrument characteristics (SNR, radiometric characteristics). The estimation accuracy of the OAS using the actual satellite instrument data, particularly in case of the inversion method, depends additionally on how well these factors can be taken into account when converting the radiance measurements at the instrument level to the subsurface reflectance. The use of the long wavelength channels (e.g. the 747 nm channel of MODIS) for the estimation of \( \text{C}_{\text{TSS}} \) by satellite remote sensing may be difficult, because of the low radiance levels. Short wavelengths (400–450 nm) were not included in our analyses. When working with actual remote sensing data this region can also be problematic due to low radiance of the CDOM-rich lakes and strong disturbance by the atmosphere. Unlike MERIS and MODIS, LANDSAT ETM+ was not designed for water applications. Because of this (e.g. low SNR, 8-bit data) the accuracy decrease can be expected to be higher than in the case of MERIS and MODIS, if actual satellite instrument data is used.
5. Conclusions

In the development of the remote sensing algorithms for water quality estimations in a specific region, there is a need to identify optimum channel configurations and interpretation methods. Such studies should be based on the knowledge of how OAS and their SIOPs influence the reflectance in different parts of spectrum. SIOPs are essential for the inversion method, but they are also important for the development and use of empirical algorithms, for example in selecting the optimum channels and with regard to the limitations of their use in a specific region or season. The lakes in this study represent the boreal region, where CDOM concentrations are typically high, and C\text{Chl-a} and C\text{TSS} can vary considerably. The high CDOM levels, for example, mean that CDOM absorption shadow the optical signature of phytoplankton in the blue region of the spectrum rendering the blue/green ratio based C\text{Chl-a} algorithms useless.

Empirical methods usually require \textit{in situ} water sampling in cloudless conditions concurrent with the satellite overpass, but they are simple to apply. Additional advantage of the empirical algorithms is that OAS can be estimated employing just a few channels (e.g. the MERIS channels 490, 665, 705 nm). The applicability of the 705 nm channel, important for C\text{Chl-a} and C\text{TSS} estimations, has been proved by airborne remote sensing (e.g. Dekker, 1993; Kallio et al., 2001), but the usability of this channel as measured from the space needs to be established. According to our results empirical algorithms were in general more accurate than the inversion method. The difference was most evident in the case of acdom(400). However, the results obtained here are preliminary, because of the low number of stations and because the same dataset was used in model calibration and in testing the algorithms. Therefore, the algorithms presented here should be further tested with an independent dataset.

The inversion method requires knowledge of the SIOPs, which should be preferably determined for each lake. The inversion also calls for a proper atmospheric correction of the satellite images. Unfortunately, the standard atmospheric corrections of the ocean colour instruments are not directly valid for areas such as the boreal region, where OAS concentrations are often high and atmospheric characteristics differ from those assumed for the standard atmospheric corrections (e.g. Ruddick et al., 2000; Siegel et al., 2000). The advantage of the inversion method is, on the other hand, that once the SIOP's (lake specific, seasonal) have been determined the inversion can be applied to satellite data without concurrent reference measurements of the OAS concentrations.

Ocean colour instruments such as MERIS and MODIS provide images on a daily basis, but their spatial resolution is suitable only for large lakes. This presents problems in Finland, where although the total number of lakes is about 56 000, most are small (95% of the lakes have an area < 1 km\textsuperscript{2}). However, the next generation ETM+ instrument, namely ALI, with its improved radiometric characteristics and a spatial resolution of 30 m, might be suitable for estimating C\text{TSS} (although not in eutrophic lakes) and C\text{cdom}.
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