A Study of Scattering, Backscattering and a Hyperspectral Reflectance Model for Boreal Waters

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Abstract

Some inherent and apparent optical properties and their relations have been studied using data from Finnish, Estonian and Swedish waters during 1997 – 2001 and a hyperspectral model for irradiance reflectance was tested. The measured characteristics were up/downwelling spectral irradiance (Licor Li-1800UW), absorption and attenuation of the water in nine wavelength channels (WetLabs, ac-9), backscattering in six wavelength channels (HOBI Labs Hydroscat 6), Secchi disk depth and the concentration of chlorophyll a, suspended matter and yellow substance. The spectral dependence of the scattering coefficient b was studied in different lakes and in different years. It was found that a power law describes best this dependency. The backscattering coefficient \( b_b \) and the backscattering probability \( B \) were studied using direct measurements and also calculated values. Lastly a hyperspectral model for reflectance was tested with new data and improved parameterization. The model has been developed for interpretation of remote sensing data collected above inland waters. A large data set of Ac-9 and Li-1800UW results was used to test and improve the model, which was run in a forward mode.

Key words: scattering, backscattering, reflectance model, optically active substances, water quality, optical remote sensing

1. Introduction

The optically active substances (OAS), chlorophyll, suspended matter and yellow substance, determine the penetration of light in the water and consequently the light available for primary production. The penetration of light also depends on how OAS absorb and scatter light at different wavelengths. The same factors also affect the reflectance from the water column, and it is important to understand the parameters that affect diffuse reflectance, since e.g. remote sensing of water quality is based on analyzing the magnitude and shape of the reflectance spectrum.

Coastal and inland waters have received increasing attention in recent years due to their importance for human activities (e.g. Kirk, 1994; Maffione, 1998; Arst et al., 1996, 1999; Lindell et al., 1999; Strömbeck, 2001; Herlevi, 2002). The optical variability in inland waters can be much larger than in different regions of open ocean (Horne and
Inland waters are optically multicomponent systems. They are often characterized by high concentration of dissolved organic matter (yellow substance), which may vary independently from phytoplankton concentration. Also the concentration of suspended inorganic particles can be very high due to river inputs and matter resuspended from the bottom (Reinart and Herlevi, 1999).

The diffuse reflectance \( R (E_d/E_0) \), scattering coefficient, \( b \), backscattering coefficient, \( b_b \) (scattering for angles > 90º), and backscattering probability, \( B (b_b/b) \), were the main optical properties that were measured and calculated. The main purpose of this work was to study the characteristics of \( b \) and \( b_b \) in different water types and the relationships between \( R \) and the inherent optical properties, absorption, \( a \), and scattering, \( b \). In general the relationships between the inherent and apparent optical properties are interesting from a physical point of view, i.e. which physical laws are governing their mutual relationships, what is the role of backscattering and absorption in diffuse reflectance \( R \) etc. The relations are also practically important, since if one is able to calculate \( R \) reliably from absorption and backscattering it is possible to derive the reflectance for remote sensing purposes.

2. Study areas and methods

Extensive measurements in 12 Finnish lakes were carried out during the European Union project SALMON (summers 1997-1998) and less thorough measurements during a Finnish-Estonian project SUVI (summers 1997-2000). The study region covers an area from Southern Estonia to Finnish Lapland (58ºN-67ºN). Lakes were selected on the basis of previous knowledge about their optical properties and trophic status. The lakes varied from clear oligotrophic lakes (Secchi depth 12 m) to turbid hypertrophic lakes (Secchi depth 0.2 m). In Sweden were measurements performed in two lakes and also on sea area outside Norrtälje.

Concentrations of the OAS were determined from water samples. These were: concentration of total suspended matter \( (C_S) \), the sum of chlorophyll-a and phaeophytin-a (further chlorophyll-a, \( C_{Chl} \)) and the absorption coefficient of filtered water (a measure of yellow substance or coloured dissolved organic matter, \( a_I \)). Concentrations of chlorophyll were determined from material collected on Whatman GF/C filters and pigments were extracted with hot ethanol (Reinart, 2000). Full absorption spectra (350-850 nm) of the yellow substance were measured in a laboratory using a spectrophotometer Hitachi U-1000. The concentrations of total suspended matter were determined from water samples using gravimetric determination with 0.45 \( \mu m \) Whatman GFC filters.

Vertical profiles of the spectral absorption and attenuation coefficients were measured in situ using a WetLabs ac-9 absorption/attenuation meter. We used the standard wavelength channels of ac-9: 412, 440, 488, 510, 532, 555, 650, 676 and 715 nm in 1997-1999. In 2000-2001 measurements the channel 532 nm was omitted and 630 nm was included. A Li-Cor Li-1800UW spectrometer was used to measure
downwelling and upwelling spectral irradiance profiles in the water with 2 nm spectral resolution in the wavelength band of 300-850 nm.

3. **The variation of total scattering with wavelength**

The spectral distribution of the total scattering coefficient, $b$, obtained from the ac-9 data was investigated from all the data collected during 1997 – 2000. Different authors have noted that the spectral distribution of $b$ is influenced by the turbidity of the water. The spectral dependence can be explained by a power law $b = b_0(\lambda_0/\lambda)^n$. Jerlov and Steemann Nielsen (1974) shows that the wavelength dependence of $b$ becomes weaker with increasing turbidity and the value of $n$ for Baltic waters is close to zero. Bukata et al. (1979) found $b$ to be spectrally invariant in Lake Ontario, as does Phillips and Kirk (1984) in Australian waters. Gould and Arnone (1998) show decreasing $b$ with wavelength the exponent $n$ being about 1.05. Kirk (1994) mentions in his book that there is evidence that $b$ varies approximately with $\lambda^{-1}$. Halturin et al. (1983) show that for the clearest ocean water $n$ is about 1.22. Thus, most of these previous results indicate that the $n$ is decreasing with increasing turbidity. In addition Kopelevich (1983) shows in his paper that the spectral distribution of $b$ depends on particle size, smaller particles influencing more.

In the present study the spectra of 98 cases were investigated and the range $n$ was between 2.42 and 0.13, with the mean value being 0.78. Remarkably there was only a poor correlation between the average scattering coefficient $b$ (and also the beam attenuation coefficient $c$) and the spectral wavelength dependency $n$ ($R^2 = 0.14$). This suggest that in our data turbidity does not affect the wavelength dependence of $b$. During the early summer (May/June) we found a clearly larger wavelength dependence than in August. The average $n$ in May/June was 0.90 and in August 0.66, while the average $b$ remained nearly the same, about 4.5, in both cases. In some cases the difference is really large in a certain lake even with comparable turbidity values, e.g. in Lake Tuusulanjärvi (a eutrophic turbid lake) the average May and August values for $n$ were 1.91 and 0.55, respectively. Also the correlation between $n$ and $b$ was positive and much better in May/June data ($R^2 = 0.43$). The best correlation was between $n$ and $b$ measured in May ($R^2 = 0.78$, Fig. 1). The correlation between the average total scattering and the concentration of total suspended matter was $Cs = 1.3 \cdot b$, $R^2 = 0.72$ (Fig. 2).

These results show that there is generally little correlation between the average turbidity and the wavelength dependence of $b$, but the correlation is in all cases positive meaning that turbidity increases the wavelength dependence of $b$. The question of why the wavelength dependence of scattering is larger in spring than in late summer can be explained at least in part by the size and type of the particles in the water. In the spring after the snow melt the water contains relatively more small mineral particles from the river runoff and the general spring runoff. In August the amount of algae is larger and algal blooms may occur. This is the case especially in the turbid lakes that are situated near both agricultural and rural areas. Alga is found in colonies, which can be larger
than small mineral particles (clay, silt). Another factor is that living cells contribute to the backscattering much less than mineral or detrital particles and that forward scattering is virtually independent of wavelength (Kirk, 1994; Jerlov, 1968). Hence smaller mineral particles contribute more to backscattering, which is more wavelength dependent than forward scattering. The results of our bio-optical determinations of the concentrations of the OAS support the fact that in August when the n was smaller in the turbid lakes the concentration of chlorophyll-a was also large. Furthermore the larger angle scattering i.e. backscattering enables the density fluctuation scattering to play a significant role in the total scattering and the density fluctuation scattering is known to be more sensitive to wavelength than particle scattering. This may be the case at least in the clear lakes, where density fluctuation may take a more significant part in the scattering process.

![Graph of b vs. n in May 1997-2000](image)

Fig. 1. Correlation between the wavelength dependence exponent, n and total scattering coefficient, b measured in May.

![Graph of b vs. CS](image)

Fig. 2. Correlation between the concentration of suspended matter, C_s, and the total scattering coefficient, b.
4. Backscattering in Finnish, Estonian and Swedish waters

Simultaneous measurements of absorption, scattering and backscattering were made in Swedish sites in 1998, 1999 and 2001. In addition simultaneous spectral irradiance measurements were performed in Sweden in 1998. The measurements in 1998 and 1999 were made in Lake Erken and at three sites in the archipelago outside of town Norrtälje. The 1998 data was used to compare the measured irradiance reflectance, \( R \) and the calculated \( R \) using the following equation developed by Gordon et al. (1975):

\[
R(\lambda) = C(\mu_0) \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}
\]

(1)

where \( b_b \) is backscattering, \( a \) is total absorption and \( C \) is a coefficient as a function of \( \mu_0 \), which is a cosine of the zenith angle of the refracted photons. The first effort was to test the values of \( C \) in Eq. (1), since all the other parameters have been measured. Results showed quite good agreement with the results found by Kirk (1984) in his Monte-Carlo studies, where \( C \) can be expressed by the following formula:

\[
C(\mu_0) = 0.975 - 0.629\mu_0
\]

(2)

This equation implies that the reflectance decreases as the solar altitude increases. The values of \( C \) calculated by Eq. (2) in our 1998 measurements were between 0.52 and 0.55 as the solar altitudes were low.

*Calculated values of \( B \)*

In the second effort \( b_b \) data was not available, and we tried to test the validity of the coefficient \( C \) in Eq. (1) using all the data of irradiance reflectance, \( R \), absorption coefficient, \( a \), and scattering coefficient, \( b \), measured in Finnish and Estonian lakes during 1997-2000. The problem was approached in a following manner. The first task was to determine a reliable backscattering efficiency, \( B = b_b/b \), for determining the backscattering coefficient in Eq. (1). Three different approaches were used: 1) All the cases where absorption, scattering and backscattering coefficients were measured in Sweden were compared to the individual absorption and scattering coefficient data measured in Finland and Estonia. The cases where both the absorption and scattering in Swedish waters were equal or very close were chosen. The backscattering probability from the Swedish data was then used to calculate the coefficient \( C \) for the Finnish/Estonian case. 2) One single representative \( B \) value based on the Swedish data was chosen for each lake for calculating the values for \( C \). 3) The value for \( C \) was calculated using a single value of \( B \) (0.019) for all cases. The \( B \) used was that found by Petzold relying on the data from the San Diego harbor (Kirk, 1994). The purpose of these tests was to find out if the value of the coefficient \( C \) changes in a logical manner from a water type to another.
The third effort was to calculate the backscattering probability, \( B = b_b/b \), from all the data collected in Finland and Estonia during 1997-2000, using the values for the coefficient \( C \) obtained from the methods described above. The results were classified using a procedure described in Reinart (2000). This classification is based on the concentrations of the OAS and apparent optical properties using five different water types with relatively complex definition of each class. The classes are:

- **C** – clear water (oligo/mesotrophic), the amount of OAS relatively small
- **M** – moderate (mesotrophic), yellow substance most important, absorption more important than scattering
- **T** – turbid (eutrophic, hypertrophic), suspended particles cause high scattering
- **V** – very turbid, very high amount of chlorophyll, shallow eutrophic lakes
- **B** – brown water (dystrophic), high amount of yellow substance.

The results can be seen in Table 1. Some comments and interpretation of these results is necessary. First, the approach of basing \( B \) values on a comparison of Fin/Est \( a \) and \( b \) values to the Swedish ones can be questioned. Certainly \( B \) is related to \( a \) and \( b \), but it also depends very strongly on the particle size and type, which cause the scattering (see Fig. 3 for variation of \( B \)). The results also indicate that the value of \( C \) is not constant or solely dependent on the solar elevation. Looking at the results of the first three methods (first three columns in Table 1) it seems that \( C \) is getting larger when moving towards more turbid waters starting from class B, except for class V. This phenomenon is the clearest in case of using a common \( B \) value (0.019) for all cases. The result appears to be clear, but the very turbid water case (V) needs further explanation. It seems that the value of \( B \) used to reach the \( C \) values have been too large in the V class. There is a reason to believe (explained later) that the backscattering probabilities for very turbid waters in our case were in reality smaller than the ones chosen or the widely used Petzold value (0.019). This study indicates, that the value of \( C \) in the Eq. (1) is changing with the water type as well as with the solar elevation.

<table>
<thead>
<tr>
<th>Water class</th>
<th>C 1)</th>
<th>C 2)</th>
<th>C 3)</th>
<th>C (Kirk)</th>
<th>B 2)</th>
<th>B (Kirk)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.34</td>
<td>0.29</td>
<td>0.16</td>
<td>0.46</td>
<td>0.012</td>
<td>0.006</td>
</tr>
<tr>
<td>C</td>
<td>0.36</td>
<td>0.37</td>
<td>0.25</td>
<td>0.45</td>
<td>0.013</td>
<td>0.011</td>
</tr>
<tr>
<td>M</td>
<td>0.38</td>
<td>0.42</td>
<td>0.37</td>
<td>0.46</td>
<td>0.016</td>
<td>0.015</td>
</tr>
<tr>
<td>T</td>
<td>0.54</td>
<td>0.49</td>
<td>0.50</td>
<td>0.45</td>
<td>0.020</td>
<td>0.023</td>
</tr>
<tr>
<td>V</td>
<td>0.15</td>
<td>0.27</td>
<td>0.28</td>
<td>0.45</td>
<td>0.020</td>
<td>0.011</td>
</tr>
<tr>
<td>Average</td>
<td>0.37</td>
<td>0.40</td>
<td>0.34</td>
<td>0.45</td>
<td>0.016</td>
<td>0.015</td>
</tr>
</tbody>
</table>

When determining the backscattering probabilities, \( B \) for different water types, we chose to concentrate on the values obtained using the known and tested equation for \( C \)
developed by Kirk (Eqs. 1-2). The results show that $B$ is growing when moving towards more turbid waters starting from class B, except in class V in a similar fashion with $C$. The same phenomenon appeared with the chosen values for $B$ ($B\ 2$, Table 1). Again the exception was in the class V for the chosen values, due to the fact that we did not have real data measured in Sweden that would belong to the class V. Moving from brown waters towards more turbid waters the backscattering increases due to the increase in the amount of inorganic particles, which scatter towards larger angles than organic particles. Nevertheless in very turbid class the concentration of chlorophyll and organic particles is so large ($C_{chl} > 40 \text{ mg m}^{-3}$ in our case) that they dominate the scattering process where forward scattering is enhanced. This is the explanation why the backscattering probability, $B$ in the class V is so small. The average value for all cases thus obtained was 0.015, which is clearly smaller than the Petzold value. Kirk (1994) states that above a certain level of turbidity, such that particle scattering is dominant at all angles, the normalized volume scattering function is not expected to alter its shape with increasing turbidity. This is why the value 0.019 (Petzold) may be applicable to the majority of natural waters other than the very clear oceanic ones. However, when the scattering is dominated by organic particles with a low refractive index a different shape of volume scattering function might be appropriate. Our results support this at least in the very turbid water case, but why is the value for $B$ in e.g. the clear water case so much smaller than Petzold’s value? It may be that even our ‘clear’ lakes contain relatively much chlorophyll or the Kirk’s value of $C$ is slightly too large. In the turbid water case (T) the inorganic particles are dominating giving the value for $B$ about 0.02.

![Graph](image_url)

Fig. 3. The total absorption, scattering and the backscattering probability at a wavelength of 412 nm along a transect for every 1000 seconds in Lake Vänern, 2002.

Some other average inherent and apparent optical properties have been classified using the classes by Reinart (2000) (Table 2). The values fall into the classes in a logical manner and the classes for $B$ are related to those for $b/a$, except in class V, which was explained above. Hence the average values for $b/a$ can also be used to classify the values for $B$ in our water types.
Table 2. Average values of all Fin/Est measurements of some inherent and apparent optical properties classified into five water types.

<table>
<thead>
<tr>
<th>Water class</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>Kd</th>
<th>b/a</th>
<th>R</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>3.263</td>
<td>1.935</td>
<td>5.198</td>
<td>3.786</td>
<td>0.577</td>
<td>0.003</td>
<td>0.006</td>
</tr>
<tr>
<td>C</td>
<td>0.672</td>
<td>0.821</td>
<td>1.493</td>
<td>0.999</td>
<td>1.322</td>
<td>0.008</td>
<td>0.011</td>
</tr>
<tr>
<td>M</td>
<td>1.316</td>
<td>2.386</td>
<td>3.702</td>
<td>1.979</td>
<td>1.968</td>
<td>0.019</td>
<td>0.015</td>
</tr>
<tr>
<td>T</td>
<td>2.058</td>
<td>8.858</td>
<td>10.919</td>
<td>3.957</td>
<td>4.495</td>
<td>0.053</td>
<td>0.023</td>
</tr>
<tr>
<td>V</td>
<td>2.346</td>
<td>13.920</td>
<td>16.265</td>
<td>4.368</td>
<td>6.474</td>
<td>0.042</td>
<td>0.011</td>
</tr>
</tbody>
</table>

Measured values of B

As mentioned simultaneous measurements of absorption, scattering and backscattering coefficients have been performed in Swedish waters in 1998, 1999 and 2001. A focus in this paper is on the backscattering and its probability, i.e. \( b_b/b \) or \( B \). The measurements in 1998 and 1999 were made in Lake Erken and at three sites in the archipelago outside of town Norrtälje. The results show that the backscattering probability can be quite variable, changing between 0.010-0.019 in Lake Erken (Er141098 etc. in Table 3). The average value for all measurements was 0.014. The measurements were made in October in 1998 and in May in 1999 and the difference due to the time of the year is clear. In Lake Erken the value of \( B \) was about 0.010 in May and 0.017 in October. This and the fact that the total absorption was clearly higher in May indicate that there were algae and chlorophyll present. Organic particles have lower refractive index, thus lower effect on backscattering. This same phenomenon showed up at other sites as well, but not as prominently. A second notable feature was that the value of \( B \) was so variable at the same site i.e. \( B \) was 0.015 at the depth of 0.5 m and 0.018 at the depth of 4.0 m and 0.019 at the depth of 0.5 m the following day. Hence it is difficult to find a reliable value for \( B \) that represents a water type or even a single lake. Still taking into account the time of the year and the general conditions of the water area under study, it is possible to find an estimate for \( B \).

Table 3. Values of n, describing the wavelength dependence of backscattering \( B \), \( B \) itself and the total scattering divided by the total absorption measured in Sweden 1998/1999 and 2001.

<table>
<thead>
<tr>
<th>1998/1999 Lakes and sea</th>
<th>n</th>
<th>B</th>
<th>b/a</th>
<th>2001 Vänern</th>
<th>n</th>
<th>B</th>
<th>b/a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Er1310 0.5 m</td>
<td>0.46</td>
<td>0.015</td>
<td>1.778</td>
<td>1</td>
<td>0.72</td>
<td>0.022</td>
<td>1.204</td>
</tr>
<tr>
<td>Er1310 4.0 m</td>
<td>0.23</td>
<td>0.018</td>
<td>1.740</td>
<td>1000</td>
<td>0.78</td>
<td>0.018</td>
<td>1.169</td>
</tr>
<tr>
<td>Er141098</td>
<td>0.58</td>
<td>0.019</td>
<td>1.430</td>
<td>2000</td>
<td>0.82</td>
<td>0.018</td>
<td>1.178</td>
</tr>
<tr>
<td>Har151098</td>
<td>0.58</td>
<td>0.016</td>
<td>4.153</td>
<td>3000</td>
<td>0.69</td>
<td>0.016</td>
<td>1.364</td>
</tr>
<tr>
<td>Kar151098</td>
<td>0.74</td>
<td>0.012</td>
<td>1.123</td>
<td>4000</td>
<td>0.59</td>
<td>0.016</td>
<td>2.052</td>
</tr>
<tr>
<td>Er070599</td>
<td>0.84</td>
<td>0.010</td>
<td>0.959</td>
<td>5000</td>
<td>0.52</td>
<td>0.020</td>
<td>2.664</td>
</tr>
<tr>
<td>Har130599</td>
<td>0.76</td>
<td>0.015</td>
<td>4.155</td>
<td>6000</td>
<td>0.51</td>
<td>0.020</td>
<td>3.055</td>
</tr>
<tr>
<td>Lid130599</td>
<td>0.85</td>
<td>0.011</td>
<td>1.496</td>
<td>7000</td>
<td>0.48</td>
<td>0.022</td>
<td>3.127</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>8000</td>
<td>0.56</td>
<td>0.017</td>
<td>2.983</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>9000</td>
<td>0.6</td>
<td>0.017</td>
<td>2.308</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>10000</td>
<td>0.77</td>
<td>0.019</td>
<td>1.536</td>
</tr>
</tbody>
</table>
In 2001 the measurements were made using a boat based flow-through system to measure \(a\), \(b\), and \(b_b\) and other parameters as well simultaneously. The results are from a 50 km long transect along Lake Vänern. The values of \(a\), \(b\) and \(B\) at the shortest wavelength (412 nm) along the transect can be seen in Fig. 3 and the spectra of \(B\) for even times (distances) of 1000 seconds in Fig. 4. The average values (over all wavelengths) of \(B\) are shown in Table 3. It can be seen that the value for \(B\) is following the overall value of scattering in the middle part of the transect, but it is rising at both ends, where the values of \(a\) and \(b\) are lowest. This is difficult to explain without knowing the details of the water conditions, but most likely the relative amount of small mineral particles is larger at both ends causing the backscattering efficiency to rise. The variation of \(B\) is between 0.016-0.022, the average being 0.019, which is exactly the value found by Petzold.

![Fig. 4. The spectra of the backscattering probability, B, measured along a transect in Lake Vänern. The spectra are plotted for every 1000 seconds.](image)

The wavelength dependence of \(B\), expressed similarly with the case of total scattering shown earlier in this paper, i.e. \(B = B_0(\lambda_0/\lambda)^n\), was also studied and the results can be seen in Table 3. It must be noted that \(B\) is not constant over the wavelengths, but diminishing with wavelength as does scattering. The values of \(n_B\) in 1998, 1999 cases are more variable (so are the water types) than in Vänern, 2001, but the average value was 0.63 in both cases. One clear feature can be seen in the results, the value of \(n\) is larger in spring than in autumn. Other interesting fact is that especially in 2001 data the value of \(n_B\) correlates well in a negative direction with the value of total \(b/a\) (or \(b\)), \(R^2\) being 0.88. The larger the scattering the smaller the wavelength dependence of \(B\), which is opposite to the behavior of \(b\) seen earlier in this study and actually this data shows also positive correlation between \(n_B\) and \(b\).

5. **A hyperspectral model**

A hyperspectral model for interpretation of remote sensing data, described in Kutser _et al._ (2001), has been improved here for simulation of watercolor spectra above
and beneath the water surface. A prototype of the model (Kutser, 1997; Kutser et al., 1997; Kutser et al., 1998a; Kutser et al., 1998b) was elaborated earlier on the basis of data available in literature (mainly from clear oceanic waters). The database for that model was insufficient to be able to improve it and it was found that oceanic water parameters cannot describe the reflectance spectra of turbid waters. The data to improve the model has been collected during 1997-2001 and the focus here is on the underwater reflectance. Some improvements and simplifications of the model are presented here.

**Basics of the model**

The basic equation of this hyperspectral model is Eq. (1) developed by Gordon et al. (1975) in their Monte Carlo study relating the irradiance reflectance just beneath the water surface with a polynomial function of absorption and backscattering coefficients, where $C$ is a function of solar altitude (Eq. 2). The variability range of $C(\mu_0)$ in our case is between 0.40 and 0.50 (latitude $58^{\circ}$N to $67^{\circ}$N; solar zenith angle $60^{\circ}$ or more). It is obvious that an expression like (1) contains assumptions regarding the light field and the average shape of the volume scattering function.

We assume that there are three optically active components in the water: phytoplankton, yellow substance and non-chlorophyllous suspended matter (tripton) and the total absorption and scattering coefficients are additive over the constituents of the medium by the definition of inherent optical properties. Under these conditions the total spectral absorption coefficient of the water, $a(\lambda)$, is described by the following formula:

$$a(\lambda) = a_w(\lambda) + a_{Ph}^*(\lambda)C_{Chl} + a_Y(\lambda) + a_{SM}^*(\lambda)C_{SM} ,$$

where $a_w(\lambda)$ is the spectral absorption coefficient of pure water, $a_{Ph}^*(\lambda)$ is the chlorophyll-specific spectral absorption coefficient of phytoplankton, $a_Y(\lambda)$ is the spectral absorption coefficient of yellow substance (coloured dissolved organic matter) and $a_{SM}^*(\lambda)$ is the specific absorption coefficient of non-chlorophyllous particles. $C_{Chl}$ and $C_{SM}$ are concentrations of chlorophyll-a and non-chlorophyllous suspended matter.

The total spectral backscattering coefficient $b_{Ph}(\lambda)$ can be described by the formula:

$$b_{Ph}(\lambda) = 0.5b_w(\lambda) + b_{Ph}^*(\lambda)C_{Chl} + b_{SM}^*(\lambda)C_{SM} ,$$

where $b_w$ is the scattering coefficient of pure water and it is assumed that backscattering probability is 50% in pure water. $b_{Ph}^*$ is the chlorophyll-specific backscattering coefficient of phytoplankton and $b_{SM}^*$ is the spectral backscattering coefficient of non-chlorophyllous particles.
**Model parameters**

Absorption and backscattering due to yellow substance and suspended matter are often expressed through empirical functions of $C_{Chl}$ (Gordon et al., 1988; Lee et al., 1994), that is acceptable in oceanic waters, but not in coastal and inland waters where concentrations of optically active substances are not correlated with chlorophyll-a concentration. It would be preferable to use spectra of specific absorption and scattering coefficients measured in the water body under investigation. Unfortunately this kind of data is unavailable in most cases and variability of the parameters is very high, sometimes varying over two-three orders of magnitude.

In this model the values of absorption and scattering coefficients of pure water, $a_w(\lambda)$ and $b_w(\lambda)$, were taken from Smith and Baker (1981). The spectral chlorophyll-specific absorption coefficient of phytoplankton is calculated using the power function recommended by Bricaud et al. (1995):

$$a'_{Ph}(\lambda) = A(\lambda)C_{Chl}^{-B(\lambda)},$$

(5)

where $A(\lambda)$ and $B(\lambda)$ are positive, wavelength-dependent parameters. The values for $A(\lambda)$ and $B(\lambda)$ used in this study were estimated by Strömbeck (2001) based on laboratory measurements of $a'_{Ph}$. For each measured $a'_{Ph}$ spectrum, regressions were used to define power functions (Eq. 5) and coefficients $A(\lambda)$ and $B(\lambda)$. While testing the effects of parameters obtained by Strömbeck and Bricaud, respectively, it was found that the Strömbeck’s values worked slightly better in this model, although the difference was quite small (both author’s parameters can be seen in Fig. 5).

![Fig. 5. Parameters A and B for calculation of $a'_{Ph}$ derived by Strömbeck and Bricaud.](image)

The absorption by yellow substance is expressed as a function of the absorption coefficient of dissolved material at a wavelength of 400 nm, $a_4(400)$, and a slope factor, $S_Y$, by the following formula:
\[ a_y(\lambda) = a_y(400) \exp[-S_y(\lambda - 400)], \]  
(6)

\[ S_y = 0.017 \] was used in this model as a result obtained on the basis of a large database from the Baltic Sea, Estonian and Finnish lakes by Mäekivi and Arst (1996).

Our data set enables us to estimate the specific absorption coefficient of non-chlorophyllous suspended matter using the same assumptions we made in the model. According to Eq. (3) the specific absorption coefficient of the suspended matter can be calculated with:

\[ a_{SM}^*(\lambda) = \frac{a(\lambda) - a_y(\lambda) - a_{SM}^*(\lambda) - a_{Ph}^*(\lambda)C_{Chl}}{C_{SM}}. \]  
(7)

The total absorption coefficient \( a(\lambda) \) was measured in situ with ac-9. \( a_y(\lambda), C_{Chl} \) and \( C_S \) (dry weight of all particles) were measured from water samples and \( C_{SM} \) is calculated using the equation \( C_{SM} = C_S - 0.07C_{Chl} \) developed by Hoogenboom and Dekker (1997), as cited in Kutser et al. (2001). Where \( C_S \) is in mg/l, \( C_{Chl} \) in mg/m³ and \( C_{SM} \) will be in mg/l. The \( a_{Ph}^*(\lambda) \) is calculated as described above.

Thus determined \( a_{SM}^*(\lambda) \) needs to be described mathematically for using it in a model. After calculating the spectra of \( a_{SM}^*(\lambda) \) they were plotted and they seemed to decrease exponentially with increasing wavelength. The usage of Eq. (7) to calculate \( a_{SM}^*(\lambda) \) produced some uneven shapes to the spectra due to the shape of the \( a_{Ph}^*(\lambda) \) spectra. However \( a_{SM}^*(\lambda) \) was described using two parameters \( a_{SM}^*(400) \) and the slope of an exponential curve \( (S_{SM}) \) analogous to those in Eq. (6). To estimate numerical values of the parameters we fit the simulated \( a(\lambda) \) (Eq. 3) to the total absorption coefficient spectra measured by ac-9.

There are four unknown parameters in Eq. (4): specific scattering coefficients of phytoplankton and non-chlorophyllous particles \( (b_{Ph}^*(\lambda) \) and \( b_{SM}^*(\lambda)) \) as well as the backscattering probabilities \( (b_{Ph}/b_{Ph}(\lambda) \) and \( b_{SM}/b_{SM}(\lambda)) \). In this study after some testing a more simple equation was chosen for backscattering i.e.

\[ b_b(\lambda) = 0.5b_s(\lambda) + b_{b,S}(\lambda)C_S, \]  
(8)

where \( S \) stands for total suspended matter including phytoplankton. Thus there are only two unknown parameters, \( b_{SM}^*(\lambda) \) and \( b_{b,S}/b_{S}(\lambda) = B_S \). This simplifies the model and it was found that including the effect of phytoplankton on the backscattering separately did not improve the results, rather the opposite. One reason for this is that there are very little results of specific absorption, scattering and backscattering coefficients of different algae species available and there was no data available on the optical properties of algae species present in the waters under this investigation.

**Results of the model**

There are two main stages in testing and applying this kind of model. The first is forward modelling: calculating reflectance spectra on the basis of known concentrations
of optically active substances. Inverse modelling, estimation of concentrations of optically active substances on the basis of reflectance spectra, can be carried out when the model works reliably in forward mode. This study concentrated on the forward modelling of the underwater irradiance reflectance.

The forward modelling was carried out in three steps. The first step was to search for $a^*_{SM}(\lambda)$. We calculated $a^*_{SM}(400)$ using Eq. (7), in situ and laboratory measurements data. After that we calculated slope factors, $S_{SM}$, fitting the simulated total absorption coefficient spectra with ac-9 data. We need functions describing the dependence of the parameters on the concentration of suspended matter in order to make the model suitable in simulation of reflectance spectra in a variety of lakes. The variation in values of $a^*_{SM}(400)$ and $S_{SM}$ was more than an order of magnitude in our study sites and dividing both parameters with concentration of non-chlorophyllous particles enabled us to obtain power functions describing the dependences reasonably well (Fig. 6). The results of the correlations are following:

$$a^*_{SM}(400) = 0.22C_{SM}^{-0.45}$$  \hspace{0.1cm} (9)

and

$$S_{SM} = 0.007C_{SM}^{0.12}$$ \hspace{0.1cm} (10)

The second step was to search for parameters necessary for a calculation of the backscattering coefficient. After making assumptions described above, the unknown parameters were the specific scattering coefficient of all particles, $b^*_{S}(400)$, and the exponent $n$ for calculating $b^*_{S}(\lambda)$. It was found that a power function $b^*_{S}(\lambda) = b^*_{S}(400)(400/\lambda)^n$ describes best the wavelength dependence of $b^*_{S}$. The specific scattering coefficient was calculated using the following formula:

$$b^*_{S}(400) = \frac{b(400) - b_w(400)}{C_S},$$ \hspace{0.1cm} (11)

where $b(400)$ was extrapolated from ac-9 data and $b_w$ was from Smith and Baker (1981). The exponent $n$ was estimated comparing $b^*_{S}(\lambda) \cdot C_S + b_w(\lambda)$ with those measured by ac-9.
The variability of these two parameters was also large, but it was possible to describe the dependence of the parameters on the concentration of all particles after dividing them with $C_S$. The dependence of $b^*_S(400)/C_S$ and $n/C_S$ on concentration of particles is shown in Fig. 7. The results of the correlations are:

$$b^*_S(400) = 0.63C_s^{-0.011}$$  \hspace{1cm} (12)$$

and

$$n = 0.49C_s^{0.11}$$  \hspace{1cm} (13)$$
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Another choice for \( n \) is to use the average value of 0.8 calculated in the case of total scattering (first chapter). Also the exponential decrease of \( b^*(\lambda) \) was tested in a similar fashion with the specific absorption of suspended matter, but it did not give better results.

We need also backscattering probability of particles to model irradiance reflectance spectra. This parameter can be calculated using Eq. (14), where \( B \) can be calculated using Eq. (1), with reflectance spectrum, \( R \) calculated from LI-1800UW data and scattering, \( b \) measured with ac-9.

\[
B_s = \frac{Bb(\lambda) - 0.5b_n(\lambda)}{b(\lambda) - b_n(\lambda)}.
\]

The backscattering probability of particles varied also more than an order of magnitude. After dividing the probabilities with \( C_s \) we get a power function that describes the dependence of the probability on the concentration of all particles. Nevertheless this dependence was not well correlated (\( R^2 = 0.5 \)), so another method was introduced. The backscattering probabilities for suspended matter (Eq. 14) were
compared to the total backscattering probabilities (Eq. 1) and the following average relation was found $B_S = 0.93B$. The average backscattering coefficients calculated for five water types (Table 1) and the above relation were used to give an approximate value for $B_S$. The model results using these average values for $B_S$ were better than using the relationship between $C_S$ and $B_S$.

The use of power functions instead of average values of $a^{*}_{SM}(\lambda)$ and $b^{*}_{b,S}(\lambda)$ improved significantly the fitting of measured and simulated spectra. Surprisingly using combined $b^{*}_{b,S}$ instead of dividing the backscattering of particles to chlorophyllous and non-chlorophyllous part as is often done produced better overall results. Fig. 8 illustrates some examples of the fitting of the measured and modelled spectra. Looking at all the results it appears that this model does not favour any water type i.e. the model does not give better results for the clear waters than e.g. for turbid waters, although the brown water case seemed to be the most difficult (Pääjärvi). The water types in Fig. 8 are from clear to very turbid starting from upper left corner. This figure shows that the model works well for other lakes than Pääjärvi (M,B) and Enäjärvi (V). All in all the results were quite varying changing from one measurement time to the next in a same lake indicating also that the measurement errors in the reflectance (Virta and Herlevi, 1999) and/or the concentrations of the optically active substances can be significant.

6. Conclusions

The spectral distribution of the total scattering obtained from the ac-9 data has been investigated. The results are somewhat contradictory to the results found by other authors. Generally there seems to be evidence that $b$ varies approximately with $\lambda^{-1}$. Our results show that the exponent of the wavelength varied between 0.13 and 2.42, with the mean value being 0.78. One remarkable result was that there was very poor correlation between the average scattering coefficient $b$ (or the beam attenuation coefficient $c$) and the spectral wavelength dependency, and that the correlation was positive in all cases. If one intends to find a spectrum for total scattering, the time of the year is crucial and also the type of water, but as a rule of thumb $b$ varies approximately with $\lambda^{-0.8}$ (or $\lambda^{-1}$).

The backscattering probability, $B$, and the coefficient $C$ in Eq. (1) were studied by different methods. The value of $C$ in the Eq. (1) seemed not to be constant, but changing with the water type as well as with solar elevation and it is slightly smaller than the value proposed by Kirk (1984) in Eq. (2). The results obtained show that $B$ increases with turbidity starting from class B, except in class V in a similar fashion with $C$. The size distribution and the type of scattering particles were thought to be crucial for the behavior of $B$. The average calculated value was found to be 0.015. Our results indicate that even our ‘clear’ lakes contain relatively much chlorophyll and yellow substance to diminish the backscattering probability, or that the Kirk’s value of $C$ is slightly too large. The average values for $B$ obtained from direct measurements in Sweden were found to be 0.014 in varying waters and 0.019 in Lake Vänern.
Fig. 8. Measured and modelled normalized underwater reflectance spectra in six different Finnish/Estonian lakes. The water type is marked in parenthesis in the title.

The wavelength dependence of $B$ was studied and it was found that a power function $B = B_0(\lambda_0/\lambda)^n$ describes best this dependency. The average value for $n$ was found to be 0.63 and it was larger in spring than in autumn. The data from 2001 show that the value of $n$ correlated negatively with the value of $b/a$ (or $b$). This is opposite to
the wavelength dependence of $b$. Our results obtained for B are valuable for remote sensing hyperspectral modeling.

The hyperspectral model introduced here works satisfactorily in most of the boreal waters examined, but there was large variation in its performance. The regression formulae for model parameters ($a*_{SM(400)}$, $S_{SM}$, $b*_{S(400)}$ and $n$) were found. Additional studies on the separation of the influence of suspended matter and phytoplankton on absorption and scattering must be carried out to improve the performance of the model. The application of inverse modelling to interpret remote sensing data is a logical next step, which will be made after the additional investigations of the parameters mentioned above.

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7. References


