Towards airborne remote sensing of water quality in the Netherlands; validation and error analysis

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Abstract

Water managers request maps of water quality parameters such as concentrations of dissolved organic matter, chlorophyll or total suspended matter. Rijkswaterstaat sets up a production chain for such maps using a hyperspectral imaging scanner installed in the Dutch coast guard aircraft. Water quality parameters are retrieved from remote sensed images using successively; 1) a module calculating the subsurface reflectance spectra and 2) a module calculating the concentrations using specific inherent optical properties of the water constituents and the Gordon reflectance model implemented in a matrix inversion technique. The accuracy of a several numerical methods for retrieval of concentrations from reflectance spectra was assessed. Also effects of instrumental noise, errors in the atmospheric correction and errors in the specific inherent optical properties on the derived concentrations were estimated. Benchmark data set was collected for Lake Veluwe in the Netherlands. For ideal circumstances, two of the tested numerical methods were able to retrieve both total suspended matter as well as chlorophyll concentration. For less favourable circumstances total suspended matter could still be retrieved, but chlorophyll became less accurate. Dissolved organic matter concentrations could not be retrieved for any case. Application of the matrix inversion technique tested on an airborne image from Lake Veluwe showed promising results.

Introduction

Water managers have a request for maps of water quality parameters such as the concentrations of chlorophyll-a (CHL), total suspended matter (TSM) and dissolved organic matter (CDOM). Currently they rely on local point measurements made from buoys or ships, the traditional monitoring techniques for coastal or inland waters. Optical imaging techniques could supply the water managers with maps of the parameters of interest making use of the information enclosed in spectra of reflected light measured above the water surface. These imaging techniques have progressed rapidly but its application retarded. Implementation of the airborne remote sensing of water quality parameters was obstructed by its relative high costs and low flexibility. Also the need of ground truth to be measured in parallel to the airborne measurements was considered as a disadvantage. Currently Rijkswaterstaat is setting up a chain for production of water quality maps using airborne imaging remote sensing where the drawbacks mentioned above have been taken away.

An imaging hyperspectral scanner (EPS-A) recently was installed in the Dutch coast guard aircraft. Multiple use of this aircraft makes exploitation of the imaging scanner more cost effective. Due to the flexibility of the coast guard aircraft it is expected that acquisition of data is easier to organise. The third drawback is removed by implementation of a matrix inversion technique to estimate concentrations of the water constituents using reflectance spectra and specific inherent optical properties (SIOP) for input. This procedure does not rely on simultaneous ground truth measurements to the airborne measurements. The procedure is explained in more detail below.

Demands on the accuracy of the production chain, user requirements for the accuracy of the concentrations of the water quality parameters, were set by the data users by interviewing several people responsible for water management in The Netherlands (van der Woerd *et al* 1998). How realistic these user requirements are remains a topic of discussion. The requirements can be summarised as follows: 10% accuracy in the chlorophyll-a pigment concentration for coastal and inland water and 10% and 25% for the total suspended matter concentration for coastal waters and inland water respectively. No clear user requirements were obtained for the dissolved organic matter concentration. The feasibility of these user requirements with the set up production chain was studied. An error analysis of the matrix inversion technique was performed where errors in the atmospheric correction procedure, errors in the SIOP, errors in the radiometric calibration and the signal to noise ratio of the detector were counted for.

The production chain was tested with a case study on the Lake Veluwe in The Netherlands. Hyperspectral images were acquired under optimal atmospheric conditions. The complementary *in situ* measurements were taken at 9 stations, including reflectance spectra and the specific absorption and back scattering spectra of the water constituents and concentration of the water constituents. The data were used to validate the system by

- a) forward modelling of the reflectance spectra based on the Gordon model (Gordon *et al* 1975) using a set of measured SIOP, concentrations of the constituents and measured reflectance spectra,
- b) comparison of the atmospherically corrected airborne measurements and reflectance spectra measured from a ship
- c) comparison of the measured concentrations with the calculated concentrations.

Methods

The retrieval of water quality parameters from hyperspectral remote sensing images is a based on the following chain of modules;

- acquisition of the airborne hyperspectral images followed by radiometric calibration and geometric correction. Thus images are obtained with data on spectral upward radiance. Radiometric calibration and geometric correction is not discussed in this paper.
- 2. calculation of $R(0^{\circ})$ from the upward radiance spectra by correction for incident light intensity, atmospheric influences and effects introduced by the air-water interface. The module uses the radiative transfer program MODTRAN embedded in TOOLKIT (de Haan *et al* 1999).
- calculation of concentrations of the water constituents using a matrix inversion technique. The specific
 inherent absorption and scattering coefficients of the water constituents and R(0°) are needed for input.
 Measurements of the SIOP are not necessarily performed simultaneously to the airborne
 measurements.

Water quality parameters are derived using matrix inversion on a pixel by pixel basis. This system is currently in a pre-operational phase.

Calculation of R(0) from airborne measurements

The airborne images were corrected for atmospheric influences using TOOLKIT (de Haan *et al* 1999). Briefly the correction procedure performs calculation of $R(0_{app}^+)$ and $R(0^-)$ respectively with

$$R(0_{app}^{+}) = \frac{c_1 + c_2 \cdot L_{rs,t} + c_3 \cdot L_{rs,b}}{c_4 + c_5 \cdot L_{rs,b}}$$
 Eq. 1

where $c_1 c_2 c_3 c_4$ and c_5 are atmospheric correction parameters and

$$R(0^{-}) = \frac{d_1 + d_2 \cdot R(0_{app}^{+})}{d_3 + d_4 \cdot R(0_{app}^{+})}$$
 Eq. 2

where $d_1 d_2 d_3$ and d_4 are the interface correction parameters. Details on the TOOLKIT and atmospheric correction procedure used can be found in de Haan *et al* (1999). The $R(0^-)$ obtained here should match to the $R(0^-)$ obtained from the Gordon model described below using actual SIOP and concentrations of water constituents. The wavelength dependence is omitted for simplicity.

Inverse modelling

The $R(0^{\circ})$ can also be calculated by the simple reflectance model suggested by Gordon (1975) which is given by:

$$R(0^-) = f \cdot \frac{b_b}{a + b_b}$$
 Eq. 3

The constant f is chosen to be 0.33 but may vary due to solar and viewing geometry. The model assumes an optically deep medium so that bottom effects can be ignored. Also stratification in the water column and inelastic scattering effects, such a Raman scattering and fluorescence are ignored. The absorption and backscattering coefficients of the natural water can be expressed in terms of the constituent of the water, as follows:

$$a = a_w + a_{CHL}^* \cdot CHL + a_{TSM}^* \cdot TSM + a_{CDOM}^* \cdot CDOM$$
 Eq. 4

$$b_b = b_{b,w} + b_{b,TSM}^* \cdot TSM$$
 Eq. 5

No scattering for CDOM and chlorophyll-*a* is assumed. Substitution of equations 4 and 5 into equation 3 yields

$$R(0^{-}) = f \cdot \frac{b_{b,w} + b_{b,TSM}^{*} \cdot TSM}{a_{w} + b_{b,w} + a_{CHL}^{*} \cdot CHL + (a_{TSM}^{*} + b_{b,TSM}^{*}) \cdot TSM + a_{CDOM}^{*} \cdot CDOM}$$
Eq. 6

This equation provides an explicit relationship between the SIOP, the concentrations of the water constituents and $R(0^{\circ})$. To determine the concentrations from $R(0^{\circ})$ the equation is rewritten as a linear system of equations: Ax = y with

$$A = \left(\frac{R(0^{-})}{f} \cdot a_{CHL}^{*} \bigg|_{\lambda=1..n} \frac{R(0^{-})}{f} \cdot [a_{TSM}^{*} + b_{b,TSM}^{*}] - b_{b,TSM}^{*} \bigg|_{\lambda=1..n} \frac{R(0^{-})}{f} \cdot a_{CDOM}^{*} \bigg|_{\lambda=1..n}\right)$$
 Eq. 7

$$y = \left(-\frac{R(0^{-})}{f} [a_w + b_{bw}] + b_{bw} \Big|_{\lambda = 1..n} \right) \text{ and } x = \begin{pmatrix} CHL \\ TSM \\ CDOM \end{pmatrix}$$
 and Eq. 9

Thus, to estimate the unknown concentrations the linear equations can be solved with a least square approach using $A^T \cdot A \cdot x = A^T \cdot b$ where A^T is the transpose of A. This can be done if observations of $R(0^T)$ are available at minimal 3 wavelengths, the SIOP are known and a fixed value for f is chosen (e.g. 0.33).

Measurements

Images of spectral upward radiance were measured of Lake Veluwe at May 26 and 27 1999, around 11:30h GMT using a hyperspectral imaging spectrometer (EPS-A) mounted into the Dutch coast guard aircraft flying at 3000m altitude. Pixels size of about $10x10m^2$ were obtained. To reduce instrumental noise of the EPS-A an averaging of 9 pixels each time was performed. Ground truth measurements were performed at May 26, 1999. Due to better optimal meteorological conditions during the second day, no clouds and very little cirrus, this image was used for further processing and comparison to the *in situ* measurements. Ground truth measurements consisted of determination of reflectance spectra (all stations), SIOP (6 stations) and concentrations of the water constituents (all stations). For comparison of the data sets the concentrations of the water constituents in the Lake Veluwe were assumed constant over time.

The $R(0^-)$ spectra were measured according to the method of Gons (1999) using equation:

$$R(0^{-}) = \frac{Q \cdot f \cdot (L_{au} - r_{sky} \cdot L_{sky})}{(E_{ad} - r_{\Theta}(1 - F) \cdot E_{ad} - r_{dif} \cdot F \cdot E_{ad}) + 0.5 \cdot E_{wu}}$$
Eq. 10

The measured parameters are L_{au} , L_{sky} and E_{ad} . The coefficient Q varied between 2.9 and 4.7 depending on solar angle and the ratio between total and diffuse downward light. The value of r_{sky} was 0.0293, f = 1.82 for fresh water, $r_{dif} = 0.06$ (Jerlov 1976), r_{Θ} was calculated from Julian day, daytime and geographical position and F was obtained from shading off measurements.

Absorption spectra of the sum of total suspended matter and algae pigments were measured using the filterpad method (Trüper and Yentch 1967) with a 0.45 μ m Whatman GF/F filters. The absorption of total suspended matter was obtained after extraction of the pigments from the filter according to method of Kishino *et al* (1985). Residual scatter was corrected for by subtraction of the value at 750nm for the whole spectrum. The absorption spectra of algae pigments were obtain by subtraction of the spectra. The absorption spectra of coloured dissolved organic matter were measured from water filtered over 0.45 μ m filters. The concentrations of total suspended matter were measured from the dried filters. Concentrations of algae pigments were measured from ethanol extracted pigments. Beam attenuation spectra were measured from unprocessed samples. The scattering coefficient of the total suspended matter was calculated from the difference between the total absorption spectrum and the beam attenuation spectrum. The backscattering to scattering ratio spectrum was estimated to be 0.027, based on an optimised fit between the ship based measured $R(0^{\circ})$ and modelled $R(0^{\circ})$, see Figure 2.

RESULTS

Match between R(0) *spectra obtained with different methods.*

The subsurface irradiance reflectance spectra were determined with the three different techniques mention above. A good correspondence between the reflectance spectra can be seen in Figure 2. The correspondence between the modelled and the ship based measured reflectance spectra was optimised was optimised with the scattering to backscattering ratio (0.027). This way the specific backscattering coefficient was obtained. The good correspondence between the ship based and the modelled reflectance validates the optical model used in the Matrix Inversion Method. The correspondence between the ship based and the airborne measured reflectance spectra validates the atmospheric correction procedure. The airborne spectra show a high spectral noise in comparison with the other spectra which is due to the instrumental noise of the EPS-A. Recently the signal to noise ratio of the EPS-A has been improved by a factor 6.

Validity of matrix inversion method

Estimation of the concentrations of the water constituents from $R(0^{\circ})$ with a matrix inversion technique using 3 ore more wavelength bands requires a least square solution. The EPS-a measures reflectance at 17 wavelengths bands between 450 and 750nm. The outcome of such a matrix inversion techniques is affected by errors due to instrumental noise, errors due to the atmospheric correction procedure and errors in the SIOP. These effects were studied by numerical modelling using the least squares method. It was found that in case of a normal distribution of noise in the SIOP its effect on the derived concentrations appeared to be of minor effect. A normally distributed noise in the $R(0^{\circ})$ was found to have its major effect in the estimation of the chlorophyll concentration. The results of the additive effects of noise in the SIOP and $R(0^{\circ})$ are shown in Figure 3.

A shift in the reflectance value may occur due to an erroneous atmospheric correction. For the example shown here it is ignored that spectral effects are stronger in the blue wavelength range. In case of a shift of 0.5 percent of the original reflectance value difficulties occur in obtaining the concentration of chlorophyll and CDOM. The obtained concentration of TSM is overestimated but remains within the required accuracy. The obtained chlorophyll-*a* concentration is out of the required accuracy. Severe difficulties in obtaining the CDOM concentration can be seen from Figure 4c. Negative concentrations are obtain due to the spectral shift. This problem is to be solved in near future. For now the problem can be get around by adapting a fixed value for the CDOM concentration. This way the accuracy of the estimated

concentrations of the other constituents is improved. A more detailed report of these findings will be published separately.

Different techniques for inversion of the matrix were tested on modelled reflectance spectra. Any error in the measured reflectance spectra must be transformed into equation 8, in the same way as the observables were transformed. If a uniform error in reflectance is assumed it leads to application of a weighted least squares method. An example of these weights is given in Figure 5 and shows that the spectrum is effectively only used between 450 and 700 nm.

It was found that application of the weighted least squares method significantly improves the accuracy of the results. In the linear method of which results were shown above this accuracy could only be achieved by deleting all reflectance below 450nm and above 700nm.

Quantifying accuracy

Quantification of the accuracy of results obtained from reflectance spectra is a fundamental problem. For our case the accuracy is to be determined for at least 2 parameters, namely: the accuracy of fitted reflectance, and the accuracy of fitted concentrations. The cost functions for quantifying the accuracy of the retrieved spectra $(L2_R)$ is defined by:

$$L2_R = \sqrt{\frac{1}{N} \sum_{j}^{N} (R(0^-)_{j}^{cal} - R(0^-)_{j}^{obs})^2}$$
 Eq. 11

where cal indicates the model reflectance and obs indicates the observed reflectance spectrum, jis the spectral band number and N is the number of bands used. The accuracy of the retrieved concentration compared to the $in \, situ$ data as a function of measurements errors $(L2_C)$ is given by:

$$L2_{C} = \sqrt{\sum_{i}^{N_{const}} \frac{1}{C_{i}^{2}} (\max(abs(c_{i}^{mod} - c_{i}^{obs}) - S_{i}^{obs}))^{2}}$$
 Eq. 12

where N_{const} is the number of water constituents distinguished. The measurement error 'S' is introduced in order to eliminate a contribution from errors in retrieved concentrations that are smaller than the measurement error. In this work, for the measurement error, the observed natural variability in the in-situ samples is taken. For all sampling stations in Lake Veluwe (see Figure 6) a plot is shown of $L2_R$ versus $L2_C$ in Figure 6.

This figure clearly shows that the errors in both norms are correlated: this implies for the present application that an accurate matrix inversion method of the reflectance spectra also guarantees accurate

concentrations. Unfortunately, this is only true for the concentration of chlorophyll and total suspended matter. Figure 6 also shows that the error L2-C can not become smaller than 0.5. This is due to the fact that CDOM can not be retrieved accurately which is mainly due to the fact that information below 450nm is not used in the applied matrix inversion. Below 450nm CDOM has the largest effect on reflectance. Probably the only way to solve the problem is to down scale the error in spectra significantly in the blue part of the spectrum. However, the following errors must be considered; 1) the accuracy of SIOP Especially the filter path method is unclear for errors at shorter wavelengths. 2) the atmospheric correction and the sky correction according to equation 10 radiance is largest at shorter wavelengths. At present we must refrain from using remote sensing for determination of CDOM.

Case study

The matrix inversion technique was applied on an hyperspectral airborne image. A fixed value for the CDOM concentration was used to circumvent the problem described above. The *in situ* measurements showed the CDOM concentration constant over the lake. The concentration of TSM and CHL obtained are shown in Figure 5 and 6 respectively. Ground truth concentrations are listed in Table 2. A close resemblance was found between the remote sensing data and the in situ data for TSM. The red colour in the lower part of the TSM image is not a high TSM concentration but is due to sunglint. No effort was made to distinguish sun glint. This will be done in the near future.

For the chlorophyll image large areas are black. These areas have been flagged due to negative values of the chlorophyll concentrations caused by a low signal to noise ratio of the EPS-A. Currently the EPS-A has been upgraded and results are expected to be not flagged of anymore. The high values for chlorophyll are caused by water plants. No effort was made yet to distinguish for water plants. The striping in figure 6 is due to the mirrors of the scanners not being 100 percent equal. Correction for this effect was omitted in this study.

CONCLUSION

A production chain for maps of water quality parameters has been defined. First results of a test on the chain using an imperfect airborne scanner show promising results. The matrix inversion method combined with the simple Gordon reflectance model proved to be sufficient for deriving concentration of total

suspended matter and chlorophyll a. More study is needed to obtain accurate CDOM concentrations from the reflectance spectra. Near future experiences with the production chain has to demonstrate the robustness of the system as a monitoring tools for water quality parameters.

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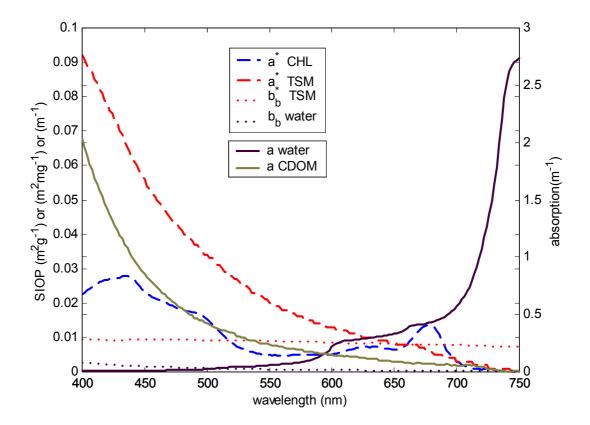


Figure 1.

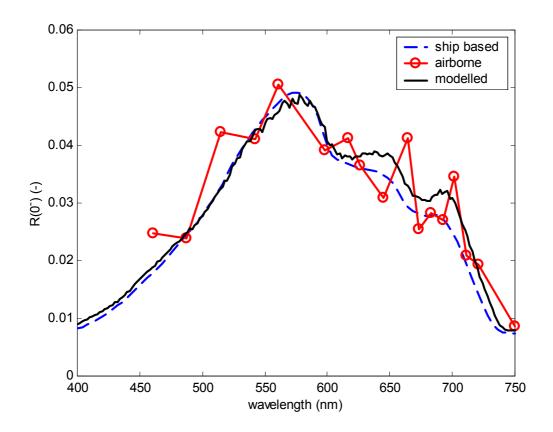


Figure 2

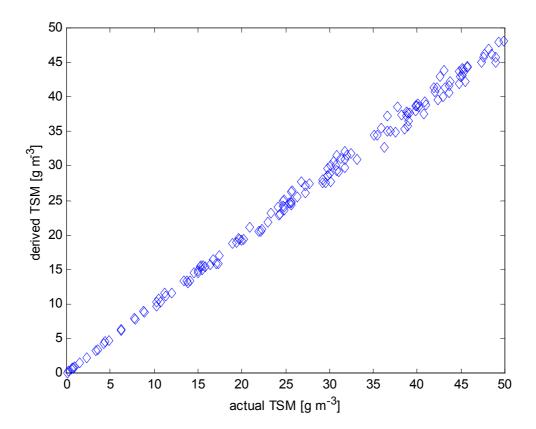


Figure 3a

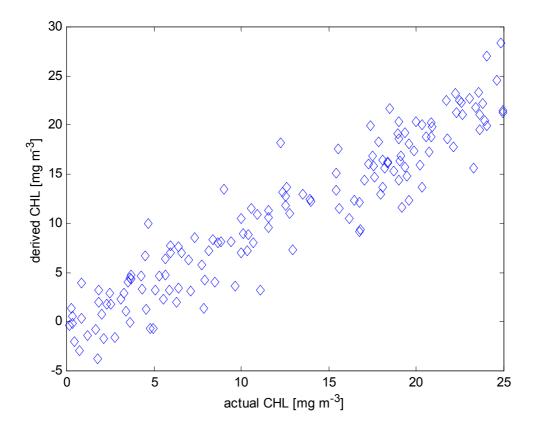


Figure 3b

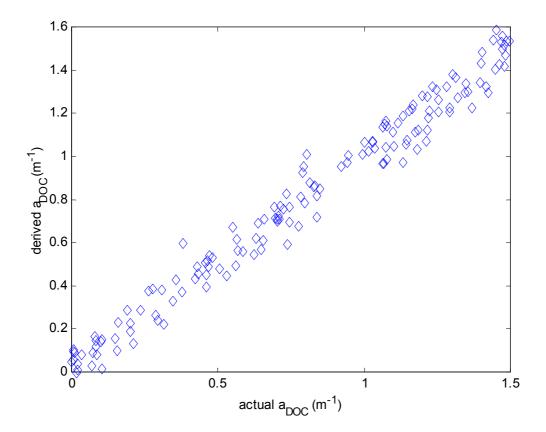


Figure 3c

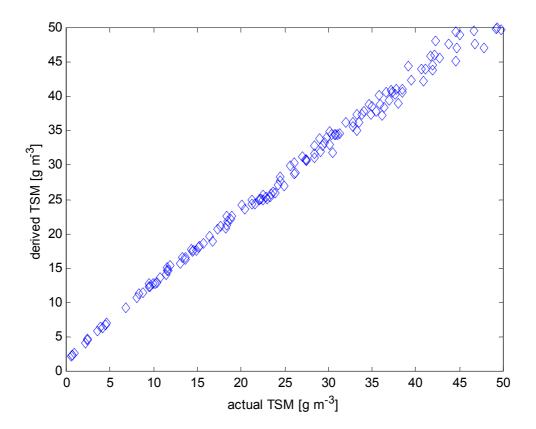


Figure 4a

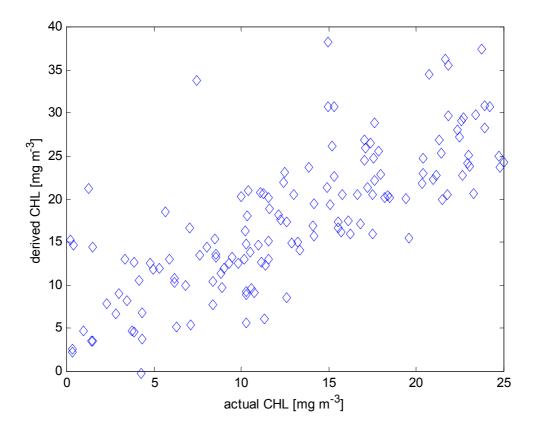


Figure 4b

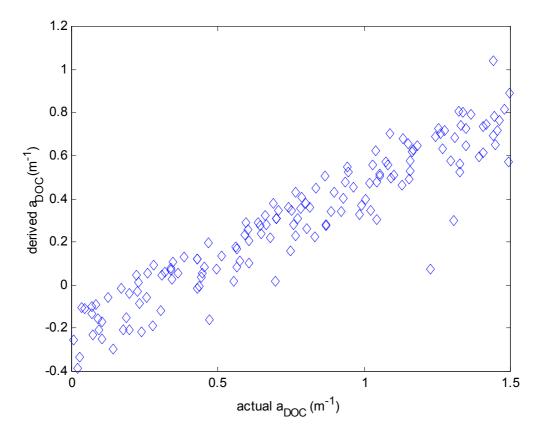


Figure 4c

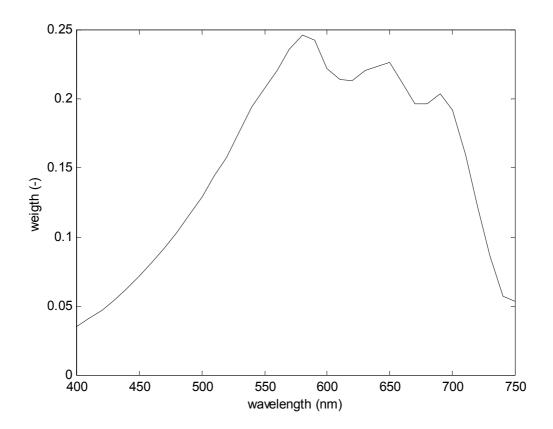


figure 5.

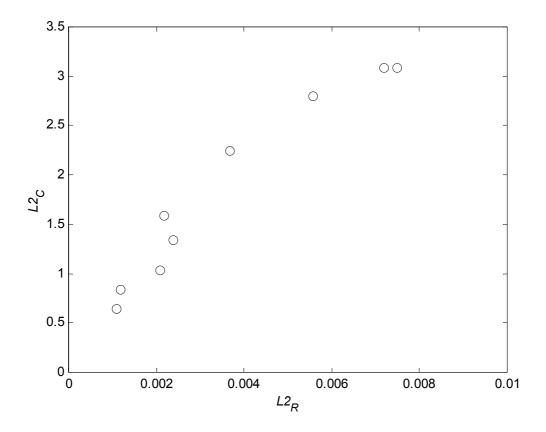
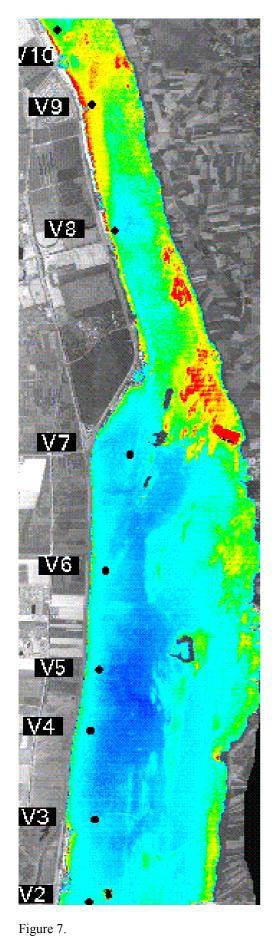


Figure 6.



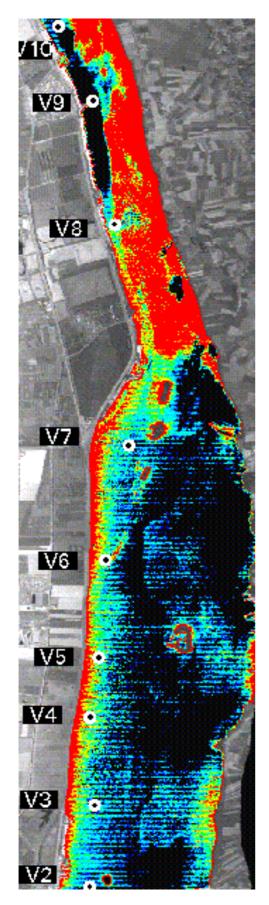


Figure 8

Figure 1. SIOP of the water constituents in the Lake Veluwe and optical properties of pure water according to Pope and Fry (1997) modified by Hakvoort and Doerffer in the near infrared part of the spectrum

Figure 2. Reflectance spectra ship based and airborne measurements and model calculations.

Figure 3. Concentrations of the water constituents as derived from reflectance spectra with a 20 percent noise in SIOP and a 5 percent noise in the $R(0^{\circ})$. The concentrations were obtained with matrix inversion based on a least square fit. a: total suspended matter b: Chlorophyll-a c: Dissolved organic carbon

Figure 4. Same notation as for Figure 3 but with an additional of 0.5 percent bias to the $R(0^{\circ})$. Note the differences in the Y-axes when compared to Figure 3, especially for CHL and DOC. a: total suspended matter b: Chlorophyll-a c: Dissolved organic carbon

Figure 5. Weights used for weighted least squares method for spectrum.

Figure 6. Correlation between L2-R and L2-C

Figure 7. Total suspended matter concentration obtained using matrix inversion. (1 <50g m⁻³)

Figure 8 Concentration of chlorophyll a obtained using matrix inversion. (1 < 50g m⁻³)

The black colour means that no accurate data were obtained from matrix inversion.

Tabel 1. Notification

Symbol	description	Units
a	total absorption coefficient	m ⁻¹
$a_{\scriptscriptstyle CDOM}^*$	absorption coefficient of CDOM	m ⁻¹
$a_{\scriptscriptstyle CHL}^*$	specific absorption coefficient of CHL	m ² mg ⁻¹
$a_{\scriptscriptstyle TSM}^*$	specific absorption coefficient of TSM	$m^2 g^{-1}$
a_w	absorption coefficient of pure water	m ⁻¹
b_b	total back scattering coefficient	m ⁻¹
$b_{b,TSM}^*$	specific back scattering coefficient of TSM	$m^2 g^{-1}$
$b_{b,\mathrm{w}}$	back scattering coefficient of pure water	m ⁻¹
CHL	concentration of chlorophyll a	mg m ⁻³
E_{ad}	downward irradiance above water surface	W m ⁻² nm ⁻¹
E_{wu}	subsurface upward irradiance	W m ⁻² nm ⁻¹
f	conversion coefficient for L_{au} to L_{wu}	-
F	fraction diffuse light of E_{ad}	-
L_{au}	upward radiance above water surface	W m ⁻² nm ⁻¹ sr ⁻¹
L_{wu}	subsurface upward radiance	W m ⁻² nm ⁻¹ sr ⁻¹
$L_{rs,b}$	average background radiance seen by detector	W m ⁻² nm ⁻¹ sr ⁻¹
$L_{rs,t}$	total upward radiance detected by sensor	W m ⁻² nm ⁻¹ sr ⁻¹
L_{sky}	downward sky radiance at 42° zenith angle	W m ⁻² nm ⁻¹ sr ⁻¹
Q	conversion coefficient for L_{wu} to E_{wu}	-
r_{sky}	Fresnel reflectance coefficient for sunlight	-
r_{dif}	Fresnel reflectance coefficient for diffuse light	-
r_{Θ}	Fresnel reflectance coefficient for sunlight	-
$R(0^{-})$	subsurface irradiance reflectance	-
$R(0^+)$	above surface radiance reflectance	-
TSM	concentration of TSM	g m ⁻³

Tabel 2. Concentrations of the water constituents measured in situ

Station	TSM (g m ⁻³)	CHL (mg m ⁻³)
V2	8.4	9.5
V3	7.4	9.6
V4	6.0	8.3
V5	8.8	10.6
V6	6.9	8.8
V7	8.5	8.0
V8	8.0	7.7
V9	43.2	8.6
V10	11.3	6.4