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FIRST DERIVATIVE INDICES FOR THE REMOTE SENSING OF INLAND WATER QUALITY USING HIGH SPECTRAL RESOLUTION REFLECTANCE

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Remote sensing is a technique with potential for monitoring the surface water quality of lakes and rivers. However, new technologies are required in order to overcome the poor spatial and spectral resolutions of conventional satellite sensors. This paper presents the results of novel derivative analyses applied to both high spectral resolution subsurface reflectance and similar data obtained at 450 m above lakes in the Netherlands. Several first derivatives, at 670, 722, and 840 nm wavelengths, showed good potential for the prediction of surface suspended matter concentrations. These were similar in strength to correlations found between reflectance in a single band and suspended sediment. First derivatives of reflectance, at 620, 638, and 661 nm in particular, showed higher correlations with chlorophyll *a* concentrations than compared with individual reflectance wavebands. The results suggest that derivatives of reflectance, calculated using high spectral resolution reflectance, may be used as the basis for indices for the detection of inland water quality and warrant further study.

INTRODUCTION

The potential of remote sensing for the monitoring of water quality in inland waters has long been recognised (Wrigley and Horne 1974). However, conventional broad band instruments currently deployed in space (Landsat TM and SPOT HRV sensors) are limited in their application to inland water systems because of a low spatial resolution and poor spectral band location with respect to the features of most interest in the reflectance spectrum (Hilton 1984; Dekker and Peters 1993). More successful applications for determining water quality have been achieved through the use of spectral bandsets specifically developed for inland waters (Dekker et al. 1991). The temporal resolution of such instruments is also a limiting factor; a high temporal frequency of measurements is needed to study the dynamic nature of inland water systems.

Reflectance from lakes is the result of both absorption and scattering processes by the optical components in the water, which include phytoplankton, suspended non-living particulate matter, dissolved aquatic humus, and the water itself (Kirk 1983). In productive inland waters, the spectrum of remotely sensed reflectance may be markedly affected in both blue and red regions by absorption of light by photosynthetic pigments in the phytoplankton. In addition, there may be strong absorption of blue light by dissolved aquatic humus. Increasing inorganic suspended sediment concentrations generally contribute to increased reflectance across the broad visible spectral region (400-700 nm, Goodin et al. 1993). Spectral reflectance from lakes is thus the result of complex absorption and scattering phenomena. For the successful application of remote sensing for the determination of water quality parameters in a range of inland waters, analytical techniques are required for the resolution of individual water quality parameters from the compound reflectance signal.

In recent years, sensors have become available which are capable of measuring reflectance at a much higher spectral resolution. Such instruments include the airborne AVIRIS, PMI, and CASI sensors, and the planned space-borne MERIS and HIRIS sensors (Gower et al. 1985; Babey and Anger 1989). Concurrent with the development of such imaging spectrometers has been the development and increasing use in the field of high spectral resolution spectroradiometers which are needed to calibrate the imaged data.

The high spectral resolution information that such instruments provide allows for the full potential of the reflectance signal from lakes to be explored. In particular, new techniques for the analysis of the data need to be developed. One potentially useful technique is derivative analysis, which is already gaining increasing attention for its application to remote sensing (Demetriades-Shah et al. 1990, Malthus et al. 1991; Goodin et al. 1993). The use of derivatives, already commonly applied in analytical chemistry, potentially allows for the elimination of background signals and for the resolution of overlapping spectral features (Demetriades-Shah et al. 1990).

In aquatic research, Maurer (1981) used derivative spectroscopy for the quantitative determination of uric acid and nitrate concentrations in polluted waters. Latterly, derivative techniques have been used to quantitatively estimate pigment concentrations in absorption spectra from both cultured and natural phytoplankton populations (Faust and Norris 1982; 1985; Bidigare et al. 1989). These workers have shown that derivatives overcame the problems of poor spectral definition in absorption spectra caused by overlapping pigment absorption bands and residual scattering due to the phytoplankton and detrital material.

In remote sensing, Philpot (1991) discussed the development of the derivative ratio algorithm as a method for providing reflectance information independent of atmospheric effects. Using an experimental approach, Goodin et al. (1993) suggested that first and second order derivative transformations reduced interference from background pure water and suspended sediment effects, respectively.

To date, no studies have investigated the application of high spectral resolution derivative remote sensing techniques for the monitoring of inland water quality parameters using data obtained at altitude. This paper reports the results of an empirical study to evaluate whether the technique was useful for estimating water quality parameters from the remotely sensed reflectance signal of inland waters. The analysis focused initially on spectroradiometric measurements of subsurface reflectance from water bodies in the central Netherlands. Comparisons were then made using spectral reflectance obtained above the lakes using an airborne imaging spectrometer.

METHODS

Subsurface optical and water quality measurements

Spectroradiometric and other limnological data were collected during August and September 1990 from a number of lakes covering a range of trophic status in the Northern Vecht and Loosdrecht regions in central Holland. Measurements were also made in the Amsterdam-Rhine canal and River Vecht, water bodies high in concentrations of suspended inorganic particles. Further information on the study area can be found in Dekker (1993).

Spectra of downwelling irradiance and subsurface upwelling radiance were measured using a Spectron SE590 spectroradiometer (Spectron Engineering, Colorado). This rapid scanning instrument is based on a linear photodiode array, measuring radiance in 252 spectral channels over the range 358-1137 nm with a nominal dispersion of 3 nm and resolution of approximately 11 nm. The instrument was configured with two sensor heads: one sensor head was fitted with a cosine corrected hemispherical receptor enabling reference measurements of above surface downwelling irradiance. Subsurface upwelling spectral measurements were made with the second sensor head using a tubular perspex guide masked with black tape and fitted onto the 15 degree receptor mounted on the head. The free end of the perspex tube was immersed just under the water surface during measurements. The use of the perspex guide did not result in significant loss of light over the wavelength range of interest (400 - 850 nm; Malthus and Dekker 1990).

Reflectances were calculated as the ratio of subsurface upwelling radiance divided by above surface upwelling irradiance.

Surface water samples were taken for analysis of water quality parameters. Chlorophyll *a* in phytoplankton collected by filtration of samples through glass-fibre filters (Whatman GF/F) was estimated spectrophotometrically following extraction in boiling ethanol (Moed and Hallegraeff 1978). Dry weight, a measure of total suspended material, was determined gravimetrically on samples collected on GF/F filters after drying at 80° C for 24 h.

Airborne spectrometer flights

Airborne spectrometer images of the lakes in the Loosdrecht/Northern Vecht region were collected on 14.9.90 using the Compact Airborne Spectral Imager (CASI, Babey and Anger 1991). This instrument has three operating modes: spatial, spectral, and full frame modes. Spectral mode data were collected in 288 discrete spectral channels at 1.8 nm intervals across the 430 to 780 nm wavelength range. For this purpose, the sensor was flown at an altitude of 450 m above ground level to reduce effects from atmospheric haze. Aircraft speed and instrument integration time were such that the along-track resolution was 13.6 m and an across-track resolution of 0.6 m. In this mode and at this altitude, the swath width of the instrument was 117 m. Five flight lines were required to cover all the water bodies, over a total spatial area of approximately 16 by 6 km.

Representative radiance spectra from the individual lakes were extracted from the spectral mode data corresponding as close as possible to the location where subsurface optical and water quality measurements were made. Three by three pixel averages were sampled to suppress instrument and environmental noise. Radiances were converted to reflectances using a measurement of downwelling irradiance made at ground level using the Spectron spectroradiometer simultaneous with the CASI flight. Further details of the instrumentation, data collection and subsequent processing to reflectance can be found in Dekker (1993).

Table 1. Range, mean, and standard deviation (S.D.) in water quality data in water bodies in which subsurface reflectance measurements were made (n = 30).

Water Quality Parameter	Range	Mean	S.D.
Secchi Disk (m)	0.35 - 4.9	1.52	1.4
Dry Weight (mg L^{-1})	1.2 - 45	15.9	11.1
Chlorophyll *a* (mg m^{-3})	1.0 - 125	39.1	40.6

RESULTS

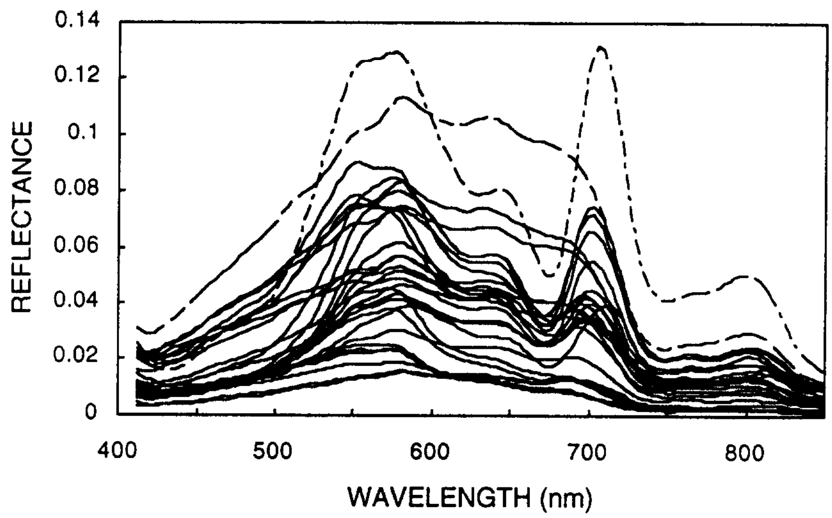
Water quality data

Subsurface reflectance spectra were obtained from 30 different locations of widely differing trophic status (Table 1). Secchi disk transparencies ranged from 4.9 m in the clearest lake (Loenderveen Water Reservoir) down to as low as 35 cm in hypertrophic Lake WijdeGat. Concentrations of chlorophyll *a* in the waters sampled spanned two orders of magnitude, ranging from 1 to 125 mg m^{-3}.

Correlations between the different water quality parameters are presented in Table 2. Secchi disk transparency was highly correlated inversely to both dry weight and chlorophyll concentrations. Sixty one percent of the variation in dry weight could be explained by variation in chlorophyll *a*, suggesting that a significant fraction (approximately 40%) of dry weight was contributed from nonliving particulate matter in these lakes.

Table 2. Correlation matrix between water quality variables.

	Dry Weight	Chlorophyll *a*
Secchi Disk	-0.65	-0.70
Dry Weight	-	0.78



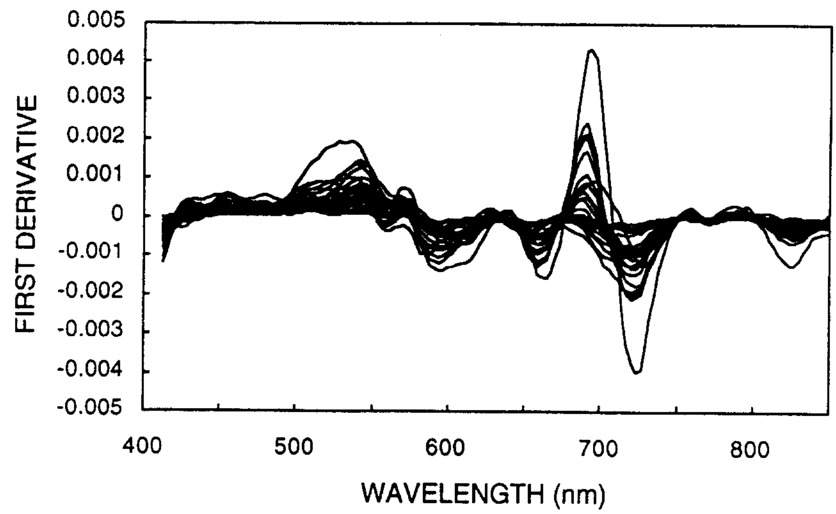


Fig. 1. a) Subsurface reflectance and b) first derivatives (dR/dλ) of subsurface reflectance from water bodies in the central Netherlands. Spectra in (a) obtained from the Amsterdam-Rhine Canal (- - -) and Lake Wijde Gat (-·-·-) are highlighted and are discussed in the text.

Subsurface reflectance spectra

Typical subsurface reflectance spectra, measured over the 400-850 nm wavelength range are presented in Fig. 1. To suppress instrumental and environmental noise, the spectra were smoothed with five passes of a three-point weighted filter. The spectra indicate several areas across the wavelength range in which reflectance is altered by differing concentrations of optical components in the water. The spectra from turbid water bodies in which suspended sediments of inorganic origin were dominant (e.g., Amsterdam-Rhine Canal, Fig. 1) showed a broad plateau of reflectance from 550-700 nm. Spectra derived from waters in which phytoplankton concentrations were high (e.g., Lake WijdeGat, Fig. 1) had reflectance peaks typically around 550-580 nm and around 700 nm. In these lakes, reflectance in the region 580-700 nm was typically reduced, the result of absorption of light by photosynthetic pigments in the phytoplankton.

First derivative spectra are presented in Fig. 1b. Peaks in the first derivative reveal the rate of change in slope of the original spectrum; spectral regions with increasing reflectance with wavelength have positive first derivative values while areas with decreasing reflectance have negative values.

To objectively determine those regions of the reflectance and derivative spectra which may be useful for the remote estimation of water quality parameters, linear correlation analysis was undertaken between water quality parameters and subsurface reflectance at each wavelength. Plots of the correlation spectra for the normal and derivative curves may subsequently

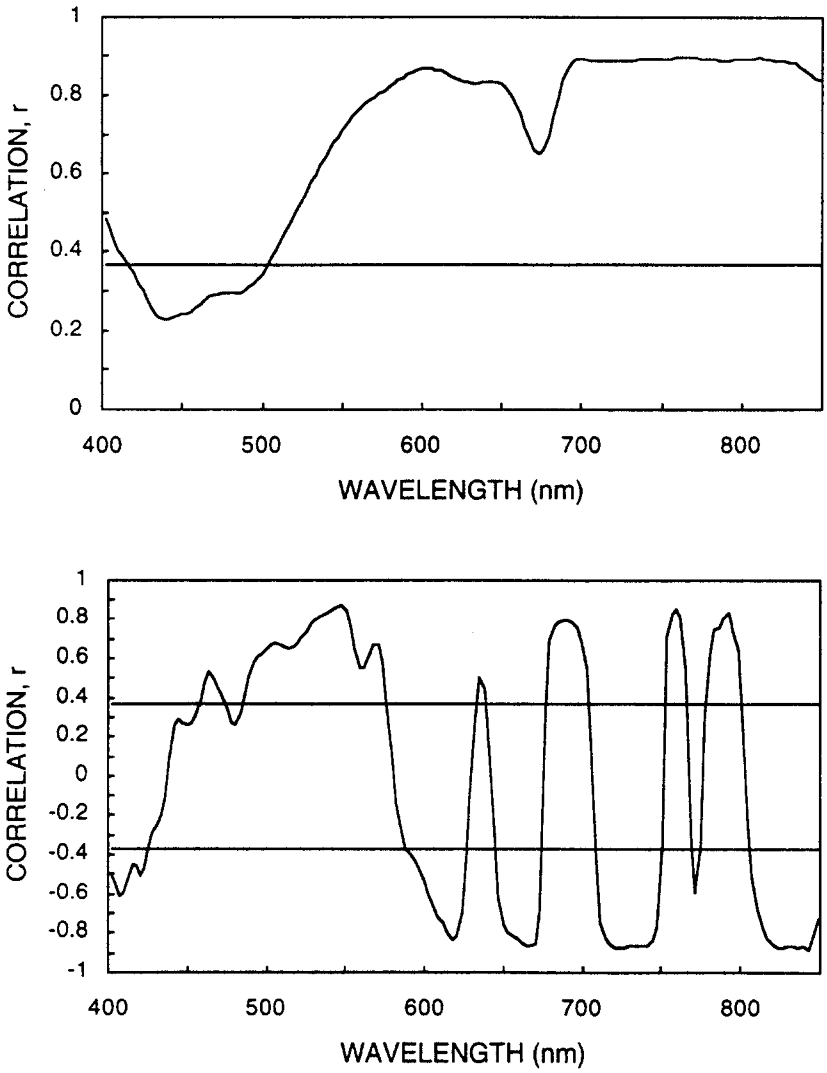


Fig. 2. Correlation spectra obtained between dry weight and a) normal reflectance and, b) first derivatives of subsurface reflectance. Horizontal lines indicate a correlation significant at the 95% confidence level.

be used to highlight those wavelengths correlating highly with water quality parameters (Figs. 2 and 3).

Dry weight was positively correlated with subsurface reflectance over the whole spectrum indicating that this water quality parameter is related to the amount of scattering material in each of the water bodies (Fig. 2a). Correlations approached r=0.9 in the 550-660 nm region in the visible region and from 700-850 nm in the near-infrared. Correlations obtained between dry weight and certain first derivative wavelengths were similar in strength to those obtained using reflectance.

Chlorophyll *a* was less highly correlated with subsurface reflectance compared to dry weight, the only regions significantly correlated being the 550-660 nm region and 700-850 nm spectral regions (Fig. 3a). However, correlations between chlorophyll *a* concentrations and the first derivative of reflectance were generally higher than those obtained with the original reflectance spectra, particularly in the visible region. High correlations were found at peaks within the region 550-730 nm, corresponding to the spectral region where peak absorption by photosynthetic pigments has its greatest impact on the reflectance spectra.

Airborne spectrometer data

Twelve reflectance spectra were obtained from the CASI spectral mode data over water bodies for which comparable water quality measurements were available (Fig. 4). Logistic constraints precluded the collection of all water quality samples at the time of the

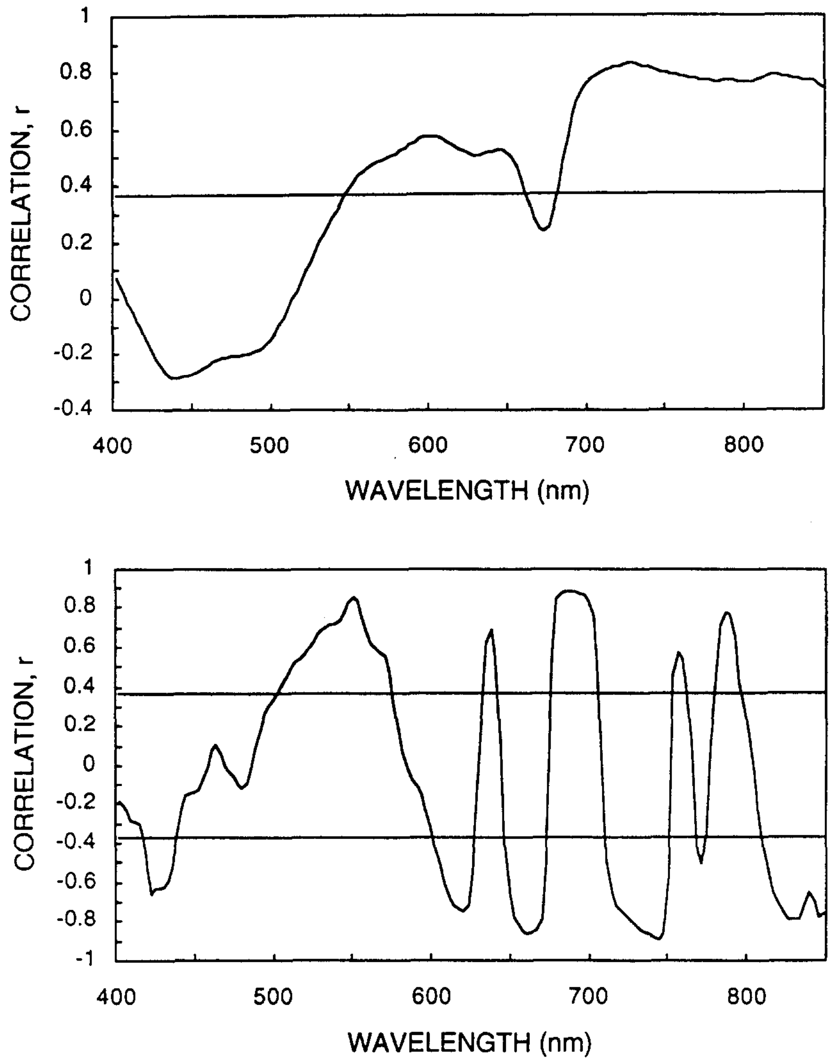


Fig. 3. Correlation spectra obtained between chlorophyll *a* concentrations and a) normal reflectance and, b) first derivatives of subsurface reflectance. Horizontal lines indicate a correlation significant at the 95% confidence level.

CASI overflight. Most samples were taken two to four days preceding the flight with two water bodies up to 14 d previously; however, it is not expected that significant changes in water quality occurred between sampling and the time of overflight.

The CASI reflectance spectra obtained at 450 m above ground level show a similar basic shape to subsurface reflectance with the exception of increased reflectance in the blue region, with a pronounced shoulder around 450 nm. This phenomenon is most likely the result of atmospheric scattering of light in the blue wavelength region. Peaks in airborne reflectance were measured at approximately 570 and 705 nm. The first derivatives of CASI reflectances (Fig. 4b) were calculated using one pass of a set of weighted coefficients over 19 spectral points, equivalent to a third order polynomial calculated fitted using least-squares. The technique is one commonly applied to spectra in analytical chemistry and the coefficients were derived from Savitzgy and Golay (1964).

Similar linear correlation analyses were undertaken between the chosen water quality parameters and normal and derivative CASI reflectances (Figs. 5 and 6). Dry weight concentrations were significantly correlated with reflectance over the 520 to 720 nm spectral region similar in strength to those obtained with subsurface reflectance. In contrast with subsurface reflectance significant correlations with dry weight were not obtained above 720 nm. Correlations between dry weight and first derivatives of airborne reflectance were obtained at similar wave-

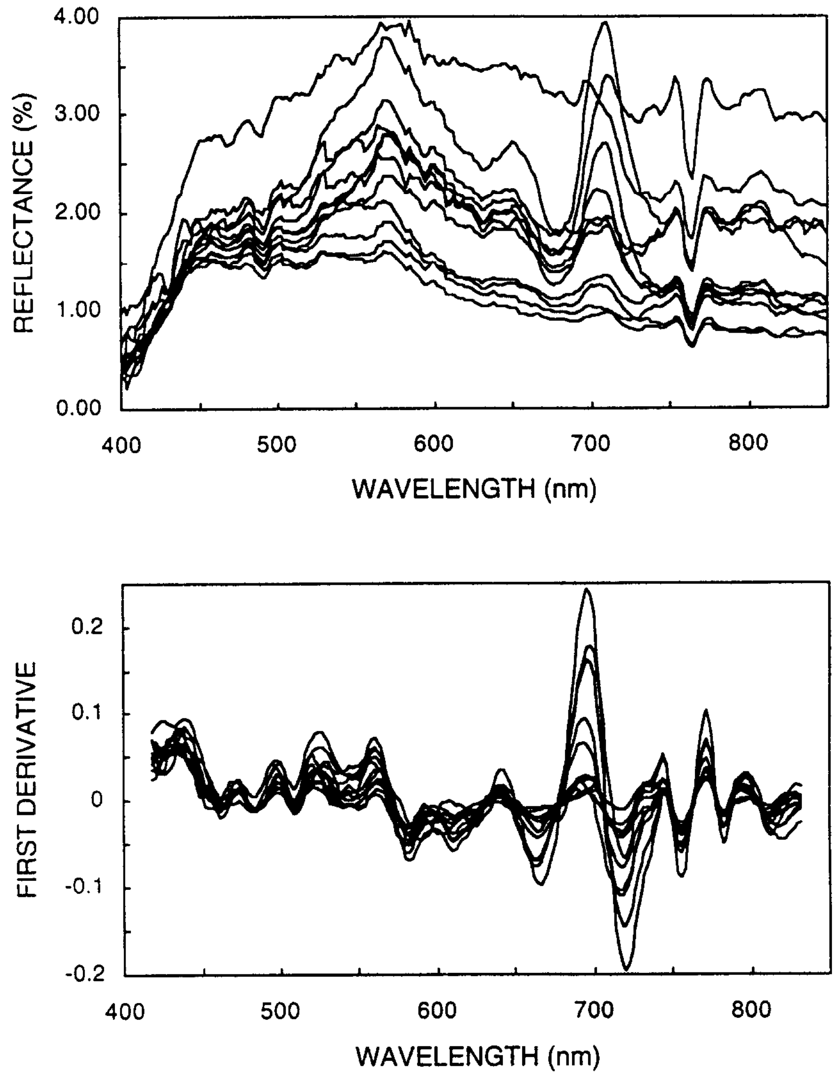


Fig. 4a) Lake reflectance and b) first derivatives (dR/dλ) of reflectance calculated from spectra obtained at 450 m altitude using the CASI instrument.

lengths and of generally similar strength to those of subsurface reflectance. Improved correlations were obtained with the first derivative at 640 nm (positive in sign) and at 675 and 720 nm (both negative in sign).

Correlations between chlorophyll *a* and CASI reflectance were lower than those obtained with subsurface reflectance. Significant correlations were only found in the 700-720 nm spectral region (approaching r=0.65). No significant correlations were observed in the 550-560 nm region and beyond 720 nm. Correlations with chlorophyll *a* were stronger at certain first derivative wavelengths (approaching r=0.85), particularly in the 600-700 nm spectral region where the absorption of photosynthetic pigments is high.

DISCUSSION

Derivatives of reflectance spectra served to highlight fine-scale differences in reflectance spectra, particularly in the 600-720 nm spectral region, as indicated by the increased number of wavebands showing correlations with the water quality parameters compared to reflectance.

Subsurface and airborne reflectance wavelengths showing highest correlations with water quality parameters are presented in Table 3. In general, blue wavelengths were poorly correlated with the parameters. This result reflects the lack of separation in subsurface reflectance spectra between lakes in this spectral region due to high light absorption by both photosynthetic pigments and dissolved aquatic humus (Kirk 1983). Atmospheric scattering also af-

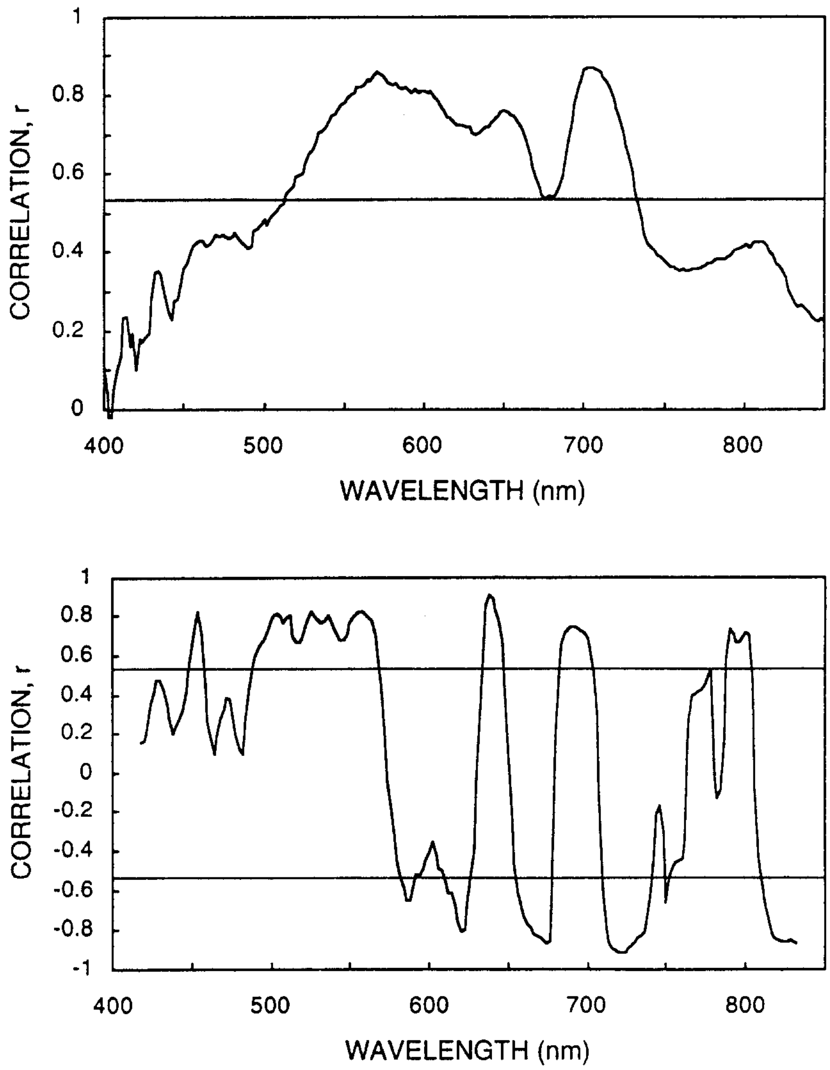


Fig. 5. Correlation spectra obtained between dry weight and a) CASI reflectance and b) first derivatives of CASI reflectance. Horizontal lines indicate a correlation significant at the 95% confidence level.

fects measurements of reflectance in this region in data derived at altitude.

Highest correlations were generally obtained in the 550-720 nm spectral region, where the greatest differences between reflectances from the lakes measured in this study were observed. This is also a region where the influence of atmospheric scattering is reduced compared to the blue spectral region. Beyond 720 nm, correlations between water quality parameters and the airborne reflectance and derivative data were generally lower than with subsurface data, presumably as a result of the low overall reflectance of light due to high light absorption of near infrared light by the water itself.

In general, dry weight correlated highly with reflectance indicating, as George and Hewitt (1989) observed, that dry weight can be reasonably predicted using reflectance in a single selected waveband. High correlations between dry weight and reflectance were obtained probably because this parameter is the best measure of the amount of living and nonliving suspended material which causes scattering of light and so contributes to high reflectance in spectral regions where absorption is low. The spectral region showing the highest correlation was the reflectance peak at 702-705 nm (Fig. 7), a region where absorption by most optical parameters is comparatively low. Correlations were only slightly improved using first derivatives, with the best wavelengths being 670, 722, and 830-840 nm. Relationships for subsurface and airborne first derivatives at 722 nm are presented in Fig. 8.

Table 3. Summary of wavelengths for both subsurface and CASI spectra in which high correlations with dry weight and chlorophyll *a* were obtained.

Subsurface (nm)	r	CASI (nm)	r
Dry Weight			
Reflectance			
603	0.87	570	0.86
703	0.89	704	0.87
First Derivative			
-	-	454	0.83
548	0.87	556	0.82
617	-0.83	620	-0.80
-	-	638	0.91
667	-0.87	674	-0.86
690	0.80	690	0.75
723	-0.88	722	-0.91
842.5	-0.89	830	0.86
Chlorophyll *a*			
Reflectance			
603	0.57	-	-
729	0.83	710	0.65
First Derivative			
550	0.85	564	0.80
620	-0.75	620	-0.81
638	0.68	640	0.85
661	-0.86	664	-0.82
688	0.88	685	0.76
744	-0.89	722	-0.67
830	0.79	810	-0.77

Chlorophyll *a* was poorly correlated with reflectance, particularly in the spectra obtained at altitude. Correlations were markedly improved when first derivatives were taken, with r values approaching 0.85 using the CASI spectra. Candidate first derivative chlorophyll indices worthy of further attention include those at 620, 638, and 661 nm (Fig. 9). These wavebands correspond to the region in the spectrum where photosynthetic pigments most markedly influence the spectral reflectance from lakes and where absorption due to other parameters (e.g., aquatic humus and the water itself) is low (Kirk 1983).

CONCLUSION

Using the reflectance spectrum from a turbid lake, Philpot (1991) suggested that useful wavebands for the detection of water quality through an atmosphere may be found in the derivatives of reflectance. However, no empirical analysis with actual water quality parameters was undertaken. This study has indicated that, using high spectral resolution data obtained from lakes covering a wide range in trophic status, first derivative indices may be successfully applied with at least the same accuracy as other methods to estimate concentrations of suspended sediment and chlorophyll *a* from remotely sensed data. Further work is required on the development of algorithms for first and higher order derivative indices, their comparison to indices based on ratios of reflectance, their sensitivity to other optical components in the water and their sensitivity to atmospheric interference if obtained at higher altitude. The results presented here should also be tested for generality using high spectral reflectance data obtained from other lake systems.

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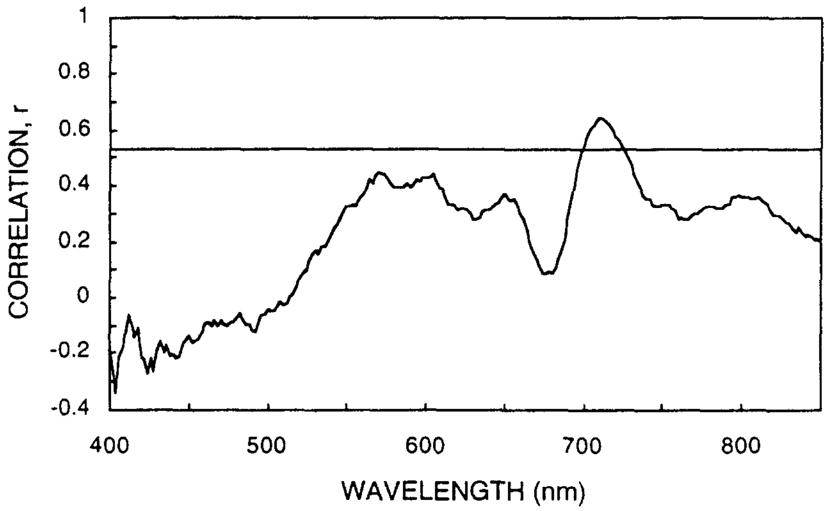

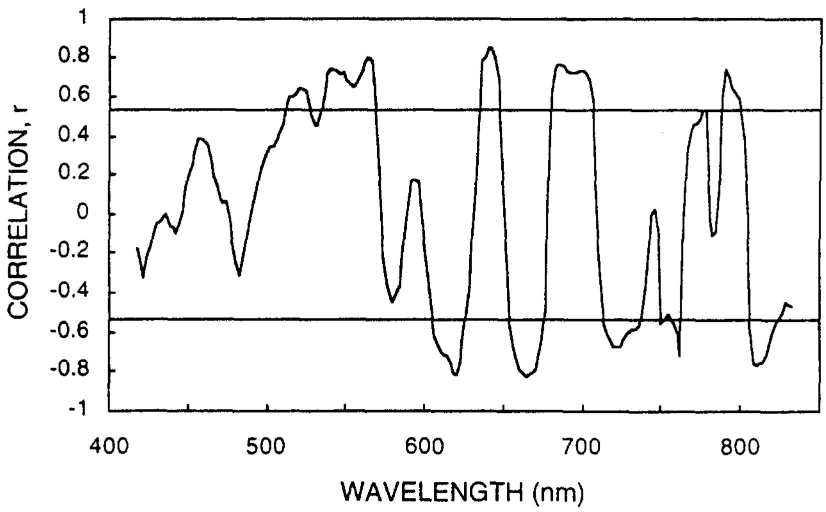

Fig. 6. Correlation spectra between chlorophyll *a* concentrations and a) CASI reflectance and b) first derivatives of CASI reflectance. Horizontal lines indicate a correlation significant at the 95% confidence level.

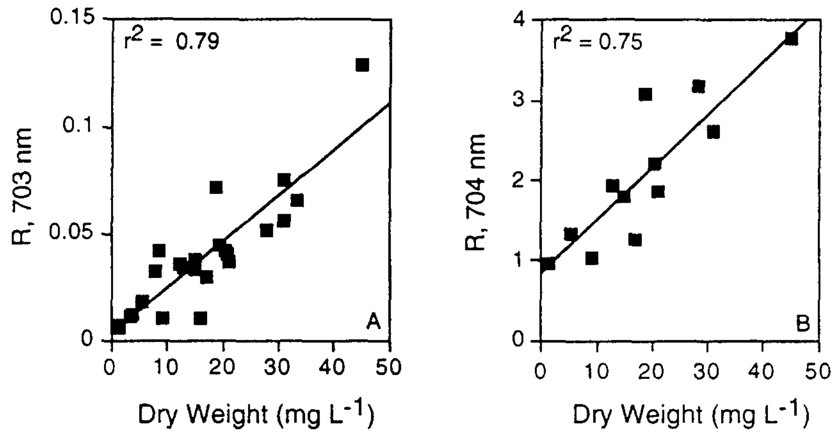

Fig. 7. Relationships between reflectances at approximately 704 nm and suspended sediment concentrations (measured as dry weight); a) using subsurface reflectance, b) using airborne CASI reflectance.

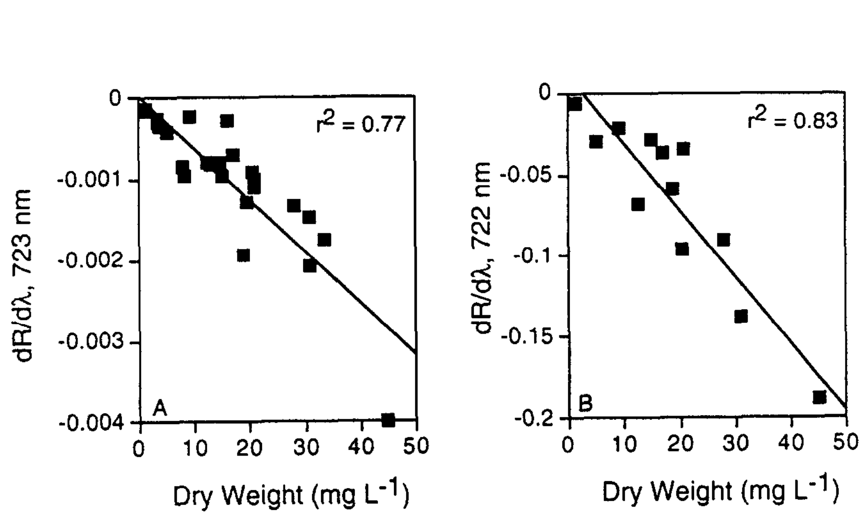

Fig. 8. Relationships between first derivatives of reflectance at approximately 722 nm and suspended sediment concentrations (measured as dry weight); a) using subsurface reflectance, b) using airborne CASI reflectance.

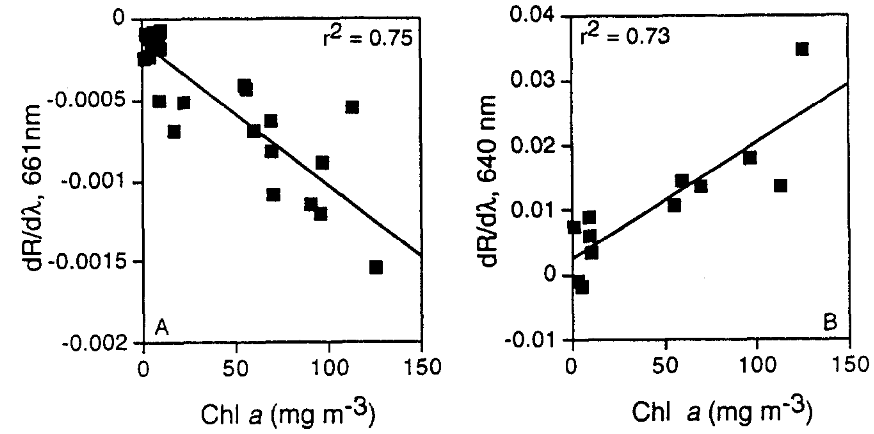

Fig. 9. Relationships between first derivatives of reflectance and phytoplankton biomass (measured as chlorophyll *a* concentration); a) first derivative of subsurface reflectance at 661 nm, b) first derivative of airborne CASI reflectance at 640 nm. The relationships are different in sign because they refer to different features in the respective first derivative spectra (Figs. 1b and 4b).

REFERENCES

Babey, S.K.; Anger, C.D. A compact airborne spectral imager (CASI). Proc. IGARRS'89/12th Canadian symposium on remote sensing. Vol. 2. Vancouver: IEEE; 1989: 1028-1031. Available from: IEEE, New York, NY.

Bidigare, R.R.; Morrow, J. H.; Kiefer, D. A. Derivative analysis of spectral absorption by photosynthetic pigments in the western Sargasso Sea. J. Mar. Res. 47: 323-341; 1989.

Dekker, A.G. Detection of optical water qualtiy parameters for eutrophic waters by high resolution remote sensing. PhD thesis, Free University, Amsterdam. ISBN 90-9006234-3; 1993.

Dekker, A.G.; Peters, S.W.M. The use of Thematic Mapper for the analysis of eutrophic lakes: A case study in the Netherlands. Int. J. Rem. Sens. 14: 799-822; 1993.

Dekker, A.G.; Malthus, T.J.; Seyhan, E. Quantitative modeling of inland water quality for high-resolution MSS systems. IEEE Trans. Geosci. Remote Sens. 29: 89-95; 1991.

Demetriades-Shah, T.H.; Steven, M. D.; Clark, J.A. High resolution derivative spectra in remote sensing. Remote Sens. Environ. 33: 55-64; 1990.

Faust, M.A.; Norris, K.H. Rapid in vivo spectrophotometric analysis of chlorophyll pigments in intact phytoplankton cultures. J. Phycol. 17: 351-361; 1982.

Faust, M.A.; Norris, K.H. In vivo spectrophotometric analysis of photosynthetic pigments in natural populations of phytoplankton. Limnol. Oceanogr. 30: 1316-1322; 1985.

George, D.G.; Hewitt, D.P. The trophic classification of lakes in the Windermere area. Proc. NERC workshop on airborne remote sensing, 23 November 1989; Windermere. Swindon, UK: NERC Scientific Services, Polaris House; 1989: 109-119.

Goodin, D.G.; Han, L.; Fraser, R.N.; Rundquist, D.C.; Stebbins, W.A.; Schalles, J.F. Analysis of suspended solids in water using remotely sensed high resolution derivative spectra. Photogramm. Eng. Remote Sens. 59: 505-510; 1993.

Gower, J.F.R.; Borstad, G.A.; Hollinger, A.B. Development of an imaging optical spectrometer for ocean and land remote sensing. In: Proc. 3rd international colloquium on spectral signatures of objects in remote sensing. 16-20 December; Les Arcs, France: ESA SP-247; 1985: 219-225. Available from: European Space Agency, Paris, Cedex 15, France.

Hilton, J. Airborne remote sensing for freshwater and estuarine monitoring. Water Res. 18: 1195-1223; 1984.

Kirk, J.T.O. *Light and photosynthesis in aquatic ecosystems.* Cambridge, UK: Cambridge University Press; 1983.

Malthus, T.J.; Dekker, A.G. Spectral light attenuation in a hypertrophic lake system (Loosdrecht Lakes, The Netherlands). Verh. Int. Verein. Limnol. 24: 711-714; 1990.

Malthus, T.J.; Andrieu, B.; Baret, F.; Clark, J.A.; Danson, F.M.; Jaggard, K.W.; Madeira, A.C.; Steven, M.D. Candidate high spectral resolution derivative indices for the prediction of crop cover. In: Proc. 5th international colloquium on physical measurement and signatures in remote sensing. 14-18 January; Courchevel, France: ESA SP-319; 1991: 205-208. Available from: European Space Agency, Paris, Cedex 15, France.

Maurer, W. Investigations on wastewater pollutants using derivative spectroscopy. Int. J. Environ. Anal. Chem. 9: 237-248; 1981.

Moed, J. R.; Hallegraeff, G. M. Some problems in the estimation of chlorophyll a and phaeopigments from pre- and post-acidification spectrophotometric measurements. Int. Rev. Ges. Hydrobiol. 63: 787-800; 1978.

Philpot, W.D. The derivative ratio algorithm: avoiding atmospheric effects in remote sensing. IEEE Trans. Geosci. Remote Sens. 29: 350-357; 1991.

Savitzgy, A.; Golay, M.J.E. Smoothing and differentiation of data by simplified least squares procedures. Anal. Chem. 36: 1627-1639; 1964.

Wrigley, R.C.; Horne, A.J. Remote sensing and lake eutrophication. Nature 250: 213-214; 1974.