INT. J. REMOTE SENSING, 1992, VOL. 13, NO. 17, 3367–3373

The peak near 700 nm on radiance spectra of algae and water: relationships of its magnitude and position with chlorophyll concentration

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(Received 5 March 1992; in final form 1 July 1992)

Abstract. To investigate the nature of the peak near 700 nm on reflectance spectrum of water, simultaneous measurements of the reflectance spectra in the region of 400 to 750 nm and relevant water quality constituent concentrations (chlorophyll, dissolved organic matter and suspended matter) were carried out. The data set cover various trophic states of water bodies, all seasons and different climatic regimes. A shift of the peak position from about 680 nm up to 715 nm and an increase of the peak magnitude when chlorophyll concentration increased were observed. The magnitude and the peak position could be used as precise indicators and predictors for the phytoplankton concentration. It contributed significantly to the increase in the accuracy of the derivation of chlorophyll values from multispectral data.

1. Introduction

The red region of the reflectance spectrum is very important for the remote sensing of inland and coastal waters. This is due to several spectral features unique to phytoplankton chlorophyll-*a* that take place in this region. A strong peak, at about 685 nm in the upwelling radiance spectrum in natural waters, was observed by Neville and Gower (1977) and Gower (1980). There have been several attempts to explain this peak: it may be due to (*a*) fluorescence of phytoplankton pigments (Morel and Prieur 1977, Gordon 1979, Carder and Steward 1985, Hoge and Swift 1987); (*b*) anomalous scattering caused by the chlorophyll absorption peak at 675 nm (Morel and Prieur 1977); and (*c*) a minimum on the combined absorption curve of algae and water for high chlorophyll values (Vasilkov and Kopelevich 1982, Vos *et al.* 1986, Kishino *et al.* 1986, Gitelson and Kondrat'ev 1991). Much of the experimental basis for testing these hypotheses was made over a very limited range of chlorophyll concentration or/and in artificial water bodies (Vos *et al.* 1986, Hoge and Swift 1987, Borstad *et al.* 1989). To date, it is not clear whether a shift of the reflectance maximum of around 700 nm, indeed, took place and how its position and magnitude depend on chlorophyll concentration.

The purpose of this research was to contribute to the understanding of the nature and features of the reflectance peak near 700 nm, and to use it to develop algorithms for the comprehensive remote sensing of water quality.

2. Methods

Several thousand spectral irradiance measurements, along with simultaneous ground-data references were taken between 1983 and 1989 in various areas of the

CIS, Hungary, Bulgaria and Germany. In the study of individual ecosystems, the phytoplankton chlorophyll ranged from 0·1 to 350 mgm^{-3}, the suspended matter ranged from 0·1 to 66 mgl^{-1}, and the dissolved organic matter absorption at the wavelength 380 nm was 0·1 to 12 m^{-1}. We also conducted experiments using enclosures. These measurements were carried out in three enclosures (each about a three-meter diameter) open to both sediments and to the atmosphere. The enclosures were installed in a small lake of the Don River system of Russia, at a water depth of 2·5 m. Each enclosure contained more than 15 m^3 of lake water. One enclosure served as a control, the other two enclosures were supplemented with essential nutrients that induced the sharp growth of the phytoplankton biomass. During ten days no change of chlorophyll concentration was noted in the lake and the test enclosure (at about 15 mgm^{-3}); while a rapid increase occurred in the enclosures supplied with nutrients reaching a level of 70 mgm^{-3} in one of them.

A radiometer, recording in the range of 400 to 750 nm, with a spectral resolution of about 1 nm and field of view 7° was used to measure the upwelling radiance and downwelling irradiance (Gitelson and Keydan 1990). Measurement of the reflectance (as ratio of upwelling radiance to downwelling irradiance) was taken at least five times over each sample of the water surface, and loaded into a data logger for processing. Radiometric readings and samples were taken from a boat. Water samples from at least three different depths in the 1·0 m layer were taken and then the acquired constituent concentrations were averaged. Measurements of chlorophyll concentration were made by use of the TURNER 10 005R and KVANT-5 fluorimeters, with the Lorenzen (1967) calibration. Suspended matter were determined by the gravimetric method (Mittenzwey *et al.* 1988). The dissolved organic matter concentration was estimated by using light absorption of the filtrate at 380 nm. Immediately after sampling the fluorescence spectrum each sample was measured using a fluorimeter in the range of 640 to 750 nm with a spectral resolution of more than 0·7 nm (Gitelson and Keydan 1990).

To explain the effect of fluorescence on the spectral behavior of the reflectance, a single fluorescence model was combined with a two-flow optical model applied by Vasilkov and Gitelson (1988). The reflectance in the region of 450 to 750 nm was calculated for various concentrations of relevant constituents. For the emission peak of chlorophyll at 680 nm a Gaussian distribution was assumed.

To determine the volume of fluorescence function Gordon's model (1979) was used. To specify cell size distribution of phytoplankton the Junge distribution $f(r) = Ar^{-\gamma}$ (where A and γ are parameters, r is cell radius) was used (Jonasz and Plandke 1986). The parameter 'γ' varied from 0·1 to 5·0. The minimum radius r_1 was assumed to be 0·5 to 1 μm, and the maximum radius r_2 varied from 2·5 to 10 μm. For non-organic suspended matter it was assumed a Junge distribution with 'γ' ranged from 0·1 to 5·0, and a refraction coefficient was taken at 1·2. Fluorescence quantum efficiency of phytoplankton was assumed to be 1 to 10 per cent (Carder and Steward 1985).

3. Results and discussion

Several spectral features of the reflectance spectra were common for waters that had different trophic states. A broad reflectance maximum of around 560 nm is caused by a low absorption of algae. A low reflectance, from 400 nm to 500 nm, is due to both chlorophyll-a and dissolved organic matter absorption. A dip at 620 nm, which is attributed to absorption by *phycocyanin*, a minimum at 675 nm, caused by

chlorophyll-*a* absorption, and a minor peak at 650 nm were observed. At 620 nm and 675 nm only shoulders were noticed when chlorophyll concentration (C_{chl}) was less than 3 mgm^{-3}. An increased C_{chl} leads to a sharp decrease in the reflectance magnitude near 620 and 675 nm. When C_{chl} was less than 3 mgm^{-3}, a shoulder at 680 nm was observed. This shoulder was transformed into a distinguished peak for $C_{chl} > 5$ mgm^{-3}. The magnitude of the peak increased and approached the value of the global maximum at 560 nm for $C_{chl} > 70$ mgm^{-3}.

The peak height was quantified by measuring the difference between reflectance at the wavelength, where the maximum reflectance is observed and the baseline interpolated from measurements at 675 and 730 nm. The reflectance value above the baseline normalized to a minimum value of reflectance (which was usually observed at 680 nm) for various water bodies as shown in figure 1. Model calculations, which were derived from Kishino *et al.* (1986) for a fluorescence quantum efficiency 2·5 per cent, and the results of Vos *et al.* (1986) measurements were also shown in this figure. It can be seen that the measured magnitude of the peak increases more sharply than was predicted by the calculations of Kishino *et al.* (1986). Our results were similar to Vos *et al.* (1986). The reflectance values above the baseline differed significantly from one water body to another. Nevertheless, the significance of phytoplankton particles was evident when observing the height of reflectance curves above the baseline at 675 and 730 nm.

Another way to quantify the peak height (R_{maxred}) was by normalizing it to the reflectance value of the global maximum of the spectrum at 560 nm (R(560)). A ratio

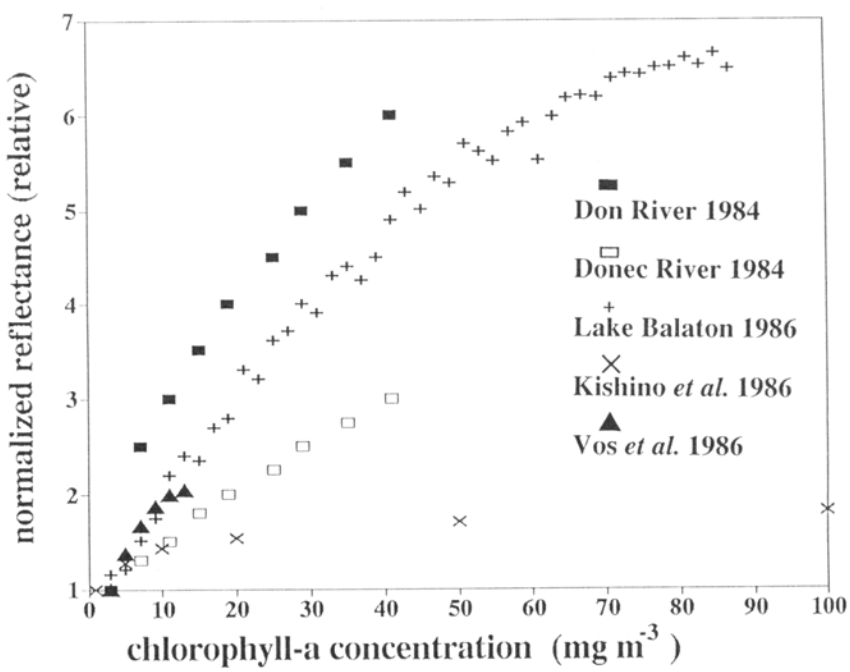

Figure 1. The peak height above baseline normalized to its minimum value for each water body, observed at 680 nm, vs. chlorophyll-*a* concentration for various water bodies. The measurements of Vos *et al.* (1986) were carried out in the cylindrical container. In Kishino *et al.* (1986) model calculations quantum fluorescence efficiency was assumed to be 2·5 per cent.

$R_{maxred}/R(560)$ vs. chlorophyll-*a* concentration for the Don and Northern Donec rivers in Russia for the different seasons and different years is described by a power function.

$$R_{maxred}/R(560) = 0{\cdot}232\, C_{chl}^{(0{\cdot}34 \pm 0{\cdot}009)} \quad (1)$$

with a coefficient of determination (R^2) of more than 0·93 for all water bodies studied (figure 2). The ratio $R_{maxred}/R(560)$ could be a precise indicator of the chlorophyll-*a* concentration for water bodies of different tropic states with a standard estimation error of less than $2\,mgm^{-3}$.

Calculations showed that the chlorophyll concentration can be derived from the radiance spectra by also using the ratio $R_{maxred}/R(675)$. The difference between these wavelengths is negligible. Therefore, the influence the dissolved organic matter and suspended matter as well is almost the same. For these reasons, the ratio $R_{maxred}/R(675)$ depends on the chlorophyll concentration only. Experimental results obtained in all water bodies which were studied confirmed this prediction (Gitelson 1991).

The increase in the peak height is accompanied by a shift in the position towards the longer wavelengths, meanwhile, the peak of the phytoplankton fluorescence had a permanent position at 680 nm for all the samples measured. The peak position for C_{chl} near $3\,mgm^{-3}$ was observed at 680–683 nm; and it shifted to a longer wavelength reaching 715 nm for C_{chl} at more than $100\,mgm^{-3}$. The position of the peak vs. C_{chl} for various water bodies are shown in figure 3. For all the considered water bodies the regression

$$\text{Peak position} = 683{\cdot}51 + (0{\cdot}268 \pm 0{\cdot}0075)C_{chl},\ \text{nm} \quad (2)$$

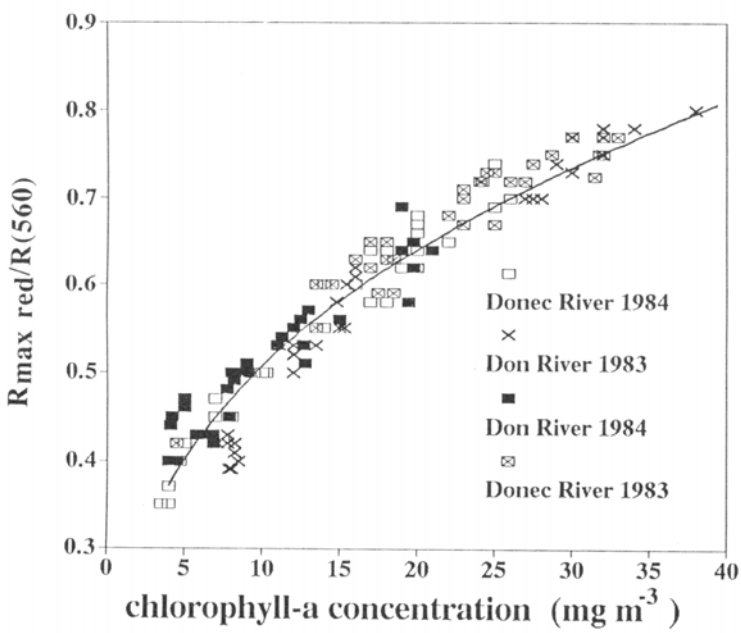

Figure 2. The peak height, normalized to value of global maximum of reflectance spectra at 560 nm, vs. chlorophyll-*a* concentration measured in various water bodies. The line presents equation (1).

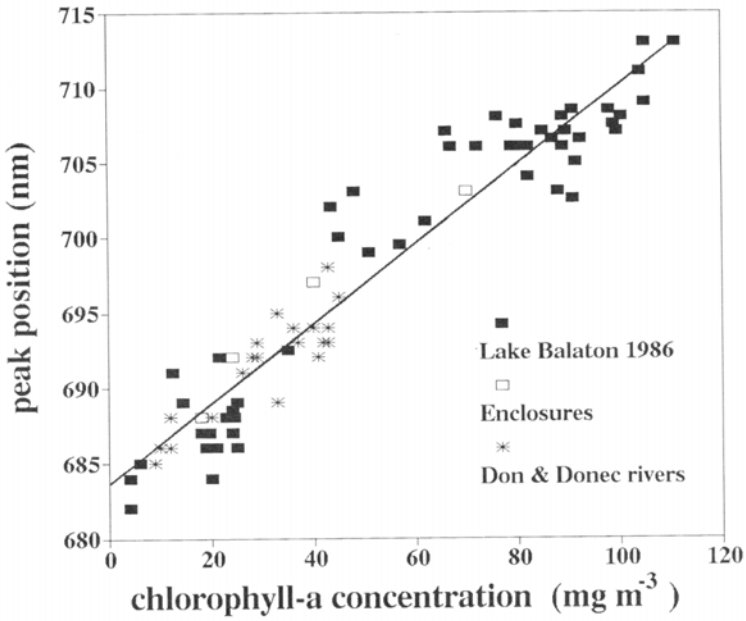

Figure 3. The relationships between the peak position and chlorophyll-*a* concentration measured in various water bodies. The line presents equation (2).

was found with R^2 higher than 0·93. It allowed the peak position to be assessed with a standard estimation error of less than 2·428 nm.

The measured values of the peak position were compared with various model calculations (figure 4). Experimental results of Vos *et al.* (1986) were also included for comparison. The measurements of Vos *et al.* 1986 (curve 4) and Vasilkov and Kopelevich's 1982 calculations (curve 2) both showed sharp shift in the peak position when chlorophyll concentration increased. The slopes of these relationships were three times more than the results of Kishino's (curve 1) and our calculations (curve 3) and measurements (curve 5). Calculation showed that the influence of phytoplankton fluorescence (for quantum efficiency less than 2·5 per cent) on the peak position for $C_{chl} > 30\,mgm^{-3}$ was negligible. The calculation of Kishino *et al.* 1986 (curve 1) was very close to our calculation (curve 3) and experimental results (curve 5). Parameters of the power function 'peak position $= a(C_{chl})^b$' were very near by: 'a' varied from 661·01 nm (present calculation) to 666·42 nm (Kishino *et al.* 1986), and it was 661·7 nm for our experiments. Parameter 'b' varied from 0·013 (Kishino *et al.* 1986) to 0.015 (present calculation) and it was 0·0145 for our measurements. It should be noted that the model calculations of Carder and Steward (1985) were quite close to our measured values.

The following conclusions can be drawn from this study:

(1) The magnitude of the peak near 700 nm in the radiance spectrum correlated strongly with the chlorophyll-*a* concentration. Peak height above the baseline and reflectance ratio $R_{maxred}/R(560)$ increased several times when C_{chl} increased and even reached a magnitude of the global maximum of the reflectance spectrum at 560 nm. Ratios $R_{maxred}/R(560)$ and $R_{maxred}/R(675)$

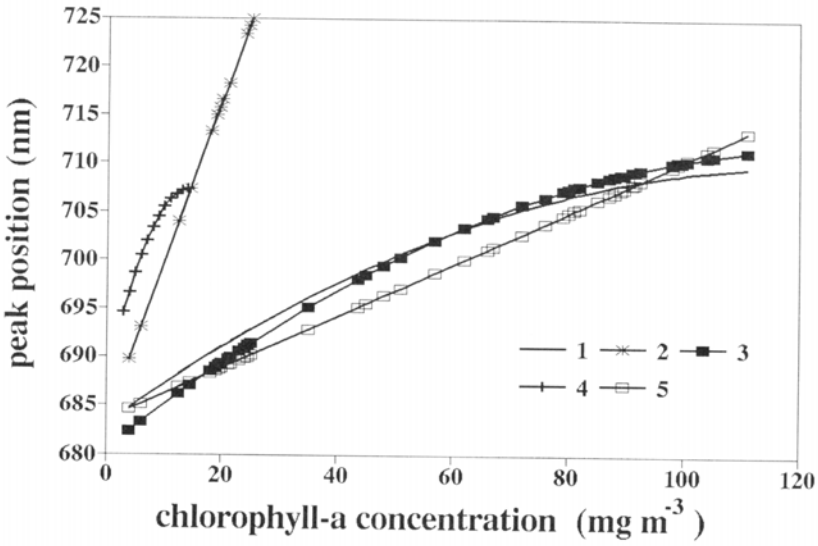

Figure 4. The relationship between the peak position and chlorophyll-*a* concentration. Comparison of the results of calculations and measurements. *Model calculations*: 1–Kishino *et al.* (1986) for quantum fluorescence efficiency 2·5 per cent; 2–Vasilkov and Kopelevich (1982); phytoplankton fluorescence was not taken into consideration; 3–present work for quantum fluorescence efficiency 2·5 per cent. *Measured values*: 4–Vos *et al.* (1986); 5, present work; the line presents equation (2).

can predict the chlorophyll concentration for water bodies of different trophic states and allowed the assessing C_{chl} value with estimation error of less than $3\,mgm^{-3}$.

(2) The position of the peak near 700 nm was very closely related to chlorophyll concentration. For all the water bodies studied linear regression for the relationship with square of correlation coefficient r^2 more than 0·9 and estimation error of less than 2 nm was obtained.

(3) The magnitude and the peak position could be used as precise indicators and predictors for the phytoplankton concentration. It contributed significantly to the increase in the accuracy of the derivation of chlorophyll values from multispectral data.

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