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Retrieval of Water Quality Parameters of Coastal Waters around Singapore from In-Situ Spectral Reflectance Data

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Abstract - A sea-truth water sampling campaign was carried out in the Johore Strait, Singapore from Dec 1996 to Dec 1998, Water leaving radiance and reflectance data were collected together with coincidental measurements of water quality parameters, including the total suspended solid (TSS) and the chlorophyl-a (Chl-a) loadings. Results of spectral analysis show that, it is possible to distinguish case II waters of different TSS and Chl-a loadings using the reflectance spectra. An algorithm for retrieving Chl-a and TSS from the in-situ reflectance spectra is tested. Attenuation coefficients of the case II waters are derived from reflectance.

INTRODUCTION

Optical remote sensing is increasingly being used for monitoring of water quality parameters in the ocean, coastal waters as well as inland lakes and rivers (Gordan and Wang 1994, Gould and Arnone 1998). In optical remote sensing of water, the spectral reflectance, i.e. the ratio of the upwelling to downwelling irradiances at the water surface, is the radiometric quantity most often used in characterising the optical properties of water. There are three main classes of optically active constituents of sea water: coloured dissolved organic matter (CDOM), phytoplanktons and non-chlorophyllous particulate matter suspended in water (Sathyendranath et al. 1989, Tassan 1994). Of these constituents, the phytoplankton concentration and its spatial distribution is of particular interst not only to the marine scientists, but also to those involved in the fishery industry. Several algorithms exist for detecting phytoplankton pigments from ocean colour (Tassan 1994, Doerffer and Fischer 1994, Sathyendranath et al. 1994)

In this work, spectral reflectance data acquired during a two-year sea-truth sampling programme in Singapore coastal waters (Lin et al. 1999) are analysed. The sea-truth water sampling campaign was carried out from Dec 1996 to Dec 1998. Reflectance spectra were acquired using a portable GER 1500 spectroradiometer. The water quality parameters measued were, among other things, the total suspended solid (TSS), chlorophyll-a (Chl-a), dissolved organic matter (DOM), total phosphate, total nitrogen and plankton cell count. Attenuation coefficients of water in the visible and near-infrared region (from 350 to 750 nm) are derived from the reflectance spectra. It is possible to differentiate coastal waters with different total suspended solid (TSS) and chlorophyll-a (Chl-a) loading from the reflectance spectra. An algorithm for retrieving water quality parameters from the spectral shape, based on the singular value decomposition technique is being tested.

REFLECTANCE SPECTRA OF CASE II WATERS

Typical reflectance spectra of the case II sea water samples around Singapore are shown in Fig. 1 for four combinations of TSS and Chl-a loading: low TSS, low Chl-a; low TSS, high Chl-a; high TSS, low Chl-a and high TSS, high Chl-a. The reflectance spectra have been normalised such that they have the same mean reflectance value, in order to compensate for the possible scaling error in the measurements of the spectra.. For the clear sea water samples (top left panel of fig. 1) of low TSS (< 10 mg/l), low chlorophyll (< 5 mg/m^3), and low phytoplankton counts (< 100 cells/l). It can be seen from the figure that there is only 1 peak at 560nm in the green region which is typical for case-II waters. When the TSS loading is increased while Chl-a remains low (bottom left panel of figure 1), the shape of the reflectance spectra is about the same, but there seems to be an increase in the reflectance at longer wavelengths in the red and near-infrared regions. For Chl-a loaded water samples (top right and bottom right panels of Fig. 1), the peak at 550 nm is narrower, and the absorption due to Chl-a at 667 nm results in a dip in the reflectance spectra.

RETRIEVAL OF WATER QUALITY PARAMETERS FROM SPECTRAL SHAPE

From Fig. 1, it is seen that the shapes of the reflectance spectra depend on TSS and Chl-a. We have tested a method based on the singular value decomposition (SVD) technique (Danaher and Omongain 1992) to retrieve TSS and Chla from the spectral shape. The measured spectra are first normalized such that each reflectance spectrum has a zero mean and unit variance. Suppose that $R(\lambda)$ is a normalized reflectance spectrum measured for a given water sample. For each water quality parameter i (i.e. TSS or Chl-a), we seek a key vector $K_i(\lambda)$ such that the dot product of $R(\lambda)$ with $K_i(\lambda)$ gives the value of the water quality parameter. Using a training set of spectra with know water quality parameter values, the key vectors for each parameter can be obtained using the SVD technique. If R is a matrix whose rows are the measured spectra, and P is a matrix whose elements are the water quality parameters

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Fig. 1: Representative reflectance spectra of coastal Case II sea water around Singapore. Top left: Low TSS (<10 mg/L) Low Chl-a (<3 µg/L); Top right: Low TSS High Chl-a (20 µg/L); Bottom left: High TSS (4050 mg/L) Low Chl-a; Bottom right: High TSS (50 mg/L) High Chl-a (40 µg/L)

corresponding to the measured spectra, then we seek a matrix ${\bf K}$ of the key vectors, such that

$$\mathbf{P} = \mathbf{R}\mathbf{K} \tag{1}$$

The matrix **K** can be found by inverting the matrix equation. In general, **R** is not a square matrix, its dimension being N_s (no. of spectra) by N_w (no. of wavelength channels in each spectrum). The SVD technique enables the matrix equation to be inverted while removing noise at the same time if only the first few significant singular values are retained.

After the key vectors have been determined, they can then be applied to each of the unknown spectra $R(\lambda)$ by forming the dot-product:

$$w_i = \sum_{\lambda} R(\lambda) K_i(\lambda)$$
⁽²⁾

The dot product w_i is then the estimate for the water parameter *i*.

Fig. 2 shows the results of retrieving TSS and Chla from measured reflectance spectra, using the SVD technique. In the left panel of Fig. 2, TSS values retrieved from in-situ reflectance spectra are plotted versus the values of the water quality parameters measured in the laboratory. The root-mean-square (RMS) error in this case is 12.5 mg/l. The

right panel of Fig. 2 shows the similar results for Chla retrieval. The RMS error is 4.9 µg/l.

DERIVATION OF SEA WATER ATTENUATION COEFFICIENT FROM SURFACE REFLECTANCE

Attenuation coefficients of sea water (for non-algal-bloom cases) were derived from the reflectance spectra using an algorithm similar to the one reported by Sydor et. al. (1998). In this algorithm, the reflectance of water is modeled by the equation (Sathyendranath and Platt 1997),

$$R(\lambda) = A \frac{b(\lambda)}{a(\lambda) + b(\lambda)}$$
(3)

where $a(\lambda)$ is the absorption coefficient of the sea water and $b(\lambda)$ is the scattering coefficient. The sum $c(\lambda) = a(\lambda) + b(\lambda)$ is the attenuation coefficient of the sea water. The parameter *A* in this equation is only weakly dependent on wavelength and can be regarded as a constant. The scattering coefficient is modeled by the power law relation (Mobley 1994)

$$b(\lambda) = B \left(\frac{\lambda_{ref}}{\lambda}\right)^{\alpha}$$
(4)

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Fig. 2: Results of retrieving water parameters from normalized reflectance spectra. Left panel: TSS; Right panel: Chl-a.

where λ_{ref} is a reference wavelength, taken to be 550 nm, *B* and α are two parameters to be determined. In the long wavelength limit $\langle \lambda > 700 \text{ nm} \rangle$, the attenuation coefficient is assumed to be due entirely to absorption by water. The product *AB* and the exponent α can then be determined by least square fitting of the observed reflectance spectra to the model relation (Eq. 3). The attenuation coefficient for the whole visible wavelength range can then be evaluated using the same model.

Fig. 3 shows the attenuation coefficients of case II water samples derived from the reflectance spectra shown in Fig. 1. For low TSS samples, the attenuation coefficient curves are close to that of pure water for wavelength above 600 nm, and increases in the short wavelength (about 0.5 m⁻¹ at 400 nm) due mainly to absorption by the dissolved organic matter present in the water. A peak at 667 nm for the low TSS but high Chl-a water sample can be observed, due to absorption by Chl-a. For high TSS samples, the attenuation at the short wavelength region increases further, due to the contribution from scattering by the suspended particulates. Influence from the particulate scattering component is evident up to wavelength of about 700 nm. The Chla absorption peak at 667 nm can clearly be seen. The results show that the influence of the TSS and Chl-a components on the attenuation spectra of c ase II waters derived from the reflectance spectra can be distinguished.

If the chlorophyll content of the sea water is not significant, then the attenuation coefficient $c(\lambda)$ of sea water can be expressed as the sum

$$c(\mathbf{l}) = c_w(\mathbf{l}) + c_1 \exp\left[-(\mathbf{l} - \mathbf{l}_1)/b\right] + c_2(\mathbf{l}_2/\mathbf{l})^a$$
(5)

where c_w is the attenuation coefficient of pure water (Hakvoort 1994), c_1 is the absorption coefficient of the coloured dissolved organic matter at λ_1 (usually taken as 400 nm), and c_2 is the scattering coefficient due to the suspended particles at λ_2 (usually taken as 550 nm). The parameter α is related to the size of the scattering particles in the water. In general, larger value of α is associated with smaller particle size. The derivation of attenuation spectrum $c(\lambda)$ from the reflectance spectrum can provide an estimate for α . Given α , the other parameters can be obtained by least-square fitting of $c(\lambda)$ to equation (5). From our results for Singapore waters, the parameter α usually ranges from 1.0 to 2.0, with a mean around 1.5. The parameter b for the coloured dissolved organic matter varies from 60 nm to 100 The parameters c_1 and c_2 should correlate nm. respectively with the coloured dissolved matter and suspended particle concentrations. The correlation is being studied. Once the correlation has been established, it can be used for retrieving the dissolved organic matter and suspended solid concentrations.

DISCUSSIONS AND CONCLUSIONS

This research studied the spectral characteristics of case II sea water. The reflectance spectra were collected during a 2-year sea-water sampling programme in coastal waters around Singapore. The attenuation coefficients of the sea water samples were derived from the reflectance spectra. Coastal waters with different TSS and Chla loadings could be distinguished from the attenuation spectra. The results indicate that it is possible to retrieve the water quality parameters from the reflectance spectra acquired above the water surface.

The spectral data used in this study were collected using a hand-held spectroradiometer, which measures light radiance in 512 wavelength bands continuously from 350 nm to 1050 nm. Currently, there is no satellite-borne sensors capable of acquiring this type of hyperspectral data. However, satellites with hyperspectral sensors will be launched in the near future (e.g. the Hyperion sensor on the planned NASA's EO-1 mission). The techniques developed here can be extended to the hyperspectral data acquired by satellite-borne sensors. An additional problem encountered in the utilization of hyperspectral data acquired by satellite

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Fig. 3: Attenuation coefficients of case II waters derived from the representative reflectance spectra shown in Figure 1. Top left: Low TSS (<10 mg/L) Low Chl-a (<3 µg/L); Top right: Low TSS High Chl-a (20 µg/L); Bottom left: High TSS (40 -50 mg/L) Low Chl-a; Bottom right: High TSS (50 mg/L) High Chl-a (40µg/L)</p>

borne sensors is the effects of atmosphere. Most of the currenly available atmospheric correction algorithms (e.g. Gordan and Wang 1994) for satellite ocean colour sensors make use of the near-infrared band to retrieve aerosol optical thickness. The assumption is that the ocean surface is dark in the near-infrared band. However, in the algorithm for derivation of water attenuation coefficient presented here, the near-infrared response is used to retrieve the water parameters. Hence, a new class of atmospheric correction algorithms that do not require the near-infrared bands to be dark will be required. This can be achieved, perhaps by considering a model that deals with the effects of both the atmosphere and water together.

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