

Water quality and optical properties of coastal waters from hyperspectral data

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Abstract— *Spectroradiometers are important tools used in the study of the optical properties of the ocean and in the validation of satellite ocean color sensors. In this paper, we present the technical characteristics of a field instrument and the methods for measuring spectral reflectance and beam attenuation coefficient. Then the inversion of a reflectance model, in terms of various relevant parameters, is exposed.*

I. INTRODUCTION

Satellite remote sensing represents the most suitable technique for synoptic monitoring of coastal zones. However a quantitative use of remotely sensed data is a difficult task and is still a challenge.

The radiometric signatures of coastal waters mainly depend on three optically active water components, namely yellow substance, phytoplankton pigments and sediment. These components are in highly variable proportions in space and time and induce a high variability of the marine water optical properties.

The number of parameters that can be determined by inversion of visible satellite imagery is limited. Consequently, for a given site, some of them or alternatively some inherent optical properties (IOP) must be known. When direct measurements are not feasible, hyperspectral data can be used for this purpose.

This paper describes a compact, portable optical equipment for in situ measurements. Then it addresses the inversion of high resolution reflectance spectra in terms of two parameters (sediment refractive index and yellow substance absorption coefficient) and three parameters (total suspended matter concentration, chlorophyll concentration and yellow substance absorption coefficient at 440 nm), which are of crucial importance for calibrating ocean color sensors in coastal areas.

II. OPTICAL MEASUREMENTS

The heart of the experimental apparatus is a spectroradiometer working in the visible, suitable for the measurements of reflectance and beam attenuation coefficient. These two optical properties are needed in radiative transfer theory as they depend on the medium.

A. The spectroradiometer

The PC1000 Ocean Optics spectroradiometer is a miniature photodiode array fiber optic spectroradiometer

mounted directly on an analogue to digital (A/D) card, installed into a personal computer. The design uses a ruled plane grating to diffract the incident light flux in the range 350-850 nm. An image of the spectrum is projected on a 1024-element photodiode array and is then transferred to the computer through the A/D card. The optical resolution, which depends on the groove density of the grating (600 lines/mm) and on the size of the entrance optics (200 μ m), is 10 nm. The sample frequency of the A/D converter data is adjusted for each experiment to maximize the detector output voltage and the S/N ratio. The detector controller is run by a clock to effectively set this value to the photodiode array detector. The operating software permits to set up the frequency (between 2 kHz and 500 kHz) and also the number of scans for signal averaging. The random noise is averaged in proportion to the square root of the number of scans averaged.

Remarkable features of the design include :

- small size (13cmx12cmx4cm). This allows the optical bench to be mounted directly onto the A/D card, for computer plug-in convenience.

- high light reception. All the light collected by the fiber is injected in the spectroradiometer, with a high luminosity : the spectrum is received in parallel by the whole detector.

- low stray light (< 0.1 %).

- possible connection of multiple spectroradiometer channels to the PC1000 via a harness cable to expand wavelength range, perform multiple tasks or make reference measurements.

- choice of spectral range and resolution. Each channel can be configured with one of 14 gratings options covering ultraviolet, visible and near infrared.

B. Reflectance measurements

The spectral irradiance reflectance, R , defined as the ratio of spectral upwelling, E_u , to downwelling, E_d , plane irradiances is an important parameter in the development of bio-optical algorithms. Experience has shown that the values of reflectance are largely determined by the IOP of the aquatic medium and are not much altered by changes in the incident radiation field (solar elevation for example). The advantage of finding R is also that it requires no absolute calibration.

The collector for irradiance measurements is a cosine corrector of opaline glass diffusing material with a SMA connector. This sensor is mounted on a perch, put at a few meters from the boat and placed in the azimuthal plane of the sun to avoid ship shadow effect. E_d and E_u are measured by pointing the perch respectively upwards (sensor horizontal) and downwards (sensor normal to the sea surface). Ideal environmental conditions are clear, uncloudy sky and smooth sea, without foam. The reflectance spectra are calculated by averaging ten spectra of E_d and ten spectra of E_u because of the great sensitivity of the sensor on its position and on environmental conditions (clouds, variations of sea surface).

C. Attenuation measurements

The attenuation coefficient only depends on the medium. Experimentally, transmission through liquid samples can be measured in a cuvette holder or via a transmission dip probe. These optical systems comprise a light source, focusing optics, lenses etc. and a detector measuring the loss of signal caused by the volume of water between the source and the detector. When compared to the transmission of pure water, the measurement is directly related to the beam attenuation coefficient c

$$c(\lambda) = \frac{1}{r} \ln \left(\frac{\phi_0(\lambda)}{\phi(\lambda)} \right) \quad (1)$$

where ϕ and ϕ_0 are the radiant flux in the beam for the sample and pure water respectively, r the beam path length and λ the wavelength of light.

The transmission probe system is composed of illumination and read fibers linked with a fiber splitter and a lensed probe with removable mirror tip. Light is transmitted through the fluid to the mirror and back to the read fiber (1 cm pathlength). The cuvette holder includes two collimators to focuss light through a 1 cm pathlength quartz cuvette.

III. FIELD MEASUREMENTS

The study area is the Ebro river plume area. The Ebro river, the main Spanish river flowing into the Mediterranean sea, is 928 km long. Its mean annual flow is only $385 \text{ m}^3\text{s}^{-1}$ as the result of the presence of many dams in the basin. The Ebro delta is located at $40^\circ 40' \text{N}$ and $0^\circ 40' \text{E}$. The tidal range along the coast of the delta is low, with values of about 20 cm (Ibañez et al. 1997). Experimental data were collected in November 1996, during a two-weeks field campaign called Fliper1, in the frame of MAST3 Program. They consist in chlorophyll concentrations, total suspended matter concentrations and reflectance spectra. A total of 29 coincident radiometric and water parameter measurements are available. Note that attenuation measurements were not carried out during Fliper1, so only inversion of a reflectance model is

done in the following.

IV. THE REFLECTANCE MODEL

Spectral light absorption and backscattering coefficients are the two IOPs directly ruling the diffuse reflectance R of the ocean (Gordon et al. 1975) :

$$R(\lambda) = F \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \quad (2)$$

where a and b_b are respectively the absorption and backscattering coefficients of the water body, and the dimensionless number F depends, in particular, on illumination conditions and water types. We take for F the commonly adopted value of 0.33 (Kirk 1994). This model is discussed in Forget et al.(1997)

A. Absorption coefficient

The total absorption coefficient, $a(\lambda)$, is the sum of the pure sea water absorption coefficient, $a_w(\lambda)$, the yellow substance absorption coefficient, $a_y(\lambda)$, and the phytoplankton absorption coefficient, $a_{ph}(\lambda)$. Absorption by sediment is neglected. Values of $a_w(\lambda)$ are taken from Smith and Baker (1981). $a_y(\lambda)$ is modelled by Bricaud et al.(1981) :

$$a_y(\lambda) = a_y(\lambda_0) \exp -S(\lambda - \lambda_0) \quad (3)$$

with wavelengths expressed in nanometers. λ_0 is a reference wavelength in the blue part of the spectrum. For a wide range of sea waters, S in the surface layer has been found to vary from about 0.010 to 0.020 nm^{-1} , with a mean value in the region of $0.012\text{-}0.015 \text{ nm}^{-1}$ (Kirk 1994). We take the commonly adopted values $S = 0.014 \text{ nm}^{-1}$ and $\lambda_0 = 440 \text{ nm}$. $a_{ph}(\lambda)$ is calculated from the common relation :

$$a_{ph}(\lambda) = a_{ph}^*(\lambda)chl \quad (4)$$

where chl is the chlorophyll concentration (chlorophyll a + divinylchlorophyll a) and $a_{ph}^*(\lambda)$ is the phytoplankton specific absorption coefficient, parametrized by the power function (Bricaud et al. 1995) :

$$a_{ph}^*(\lambda) = A(\lambda)chl^{-B(\lambda)} \quad (5)$$

where A and B are positive, wavelength-dependent parameters.

B. Backscattering coefficient

Backscattering of light comes from molecular backscattering (water molecules) and particular backscattering (sediment particles and phytoplankton), the total backscattering coefficient, b_b , is expressed by :

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bs}(\lambda) + b_{bph}(\lambda) \quad (6)$$

It can be assumed that the amount of light diffused by sea water in the forward and backward directions is the same

(Morel 1974). Then $b_{bw}(\lambda)$ is equal to one-half the total scattering coefficient of water, whose values are taken from Smith and Baker (1981). Light scattering by suspended particles in the sea is described by Mie theory (Van de Hulst 1957), which permits to calculate $b_{bs}(\lambda)$. Ocean waters can be treated as a very dilute suspension of random scatterers, and consequently the intensity of light scattered by an ensemble of particles is given by the sum of the intensities due to the individual particles. For a collection of particles with size distribution $n(D)$ ($n(D)dD$ is the number of particles per unit volume with diameters between D and $D+dD$) and refractive index relative to water m_r , b_{bs} can be written as :

$$b_{bs}(\lambda) = \int_{m_r} \int_D Q_{bb}(D, m_r, \lambda) \frac{\pi D^2}{4} n(D) dD dm_r \quad (7)$$

Q_{bb} is the backscattering efficiency. The particle size distribution is modelled by a Junge law of slope -4 , $n(D) = kD^{-4}$ which approximates well both biological and mineral distributions (Bader 1970, Nanu and Robertson 1993). Considering spherical particles, we find the following expression for the mass concentration C of sediment

$$C = \int_{D_{min}}^{D_{max}} n(D) \rho_s \pi \frac{D^3}{6} dD \quad (8)$$

where ρ_s is the sediment density. From the Junge law and equation (8), we obtain :

$$k = \frac{6C}{\pi \rho_s \ln \left(\frac{D_{min}}{D_{max}} \right)} \quad (9)$$

From (7) and (9), b_{bs} is finally expressed by :

$$b_{bs}(\lambda) = \frac{3C}{2\rho_s \ln \left(\frac{D_{min}}{D_{max}} \right)} \int_{D_{min}}^{D_{max}} Q_{bb}(D, m_r, \lambda) D^{-2} dD \quad (10)$$

b_{bph} is calculated from the chlorophyll concentration chl and a mean value of the chlorophyll specific backscattering coefficient (b_{bph}^*), measured for 9 species of phytoplankton (Ahn et al. 1992) :

$$b_{bph}(\lambda) = b_{bph}^*(\lambda) chl \quad (11)$$

V. INVERSION OF THE MODEL

The reflectance model depends on the following parameters : $a_y(440)$, m_r , chl , C , D_{min} and D_{max} . The method of inversion presented here consists in assimilating experimental reflectance spectra in a model. Forget et al.(1997) discussed the inversion of $a_y(440)$ and m_r from reflectance spectra of non-chlorophyllous turbid coastal waters. The study area was the Rhône river

mouth area during a flood event. The optical properties of the waters were then essentially influenced by nonchlorophyllous matter : mineral particles, particulate and dissolved organic matter of terrigenous origins. A simple two-components, namely yellow substance and total suspended matter, reflectance model was developed. The optical effect of phytoplankton is taken into account in the present study of the Ebro river mouth area, making our reflectance model now suitable for a broad variety of coastal waters. The inversion procedure is first applied to the determination of two unknown parameters of the model and then to the retrieval of water quality parameters together with an IOP.

A. Determination of m_r and $a_y(440)$

To estimate the values of $a_y(440)$ and m_r from experimental reflectance spectra, the other model parameters are fixed. Here C and chl are known. Considering that most of backscattering is due to particles smaller than $1\mu m$ and that the choice of the upper limit is not critical, we have chosen a realistic particle size range (D_{min}, D_{max})= $0.1-100\mu m$ (Mobley 1994). The procedure consists in minimizing the quadratic difference between experimental reflectance data, $R_{exp}(\lambda)$, and modelled reflectance data, $R_{th}(\lambda)$, calculated by varying the values of $a_y(440)$ and m_r :

$$G(a_y(440), m_r) = \sum_{\lambda} [R_{th}(\lambda) - R_{exp}(\lambda)]^2 \quad (12)$$

In practice, the minimisation of G is done by varying m_r from 1.05 to 1.45 by step of 0.01 and $a_y(440)$ from 0 to $2m^{-1}$ by step of $0.01m^{-1}$. 5 stations, among the 29 sampled, are arbitrary chosen to represent the variety of the reflectance spectra in shapes and amplitudes. In Table 1, measured and inverted parameters are presented for 5 stations, denoted from A to E in the following, together with the values G_{min} of the minimum of G .

Table 1 : Values of $a_y(440)$ and m_r minimizing G

	A	B	C	D	E
C ($mg.l^{-1}$)	0.31	0.76	1.28	1.48	1.74
chl ($\mu g.l^{-1}$)	0.38	0.64	1.40	1.36	1.44
m_r	1.14	1.13	1.14	1.15	1.16
$a_y(440)$ (m^{-1})	0.05	0.06	0.08	0.10	0.11
G_{min}	0.9	0.6	0.6	0.5	0.8

Measured and computed (using optimized values of $a_y(440)$ and m_r) reflectance spectra have similar shapes (Fig.1). For the five simulations, G is less than 1 and has only one minimum. In other cases, in particular when G is greater than 1, there can be multiple solutions but the inverted parameters are found varying with small intervals. Typical values of m_r are 1.05 for phytoplankton

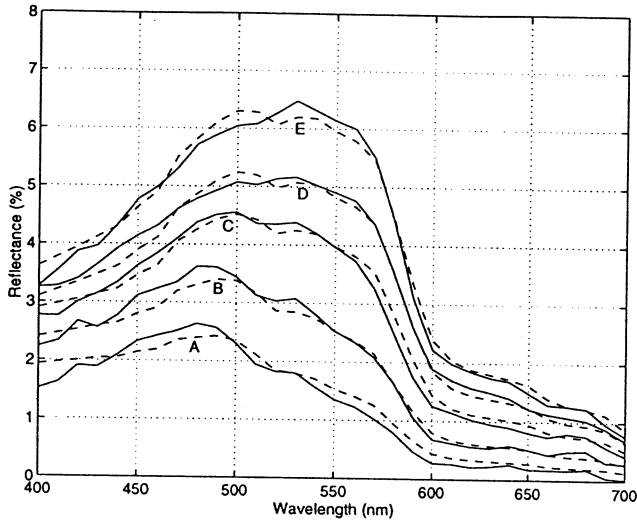


Fig.1 : $R_{exp}(\lambda)$ (full lines) and $R_{th}(\lambda)$ (dashed lines)

and 1.16 for inorganic particles (Mobley 1994). Reported values $a_y(440)$ in the Mediterranean sea are from 0 to $0.03 m^{-1}$ in oceanic waters and from 0.06 to $0.64 m^{-1}$ in coastal waters (Kirk 1994). So the inverted values are realistic.

B. Determination of C , chl and $a_y(440)$

In this part, the inversion procedure is extended to the determination of the 3 parameters, C , chl and $a_y(440)$, which are important water quality parameters. The input parameters are m_r , D_{min} and D_{max} . We keep the range of diameters $(D_{min}, D_{max}) = (0.1, 100) \mu m$. The values of m_r are obtained from a statistical analysis of the optical properties of our water samples, detailed in Lahet et al. (1998). Examination of the collection of reflectance spectra acquired during the field campaign exhibits characteristic shapes corresponding to various water colors : brownish Br, intermediate Br-G, green G, green-blue G-BI and blue-green BI-G. Each class can be characterized by a typical value of m_r (Table 2). It can be noticed that m_r decreases from sediment-dominated waters (Br, Br-G) to phytoplankton-dominated waters (G, G-BI, BI-G).

Table 2 : Classification of Ebro river waters.

Color	Br	Br-G	G	G-BI	BI-G
m_r	1.18	1.16	1.16	1.14	1.12

The results of inversion obtained at stations A-E are given in Table 3. The corresponding measured and computed reflectance spectra are shown in Fig.2.

The uncertainty of the measured values of C is $\pm 0.05 mg.l^{-1}$ for $C < 1 mg.l^{-1}$ and $\pm 0.1 mg.l^{-1}$ for $C > 1 mg.l^{-1}$. The experimental and computed values of C are seen in good agreement. For stations A, C and E, experimental values are perfectly retrieved and for the other two, the difference is only $0.1 mg.l^{-1}$ corresponding to

errors of 12% (B) and 7% (D). The retrieval of chl is far from being satisfactory. It is explained by the very low sensitivity of the model to this parameter. Nevertheless the inverted values are quite realistic.

This study also shows that the restitution of concentrations is more especially performant as the water is more turbid.

Table 3 : Values of inverted C , chl and $a_y(440)$. In italic : values measured at sea

	A	B	C	D	E
m_r	1.12	1.12	1.14	1.16	1.16
C ($mg.l^{-1}$)	0.4	0.9	1.2	1.3	1.8
	<i>0.31</i>	<i>0.76</i>	<i>1.3</i>	<i>1.5</i>	<i>1.7</i>
chl ($\mu g.l^{-1}$)	0.1	0.5	0.8	1.5	1.1
	<i>0.38</i>	<i>0.64</i>	<i>1.40</i>	<i>1.36</i>	<i>1.44</i>
$a_y(440)$ (m^{-1})	0.06	0.06	0.08	0.08	0.12
G_{min}	0.3	0.3	0.3	0.3	0.7

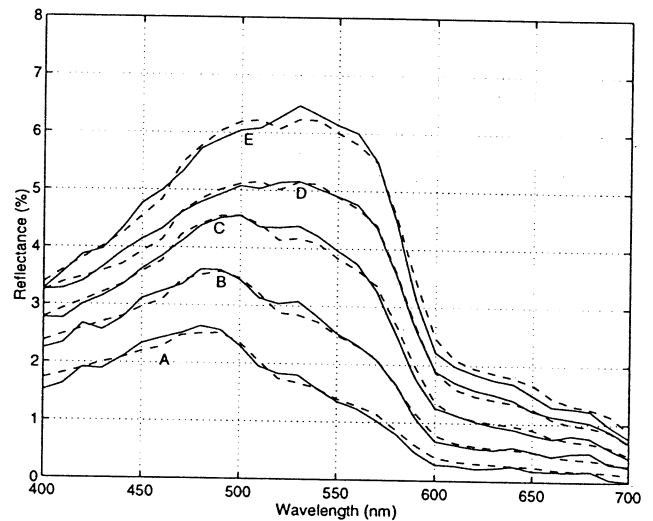


Fig.2 : $R_{exp}(\lambda)$ (full lines) and $R_{th}(\lambda)$ (dashed lines)

C. Discussion

Comparison of Fig.1 and Fig.2 exhibits that the procedure of inversion gives better results to estimate water quality parameters rather than optical parameters. Other couples of parameters than $a_y(440)$ and m_r such as C and $a_y(440)$, C and chl , $a_y(440)$ and s , $a_y(440)$ and chl , m_r and chl , chl and s can be deduced. The reflectance model is the most sensitive to variations of $a_y(440)$, m_r and C but, as m_r and C have similar spectral effects, they cannot be inverted at the same time (Forget et al. 1997). The inversion method could also be applied to obtain other triplets than C , chl and $a_y(440)$ such as m_r , $a_y(440)$ and chl . In fact the combination of parameters to be considered depends on the experimental data available.

C , chl and $a_y(440)$ can be easily measured with appropriate instruments, whereas m_r cannot be measured directly. This quantity is very sensitive to environmental conditions, mainly to the particulate matter, and to a lesser extent, to pressure, temperature and salinity. We propose in this paper a statistical approach to deal with this parameter, consisting in a classification of water types, each class being characterized by a typical value of m_r . This value is derived from the reflectance spectra corresponding to the class. For this, C and chl must be known. This strategy requires intensive in situ measurements over a given site and during a given period. In situ sizing of particles is a difficult task for instrumental reasons. It is only recently that information on sub-micrometer particles became available. A simple hyperbolic size distribution can fail to represent oceanic conditions, e.g. during the growth phase of a phytoplankton bloom, but it seems relevant to describe coastal particulate matter in the optically active size range 0.1-100 μ m (Stramski and Kiefer 1991).

V. CONCLUSION

A miniature spectroradiometer, described in this paper, was used to measure reflectance spectra of coastal waters. The fiber optic system provides flexibility for measurements at sea and delivers quality spectra. A reflectance model for coastal waters, including sediment, chlorophyll and yellow substance, is presented to estimate two parameters, m_r and $a_y(440)$, from experimental reflectance spectra. We show that the inverted values are realistic compared to those reported in literature. Extension of the method to the inversion of the three parameters C , chl and $a_y(440)$ gives encouraging results especially for the retrieval of total suspended matter concentration. Suspended matter strongly influences water quality, e.g. suspended particles can play a positive role in fertilizing coastal waters and a negative role by transporting pollutants. The low sensitivity of the model to chlorophyll concentration implies a poor accuracy in the determination of this parameter. We think that much work is needed for improving the inversion procedure. This can be done in particular by taking into account the vertical profiles of concentration (Ouillon and Forget 1998). Furthermore the success of inversion of the model in terms of C and chl demonstrates the suitability of using optical measurements to estimate important water quality parameters.

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