Water spectral libraries for the interpretation of image spectrometric data

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ABSTRACT

This paper reports the assessment of water reflectance spectra measured under controlled condition for analysis of the imaging spectrometry data of inland waters. The application of imaging spectrometry to the study of inland waters depends on a better understanding of the optical properties of the water components. To increase this understanding, a collection of water spectra has been measured under laboratory and ground controlle conditions as a part of an EOS interdisciplinary investigation. The radiometric measurement derived from those experiments is known as the Bidirectional Reflectance Function (BRDF). R was simulated using variations of a model derived from the two stream approximation of the radiative transfer equation (RTE) and compared to the BRDF. BRDF was also measured "in situ" from a boat based spectrometer (BoaR) and from an helicopter based spectrometer (HelR). Modelled R (MolR), laboratory measured BRDF (LabR) and ground measured BRDF (BoaR and HelR) were compared. They were also used to unmix the spectra of two different aquatic systems. Preliminary results show that at low chlorophyll and gilvin concentration, there is a good agreement between ModR and LabR, regardless of the model variation used. For both low and high inorganic matter concentration, the agreement between ModR and LabR is poor. All sets of data present the main features which characterize the high chlorophyll concentration reflectance spectra, but the amount of reflectance displayed by LabR and ModR is 50 times smaller than that measured in situ. When the different sets are used as input to unmixing algorithms they also yield different results.

1.INTRODUCTION

Results of a project carried out in tropical inland waters¹ since 1989 showed that there were statistically significant correlations between the concentration of optically active components and TM/Landsat reflectance in only 30 % and 45 % of the winter and summer data sets, respectively. The significant correlations occurred between suspended inorganic matter (SIM) and various reflectances and reflectance ratios in 60 % of the winter data set and 80 % of the summer data set. Total chlorophyll (CHL) occurring in concentrations between 4 mg/m³ and 20 mg/m³, could not be consistently related to TM reflectance or reflectance ratios. The high concentrations of dissolved organic matter (DOM) and high concentrations of SIM (between 5 mg/l and 26 mg/l) make it difficult to unmix the CHL signal out of the reflectance measured by broad band sensors.

Use of image spectrometric data for the remote sensing of water environments improve the discrimintion among the water constituents ². Application of image spectrometric data to water environments is ,at present, more complex than to the terrestrial environment ³ because of 1- the low reflectances (in the range of 2 % to 7%); 2- the lack of narrow absorption bands related to the presence of similarly-shaped or overlapping absorption spectra of the various components occurring simultaneously within the water

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column; 3- the uncertainty of atmospheric correction in the spectral region with information concerning water components. Additional factors in tropical environments are the high complexity of inland tropical waters and the lack of information about their spectral behavior.

As most of the research in imaging spectrometry ², water studies are focused on coupling spectroradiometric data with in-situ data for development of spectral unmixing algorithms. The problems of testing them to decompose the water spectra are: 1- there are no water spectral libraries such as those organized over the last decades for mineral and plants; 2- there is not a clear concept of what a pure endemenber to unmix the water spectra really is.

Laboratory derived spectra were used as input to an unmixing algorithm 4 to determine the suspended sediment concentration(SSC). The unmixed spectra estimated SSC with an error of + /- 13 mg/l for the range of concentrations from 0 to 200 mg/l. The model was applied to unmix TM/Landsat data collected over the Amazon river. As the SSC in the Amazon river has a large amount of SIM correlated in 90 % of the cases with TM reflectance, it is hard to judge from these results how much this approach can be extended to the unmixing of other water components with more subtle spectral features. The application of the same pair of endmembers to the Bay of Fundy, however, overestimated the SSC. The reason for that was the high concentration of suspended organic matter (SOM) in relation to the SIM present in the samples.

Attempts of retrieving chlorophyll concentrations using a library of absorption and backscattering coefficients as input to a model based in the two-stream approximation to the Radiative Transfer Equation (RTE) yielded an overestimation of 33 % in the chlorophyll concentration in the Monterey Bay ⁵. Changes of 5% in R at 450 nm cause up to 10 % change in the predicted chlorophyll.

The weaknesses of these modelling approach are: 1- the need of accurate measurements of the inherent optical properties; 2- assumption of constant thickness of the upper layer; 3- assumption of flat water surface (no winds) and uniform sky; 4 - assumption of scattering albedo (ω_0) smaller than 1⁶; 5- assumption that the Beer's law applies to scattering mediums. In spite of these problems, various versions of those models have been applied to the study of water masses ^{8,9,10,11}.

The simulation of water masses in laboratory is another method for building water spectral libraries. In spite of the problems of simulating the water light field under laboratory conditions¹², during the last decade several attempts were made to measure the effect of SIM ¹³ and DOM ¹⁰ concentrations on the shape and magnitude of the water spectral reflectance. The effect of sediment color ¹⁴ and size distribution ¹⁵ on the water spectra was also measured in laboratory. With the availability of more sensitive spectroradiometer, the effect of different species of phytoplankton suspensions on the water reflectance has been measured in laboratory^{16,17,18}.

Another method of building spectral libraries is to perform *in situ* measurements of the spectral reflectance. Measuring *in situ* water reflectance is very complex, since there is a number of factors affecting the measurements such as wind speed, sky conditions, Sun angle, ship motion and ship shadow. Several methods have been proposed to overcome those factors ¹⁹. The most common measurement reported in the literature is the Bidirectional Reflectance Function (BDRF). Those measurements consist of the ratio between the water radiance and the radiance of a BaSO4 standard. Those measurements are made from

boats ^{20,21,22} and from helicopter ^{23,24}. In some experiments, polarization filters are used to remove the surface reflectance ^{20,22}. The measurements are made with the sensor at 45° from the nadir to avoid ship shadow and to increase the sampled area, and looking into plane perpendicular to the Sun ^{20,22,25}. The problems involving this method are: 1- impossibility of measuring "unique component" spectrum; 2- impossibility of keeping the water optical thickness constant.

Table 1 illustrates the problem of identifying pure endmember on the ground. In this case the only possible definition of "pure endmember spectrum" is the spectrum with the "highest concentration of a given optically active component", since in each station there are variable amounts of each endmember

Table 1 - Water components and optical conditions at 11 limnological stations located in the UHE Tucurui Reservoir (Brazil) in April, 1992 (Source: Steffen et al., 1992). Kdpar is the average downwelling diffuse attenuation coefficient of the euphotic zone for the photosynthetically active radiation in 1/m, CHL is the chlorophyll a and phaeopigment concentration in mg/m³. Fe is the iron concentration and represents the fraction of the inorganic matter in the TSS in mg/l; TSS is the total suspended solids (organic and inorganic) in mg/l, and G440 represents the absorption of the dissolved organic matter at 440 nm in 1/m.

Station	Kdpar	CHIL	Fe	TSS	G440
1	1.80	2.86	0.73	6.00	1.55
2	1.44	2.98	0.73	5.60	1.94
3	1.10	4.28	0.63	3.60	1.42
4	0.48	4.28	0.22	1.20	0.69
5	0.48	4.64	0.23	1.60	0.38
6	0.50	3.93	0.24	1.50	0.65
7	0.55	4.17	0.34	2.20	0.43
8	0.48	3.57	0.40	1,40	0.99
9	0.57	3.93	0.42	1.10	0.94
0	0.62	2.74	0.53	1.30	1.20
.1	0.72	1.79	0.83	1.10	1.89

In this paper the spectra derived from these different methods are compared. The linear correlation coefficient is used to express the shape agreement between them. The root mean squared difference (RMS) is used to quantify the average absolute difference in the amount of reflectance yielded by the different methods. Sets of those different spectra were then tested to unmix ground reflectance spectra measured in Tucurui, a tropical aquatic system, and to unmix the reflectance spectra derived from the September 30, 1991 AVIRIS data from Mono Lake (CA).

2. METHOD

2.1 - BDRF spectra from laboratory simulations of water masses

BDRF measurements(LabR) of water masses were measured in laboratory ¹⁷ A culture of a blue-green algae was grown in laboratory and controlled amounts of it transferred to a constant water volume to produce the desired CHL concentration. SIM simulation was obtained by adding known amounts of caulinite to the water tank. Commercially available humic matter was used to produce DOM. The actual concentration of each component was checked by taking water samples for laboratory determinations. DOM concentration was expressed as the absorption coefficient at 440 nm (g440). The setup for the radiometric measurement was not a precise duplication of the natural environment (no skylight illumination) ²⁵. A comprehensive description of the experiment and the background for the experimental procedures are found elsewhere ¹⁷.

2.2 Modelling of R as a function of the water optical properties.

Three models based on the two-stream approximation to the radiative transfer equation were examined as potentially useful to derive the Irradiance Ratio (R) from the inherent optical properties. Those models are based on the following assumptions: 1- the water body is infinitely deep; 2- the water surface is flat; 3- the inherent optical propertied of the body are known. Two out of three assumptions are met by the laboratory simulation, since the tank was coated with black paint, and the measurements were performed with a flat water surface. The inherent optical properties of the water, however ,were not measured. To overcome this problem, available data in the literature were used. In some cases, numerical models were also used to derive those optical properties.

The first version of the model ²⁶ is suitable for water masses characterized by absorption coefficients larger than the scattering coefficient and expressed by equation (1):

$$b_{b}(\lambda)$$

$$R(\lambda) = 0.33 \quad ------ \qquad (1)$$

$$a(\lambda)$$

where R(2) is the irradiance ratio, $b_b(\lambda)$ is the backscattering coefficient and $a(\lambda)$ is the absorption coefficient. A second version of the two- stream model is expressed by the equation (2) and is suitable for water with high backscattering coefficient ²⁶.

$$R(l) = 0.33 \qquad (2)$$
$$a(\lambda) + b(\lambda)$$

A third model ²⁷ was tested, but the results were similar to (2). The analyses were limited to the two models. A complete discussion about those simplified models ²⁸ and the assessment of the complete solution of the radiative transfer models can be found in the literature ²⁹. $R(\lambda)$ just bellow the surface was converted to the $R(\lambda)$ just above the surface ³⁰ to become comparable to the BDRF.

To model R (ModR) the following assumptions were made: 1- the pure ocean water absorption coefficient 32 is an accurate measure of pure fresh water absorption; 2- the pure freshwater backscattering can be expressed as 70 % of the clearest ocean water scattering coefficient to compensate for the lower salinity 7; 3 - the chlorophyll specific absorption coefficient 33 is a good approximation of the species used in laboratory simulations; 4 - the dissolved organic matter spectral absorption can be estimated from measurements at 440 nm^{34;} 5 - the chlorophyll backscattering coefficient can be numerically modelled 7: 5 - the inorganic particle backscattering can be approximated by linear interpolation of values found in the literature 27 .

2.3 - BDRF from ground measurements

Two sets of BDRF were measured at the Barra Bonita reservoir (Brazil). One set was obtained from a boat (BoaR), with the sensor at a viewing angle of 45° off nadir. A polarizer was attached to the optical system to reduce the Fresnel reflectance ²⁰. Another set of BDRF was measured from an helicopter (HelR) using a data collection system developed by Laboratory Radiometry at the National Institute for Space Research (Brazil). Among the capabilities of this system are: 1- compensation for tilting of the spectroradiometer related to the instability of the helicopter; 2- simultaneous acquisition of 35 mm photographies. The helicopter was flown at nominal altitude of 70 m. Measurements of radiance from a calibrated BaSO4 panel were recorded by a ground based radiometer at three ground bases located at a maximum distance of 5 km from the water sample stations ²⁴.

2.4 - Data Analyses

In order to compare the four set of data, laboratory simulated BDRF (LabR), the modelled irradiance ratio R(ModR), the boat measurement (BoaR) and the helicopter measurements (HelR) were resampled to the spectral response of the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) ³ in the range of 400 nm to 850 nm.

The LabR and the ModR were compared using: 1- the correlation coefficient to express the shape agreement between the sets of spectra; 2- the root mean squared (RMS) to express the absolute differences between LabR and ModR. The remaining set of data were compared only by using the RMS statistic ³¹.

These different data sets were tested as input to spectral unmixing models currently used for the interpretation of image spectrometric data ². A linear unmixing algorithm ⁴ was applied to spectral data from two different aquatic environments: the Tucurui reservoir, tropical aquatic system where the three optically active component are simultaneously present in the water and the Mono Lake, an eutrophic system where the main optically active component is the phytoplankton CHL.

3. RESULTS

The results (Table 2) show that the LabR and the ModR do not agree either in shape or in the absolute values of reflectance. For the high scattering component (SIM) LabR and ModR presented no shape agreement at high concentrations, and a RMS difference of 13 % in the reflectance. The fact that the shape agreement was larger for the lower concentrations, suggests that the main problem of ModR is the set of input data to derive the reflectance. At low concentrations, the water spectra are dominated by the optical

properties of the pure water which are well known ⁷ but when the component concentration increases and the water spectrum starts to be modulated by the component optical properties, the available models and published data fail to reproduce them. On the other hand, the lack of complete agreement even at small concentrations makes one to suspect that LabR also might not be a good simulation of the water spectra.

LabR and ModR were compared to BoaR and HelR (Table 3). The ground measurements, however, were limited to high concentration of CHL. The differences between those sets of measurements are larger than those found between LabR and ModR. Those differences in the absolute reflectance are expected since changes in wind velocity and direction can introduce changes in the Fresnel reflectance. LabR and ModR (Figure 1) are in average 50 times smaller then BoaR and HelR. The shape of the spectra is also different, but they present some common features such as: 1- the minimum reflectance in the blue; 2 - the maximum reflectance in the green; 3 - the chlorophyll fluorescence peak diagnostic of high chlorophyll concentration.

Both sets of ground reflectance are very similar in shape, but they present differences in the amount of reflectance in the green and red regions which can be related to the optical conditions during the radiometric data acquisition. Although the CHL concentration is in the same range (40 mg/m3), the SIM when BoaR was measured was 3 times higher than that found when the HelR was carried out. It can explain the higher reflectance of BoaR in the green, red and near-infrared, where the impact of inorganic matter is easily sensed 10,15,30.

The different sets of reflectance data were used in an unmixing algorithm to decompose the reflectance spectra measured at the Tucurui reservoir and to decompose the September 30, 1991 AVIRIS derived reflectance measured at Mono Lake ³⁶. The fractions of each "selected pure endmember" present in the spectra of the various sample stations were then correlated to the concentration of the water component represented by each selected endmember. The results can be observed in table 4. Each set of endmembers yields completely different correlations between the fraction of the pure CHIL reference spectrum explaining the sampled spectra (FRCHIL) and the actual concentration of CHIL in the limnological stations where those spectra were measured.

At the Tucurui reservoir the only significant correlation between CHL and FRCHL was obtained when "in situ" spectra were used as "pure reference spectra or endmembers". The CHL could not be "unmixed" when LabR and ModR were used as reference spectra to represent the three optically active component present in the water (CHL, SIM, DOM). The correlation between the CHL and the FRCHL however was inverse ! As measured CHL increased, the fraction of the measured spectrum explained by the pure CHL reference spectra decreased ! The reasons for that are: 1- the in situ spectrum used as CHL pure reference was not a pure CHL spectrum as seen in table 1 (station 5); 2- there is an inverse correlation between CHL and DOM in the reservoir; as the DOM increases, the CHL decreases; as DOM affects the water spectrum almost in the same region as CHL, the presence of both components in the water, covarying inversely produces the inverse correlation between the fraction of CHL responding for the spectra and the concentration. As the CHL concentration decreases, the DOM increases adding its effect upon the absorption of light in the blue region. The net effect of both components is to increase the fraction of the pure CHL reference spectra explaining the spectrum of the various sample stations, as CHL decreases.

Water	RI		R2	
Component	r	RMS	r	RMS
0.74 mg/m3 of CHL	0.66	0.37	0.66	0.34
47.79 mg/m3 of CHIL	0.63	0.14	0.63	0.14
1.0 mg/l of SIM	0.75	3.31	0.75	0.31
20.0 mg/l of SIM	0.50	13.30	0.50	13.30
DOM (g440 = 4/m)	0.64	0.18	0.64	0.18
DOM (g440 = 9.4/m)	0.26	0.17	0.26	0.17

Table 2 - Statistical Results for LabR and ModR R1 and R2 refers to the use of equation 1 and 2 to model the water reflectance.

Table 3 - RMS for pair of reflectance measurements. The subscript 1 refers to the high CHL concentration (40 mg/m3), and the subscript 2 to the low CHL concentration (9.0 mg/m 3).

Reflectance Set	RMS
HelR ₁ / BoaR ₁	0.57
HelR ₂ /BoaR ₂	2.36
HelR ₁ /ModR ₁	1.63
HelR ₁ /LabR ₁	1.13
BoaR ₁ /LabR ₁	1.18
$BoaR_1/ModR_1$	2.60
LabR ₁ /ModR ₁	0.16

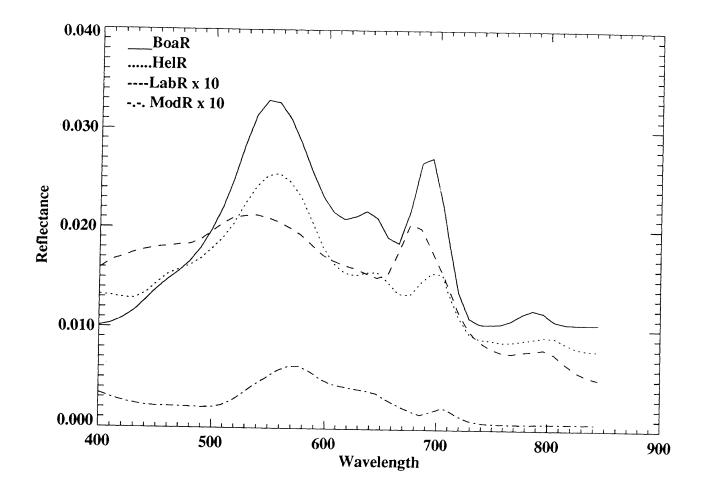


Figure 1 - Spectral Reflectance of 40 mg/l Chlorophyll concentration derived from boat measurements (BoaR), helicopter based measurements (HelR), laboratory simulation (LabR) and modelling as a function of inherent optical properties (ModR).

Table 4 - Correlation Coefficient between the fraction of the "pure CHL endmember spectrum" (FRCHL) in a given spectrum and the CHL concentration at the station where the spectrum was measured, when different pure reference endmember are used.

Data Set	Correlation between CHL and FRCHL		
	Tucurui	Mono Lake	
 LabR	-0.21	0.49	
 ModR	0.24	0.76	
 BoaR	-0.73		

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The same unmixing algorithm was applied to the spectra derived from the September 30, 1991 AVIRIS flight over Mono Lake. In this case, the only significant correlation between CHL and FRCHL was found when LabR was used as an endmember. At Mono Lake, however, the correlation between CHL and FRCHL was positive: as measured CHL increased, the fraction of the measured spectrum explained by the pure CHL reference spectra increased, which is the expected result. The reasons for these different results are: 1- the set of pure endmembers used to unmix the Mono lake spectra, which were: Low CHL, High CHL and Low SIM; 2 - at Mono Lake, CHL was the main optical component in the water, with no significant DOM. This made the LabR a reasonable description of the CHL.

From those preliminary results, one can observe that the method of producing the library of reference spectra to be used in unmixing algorithms affects the interpretation of the fractional spectra derived at each sample site. It a fractional image of the CHL component had been produced for the Tucurui reservoir using the "in situ pure endmembers", the highest fractions would be interpreted as the lowest CHL concentration. If the same image could be derived for the Mono Lake data, using LabR as endmembers, the interpretation would be different. The aquatic environment is too complex, and the unmixing capability of a given "set of endmembers" is not a function only of the presence or absence of a given water component, but also is a function of its concentration and its covariance with the remaining components. Before a final method can be defined as suitable for general application, much more data, from a broader range of environments must be obtained and analyzed to get better understanding of the interaction between the various water optical components in the various environments and between them and the light field.

The availability of numerical models for computing the underwater light fields opens a new era of research, since those models are not limited to the simple assumptions of those derived from the two-stream approximation to the RTE. But before those numerical models can be used to generate spectral libraries the inherent optical properties of the inland waters must be extensively measured simultaneously to the BRF.

4.CONCLUSIONS

The results of this study shows that laboratory simulations of pure endmembers should be improved at least in two aspects: 1- a better simulation of the downward irradiance accounting for both, the diffuse (skylight) and the direct light field; 2 - a better simulation of the underwater light field using larger container for the water: 3 - a better characterization of the simulated water masses including measurements of the some inherent optical properties.

The results also show that the simplified models based on the two-stream approximation can not be used for predictive purposes, but they are useful as an exploratory tool. To predict the reflectance as a function of the inherent optical properties, the numerical models with the complete solution of the RTE should be used. Before those models can be used, however, the inherent optical properties of inland waters must be measured for a large set of environmental conditions. The numerical models and the measurements available in the literature do not apply to the tropical inland waters. The results also suggest that the question of which is the best method of building a spectral library can not be answered at this moment.

High spectral resolution data are extremely important to the study of tropical inland waters. So there is an urgent need for high spectral and spatial resolution spaceborne systems.

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