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MODELIZATION OF LEAF OPTICAL PROPERTIES FOR INTERPRETING HIGH SPECTRAL RESOLUTION REFLECTANCE MEASUREMENTS

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ABSTRACT : A general radiative transfer model, representing the leaf optical properties from 400 to 2500 nm, is presented. It is based on the generalized "plate model" proposed by ALLEN : it provides a leaf structure parameter N. A spectrum of refractive index for leaf material is given in the 400 – 2500 range. The second part of the work consists in introducing pigment and water absorption in order to determine extinction coefficients of leaf components. This model has been fitted on experimental data corresponding to a wide range of leaf types and states. Il gives a good representation of the whole reflectance spectra with only three parameters.

KEYWORDS : High Spectral Resolution, Leaf anatomy, Reflectance, Transmittance, Absorption, Refractive Index, Model

1) INTRODUCTION

The understanding of plant canopies reflectance is necessary for an efficient use of remote sensing in agriculture. The physiological and physical processes which control spectral reflectance of vegetation are studied since many years. Recently, investigations using high spectral resolution measurements were developped and have induced improvements in interpreting the spectral information obtained on plant canopies. However the interpretation is actually limited by the need of detailed information on leaf optical properties.

Leaves represent the area where light interacts with matter and gives back a signal which depends on the characteristics of these area. The modelization of leaf optical properties represent the first step of the simulation study engaged about the understanding of the determinism of spectral deformations which can be recorded using high spectral resolution instruments. Simulated reflectance and transmittance spectra can be introduced into vegetation reflectance model to compute reflectance spectra at the scale of the canopy. This paper is a contribution to the improvement of our knowledge about leaf optical properties and it's modelization.

The incident radiation upon the leaf surface can be reflected, transmitted or absorbed. The absorption is essentially function of changes in the spin and angular momentum of electrons, transitions between orbital states of electrons in particular atoms (visible : chlorophylls a and b, carotenoïds, brown pigments and other accessory pigments) and vibrational – rotational modes within the polyatomic molecules (near infrared and middle infrared : water) (HODANOVA, 1985). There are also scattering phenomena (Rayleigh and Raman scattering). The diffuse character of reflectance is due to leaf internal structure which is the only factor determining the leaf optical properties in the near infrared (GRANT, 1987).

GAUSMAN et al. (1970) found a good relationship between the reflectance level and the number of air spaces in the leaf. Diffusion is due to air – cell wall interfaces : the light passes often from a high refractive index ($n \approx 1.4$ for hydrated cell wall, $n \approx 1.33$ for water at 1 µm) to a lower value ($n = 1.0$ for the air). Monocotyledonous leaves which have a compact mesophyll reflect little NIR radiation (≈ 40%). Dicotyledonous leaves reflect more than the previous ones because they present a spongy mesophyll with air cavities. For this reason the number of reflections on air – cell wall interfaces and the changes in the direction of light beams increase and the resulting effect is an increase of the reflection (≈ 50%). If leaves are infiltrated for example with oil ($n \approx 1.48$), the reflectance value decreases 15 % (WOOLEY, 1971 ; GAUSMAN et al., 1974).

In order to get a more accurate and exhaustive description of leaf optical properties, the development of physical models appeared rapidly as a necessity.

ALLEN et al. (1969) explain the diffuse reflectance and transmittance of a typical compact plant leaf by the means of the plate model specified by two optical constants : an effective index of refraction n and an effective coefficient of absorption k. This model applies only to a compact leaf. ALLEN et al. (1970) and GAUSMAN et al. (1970) later extend the model for N layers. They introduce the concept of Void Area Index (VAI) given by $VAI = N - 1$. They show that a monocotyledonous leaf has a VAI equal to zero and can be considered as a unic compact plate. At the opposite, for dicotyledones, it increases from zero to a maximum value, characteristic of the species, during the leaf development.

The generalized "plate model" is a discrete approach of the problem. An equivalent continuous theory has been used to explain the propagation of diffuse light in a leaf. In 1968, ALLEN and RICHARDSON published a model of leaf reflectance and transmittance based on the theory of KUBELKA and MUNK (1931) which described the transfer radiation in diffuse scattering media with two parameters : the scattering and the absorption coefficients. BARET et al. (1988) have simplified this model and have successfully applied it to single wheat leaves. More recently YAMADA and FUJIMURA (1988) have proposed a mathematical model which applies for different leaves : they consider four inhomogeneous layers (two cuticles, a palisade parenchyma, a spongy mesophyll) described by the KUBELKA – MUNK theory. In the same way,TUCKER and GARRAT (1977) have represented the interactions between and within the leaf compartments by using a Markov chain approach. But to solve this problem, it is necessary to have a very good description of the leaf internal structure and many other input variables.

The advantage of radiative transfer models is that they need only a limited number of input parameters. Other theories have been developped to describe the optical properties of leaves. ALLEN et al. (1973) proposed a ray tracing method. But this way requires a long computation time.

All of these works are adapted to specific conditions and restricted to a limited number of kinds of plants. Relatively little work has been done which tries to generalize the results obtained on particular plant species. If the leaf absorption coefficient is often given in the litterature, we rarely see the associated in vivo extinction coefficients which are obtained from pigments concentration or water content.

The aim of this paper is to present a general model describing leaf optical properties from 400 to 2500 nm using a minimum number of parameters in order to facilitate its inversion. The model presented is a generalized "plate model" where the leaf is assumed to be a pile of N homogeneous elementary plates. We will try to provide a refractive index n, a structure parameter N and extinction coefficients spectra.

2) MATERIALS AND METHODS

Theoretically, a plant leaf presents two kinds of tissues:

- an epidermis which contains a few chloroplasts
- a mesophyll which is a chlorophyllian parenchyma

According to the plant species, the internal structure is different : monocotyledones present a compact mesophyll with few intercellular spaces; dicotyledones have a palisade parenchyma with one or more layers of elongated cells on the adaxial (upper) face and a spongy parenchyma with intercellular spaces on the abaxial face (dorsiventral parenchyma). Some dicotyledones which have a palisade parenchyma on both side of the blade are called isolateral leaves.

In order to have a large range of variation (structure, pigmentation, water content), we have chosen different plant species with leaves corresponding to different states : maize (*Zea mays*), wheat (*Triticum aestivum*, PRINQUAL), tomato (*Lycopersicon esculentum*, EARLYMECH), soybean (*Glycine max*, VERDON), sunflower (*Helianthus annuus*, MIRASOL) have been cultivated in a greenhouse. Oak, maple and succulent plants leaves were also collected outdor.

We have also used etiolated seedlings (grown in the dark) which contained carotenoids but no chlorophylls, albino seedlings produced by treating seeds with fluridone (a strong herbicide) which contained no coloured pigments (MAAS and DUNLAP, 1989).

All of the plants are brought immediately to the laboratory after being collected and several measurements are performed on each leaf : weight, thickness, water content, specific leaf area, pigments concentration. We determine chlorophyll a, chlorophyll b and total carotenoids according to the methodology defined by LICHTENTHALER (1987). For brown pigments appearing during senescence, it does not exist any method for determining their concentration. For this reason we have proposed to use a brown pigments index based on spectrophotometric measurements (JACQUEMOUD, 1988). Directionnal–hemispherical reflectance and transmittance of the adaxial faces are measured with a Varian Cary 17 DI spectrophotometer equiped with an integrating sphere coated with $BaSO_4$ paint. The accuracy of the measurements is about 1%. The spectral bandwidth varies from 1 nm in the visible to 2 nm in the infrared. Spectra are sampled over the 400–800 nm wavelength interval with 4 nm steps and from 800 to 2500 nm with 17 nm steps. Data are corrected for the reflectance of a $BaSO_4$ reference and the geometry of the sphere.

3) THEORY

The plate model developped by ALLEN et al. (1969) gives a good representation of the optical properties of a compact plant leaf. It provides a refractive index n and an absoption coefficient k. A compact leaf is considered as a transparent plate with rough plane parallel surfaces. In the most general case, we shall assume that the radiant flux Io of the spectrophotometer is not exactly normal to the leaf surface but is inscribed in a solid angle Ω. This assumption takes into account the roughness of the leaf surface by adjusting the solid angle Ω to an optimal value. The light emerging from the spectrophotometer is normal to the leaf blade. Nevertheless, at microscopic scale, due to the ondulating shape of the surface (GRANT, 1987), the incoming beam penetrates the leaf with incident directions which can be included into a solid angle Ω. Inside the leaf, the flux is assumed to be diffuse and isotropic. The general formula of reflectance ρ and transmittance τ can be written in the form (JACQUEMOUD, 1989) :

$$\rho = [1-t_{av}(\alpha,n)] + \frac{t_{av}(90,n)t_{av}(\alpha,n)\theta^2[n^2-t_{av}(90,n)]}{n^4-\theta^2[n^2-t_{av}(90,n)]^2} \quad [1]$$

$$\tau = \frac{t_{av}(90,n)t_{av}(\alpha,n)\theta^2 n^2}{n^4-\theta^2[n^2-t_{av}(90,n)]^2} \quad [2]$$

where n = refractive index
θ = transmission coefficient of the plate
$t_{av}(\alpha,n)$ = average transmissivity of a plane dielectric surface for incident light (α = incidence angle)

The form of $t_{av}(\alpha,n)$ is rather complex but it can be exactly calculated (ALLEN, 1973). Fig.(1) shows the variation of $t_{av}(\alpha,n)$ for different values of n and α (α is the incidence angle and also the half value of the solid angle). We can notice that the average transmissivity is pratically equal to the normal incidence value for a large angular range ($\approx 60°$) but this effect decreases when the refractive index increases.

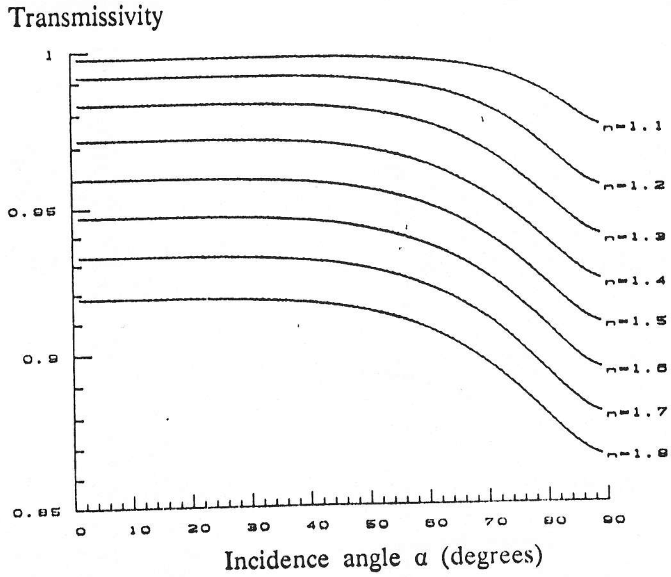

Fig.1 Average transmissivity as a function of the refractive index n and the incidence angle α

The "plate model" can be described by three parameters : a refractive index n, an incidence α and a transmission coefficient θ. Unfortunately, dicotyledonous and senescent leaves cannot be described as a unic compact layer and this model doesn't works in this case.

The generalization of the "plate model" which consists in stacking elementary layers is a physical problem studied for many years (STOKES, 1862). A leaf is assumed to be composed of a pile of N homogeneous layers separated by $N-1$ air spaces. The discrete approach can be extended to a continuous one where N needs not to be an integer. If $R_1=\rho$ and $T_1=\tau$ are the respective reflectance and transmittance of an elementary compact layer, the total reflectance and transmittance for N layers are given by the following equations :

$$R_N = \rho + \frac{\tau^2 R_{N-1}}{1-\rho R_{N-1}} = R_{N-1} + \frac{\rho T_{N-1}^2}{1-\rho R_{N-1}} \quad [3] \quad \text{and} \quad T_N = \frac{\tau T_{N-1}}{1-\rho R_{N-1}} \quad [4]$$

The solution of the Eqs. [3] and [4] was given by STOKES (1862) :

$$\frac{R_N}{b^N-b^{-N}} = \frac{T_N}{a-a^{-1}} = \frac{1}{ab^N-a^{-1}b^{-N}} \quad [5]$$

where $a=(1+\rho^2-\tau^2+\sqrt{\delta})/2\rho$
$b=(1-\rho^2+\tau^2+\sqrt{\delta})/2\tau$
$\delta=(\tau^2-\rho^2-1)^2+4\rho^2$

The starting values ρ and τ can be the reflectance and the transmittance of a single compact leaf at a given wavelength ($\rho\approx40\%$ and $\tau\approx60\%$). Fig.(2) shows that R_N rapidly increases and can be equal to T_N for a value of N which can be calculated. For infinite values of N, Eq. [5] leads to $R_\infty=a^{-1}$ and $T_\infty=0$. The absorption $A_\infty=1-R_\infty-T_\infty$ tends towards the constant value $1-a^{-1}$.

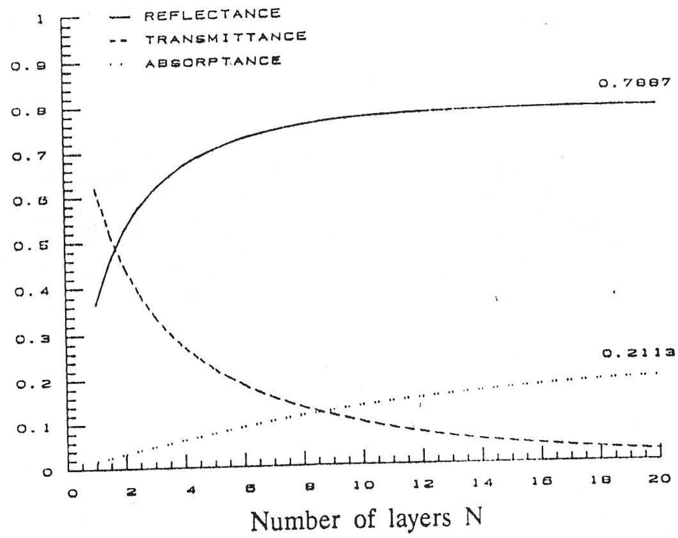

Fig.2 Variations of total reflectance R_N, transmittance T_N and absorptance A_N when the number of elementary layers increases

4) RESULTS

We shall first study the mesophyll structure effect which is particularly important when there is no absorbing materials in the leaf. This will allow us to determine a refraction index, a characteristic of the surface roughness α and a structure parameter N for each leaf. In a second step, we shall study the absorption processes and try to determine extinction coefficients for water and pigments.

4 – 1) Determination of a refraction index

In order to determine the parameters characteristic of leaf mesophyll structure, it is necessary to know the reflectance and transmittance of an ideal compact plant leaf without the effect of water and pigments. We have chosen an albino maize leaf in the 400 – 800 nm region and a dry (16 hours at 80°) maize leaf in the 800 to 2500 nm region. The albino leaf shows extrema of reflectance and transmittance and will be considered as the reference compact layer. The dry maize leaf is not compact but we have adjusted at 796 nm (wavelength of the albino maize leaf minimum absorption) the equivalent number N of elementary layers which have the closest reflectance and transmittance values to the albinos one. Then, we have inverted the STOKES model to calculate the equivalent reflectance ρ and transmittance τ of a single layer over the 800 – 2500 nm wavelength intervall. For the inversion, we have used the procedure proposed by ALLEN et al (1970).

On the homogeneous elementary layer (reflectance ρ_e, transmittance τ_e), we can apply the "plate model". This model provides a refractive index n and a transmission coefficient θ if the incidence angle α of the incident light is known (solid angle Ω). ALLEN et al. (1969) considered an isotropic incident light : that means $\alpha=90°$ for Eqs. [1] and [2]. The problem is that, for refractive index values of the litterature (GAUSMAN et al, 1974), we cannot define the transmission coefficient θ. However, the transmission of the plate can be obtained from Eq. [1] in the form [6] :

$$\theta^2 = \frac{n^4[\bar{\rho}-1+t_{av}(\alpha,n)]}{t_{av}(90,n)t_{av}(\alpha,n)[n^2-t_{av}(90,n)]+[n^2-t_{av}(\alpha,n)]^2[\rho-1+t_{av}(\alpha,n)]}$$

For the lowest experimental values of reflectance in the strong absorptions domains, the numerator of Eq. [6] is negative. That means that the average reflectivity $r_{av}(\alpha,n)=1-t_{av}(\alpha,n)$ is higher than the leaf reflectance . It follows that equation [6] has no solutions. We have adjusted α for the lowest value of reflectance and found $\alpha=59°$. So the real incidence angle is not 0°(normal incidence) nor 90° (isotropic light) but depends on the geometry of the reflecting surface. In order to adjust the α value, we have considered the reflectance of a real leaf and not of an equivalent compact layer. This hypothesis has been justified a posteriori because the inversion of the STOKES model has little effect on very low values of reflectance.

Equations [1] and [2] are used to evaluate the refractive index n if α, ρ_e and τ_e are known. If we eliminate θ from Eqs. [1] and [2], we obtain the relation :

$$[\tau_e^2-[\rho_e-1+tav(59,n)]^2].[n^2-tav(90,n)] - tav(90,n)tav(59,n)[\rho_e-1+tav(59,n)] = 0 \quad [7]$$

Equation [7] is solved by numerical methods. The adjusted refractive index of mesophyll interface material is close to 1.4 and regularly decreases from 400 to 2500 nm (Fig.3) as the refractive index of water (PALMER and WILLIAMS, 1974). These experimental values are in very good agreement with the litterature (GAUSMAN et al., 1974).

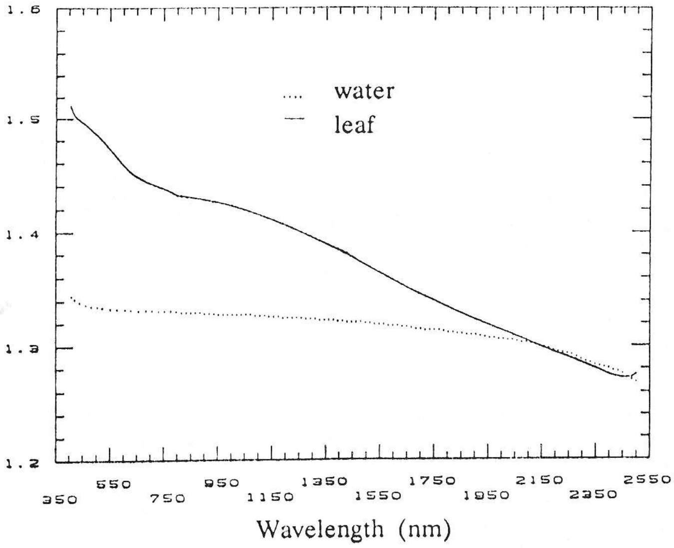

Fig.3 Refractive indexes of an ideal leaf and of water (PALMER and WILLIAMS, 1974)

The transmission coefficient θ has been assimilated, with a good accuracy, to a straight line :

$$\theta = 1{,}011.10^{-5}\,\lambda + 0{,}977 \quad \text{where } \lambda \in [460\text{nm}-2177\text{nm}]$$

These values will be supposed constant for all leaves.

4 – 2) Characterization of leaf structure

We can now adjust the structure parameter N for each leaf at the minimum absorptance wavelength. The adjustement of the N variable can be made by minimizing $(R-R_N)^2+(T-T_N)^2$ where R and T are experimental data, R_N and T_N are theoretical data. This means that :

$$\frac{d[(R-R_N)^2+(T-T_N)^2]}{dN} = 0 \quad [8]$$

As it was anticipated, we find N = 1.0 for the albino maize leaf. More generally, $N \in [1,1.5]$ for leaves with a compact mesophyll, $N \in [1.5,2]$ for dicotyledones and finally $N > 2$ for brown and senescent leaves. The parameter N gives a good representation of the different leaves studied (Fig.4).

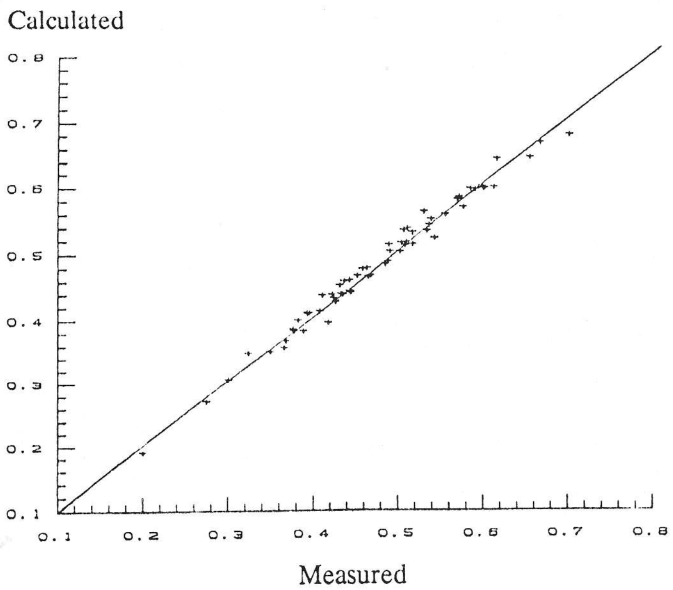

Fig.4 Comparison between reflectance and transmittance data simulated (Eq.5) and measured (64 data)

This parameter is well correlated with the Specific Leaf Area (SLA : leaf blade area per unit blade dry weight). Assuming that the cell walls have a constant weight per unit area, we can see that an increasing of the SLA corresponds to a decreasing of the number of cell−wall interfaces inside the leaf and then a decreasing of intercellular spaces. In consequence, the reflectance will be lower, the transmittance higher and N will decrease. We have observed an hyperbolic relationship between the SLA and N (Fig.5). The knowledge of specific leaf area is of importance : plant physiologists (RAWSON et al., 1987) have shown that it might be correlated with the CO_2 exchange rate per unit area (CER). Furthermore, it is the key parameter which transforms leaf biomass production into leaf area in most of the growth models.

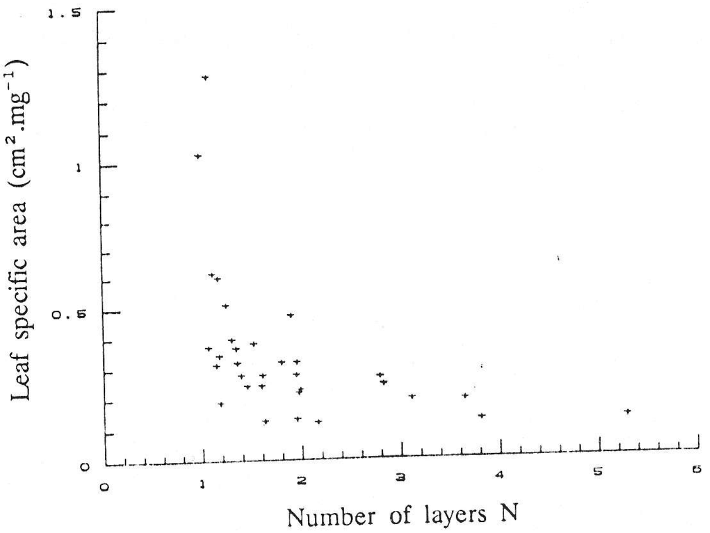

Fig.5 Relationship between number of layers and leaf specific area

As we have determined the structure parameter N, we can invert the STOKES model using measured reflectance and transmittance values, and calculate the equivalent reflectance and transmittance of the corresponding compact layer.

This will allow us to estimate the intrinsic absorption characteristics of leaf components.

4 – 3) Absorption characteristics

On this elementary layer, the "plate model" can apply. With Eq. [6] we can calculate the transmission coefficient θ which is related to the absorption coefficient k through the following equation (ALLEN et al., 1969) :

$$\theta-(1-k)e^{-k}-k^2\int_k^{\infty} x^{-1}e^{-x} \, dx = 0 \quad [5]$$

This approach represents the necessary first step before introducing pigment and water absorption.

We have to separate water (middle infrared) and pigments effects (visible). If we consider the absorption spectrum of the compact elementary layer, we can notice that absorption is not equal to zero particularly under 450 nm where the absorption values k_o correspond to the albino maize leaf. That means that other biological compounds are potential light receptors. Optical activities of some of these photoreceptors may protect the leaf from light damage when approaching the ultraviolet. We have also substracted these values from the absoption spectra of all of the leaves.

If we assume that absorption of leaves in the spectral range 1 – 2.5 µm is caused principally by pure liquid water, we can write that $k=K_w.C_w+k_o$

where k = absorption coefficient
k_o = absorption coefficient of the elementary plate
K_w = water extinction coefficient ($cm^2.g^{-1}$)
C_w = water weight per unit area ($g.cm^{-2}$)

The slope of the linear regression between k and C_w with a fixed intercept k_o gives the values of K_w whose spectrum (Fig.6a) is in good agreement with the fundamental constants for pure liquid water (PALMER and WILLIAMS, 1974).

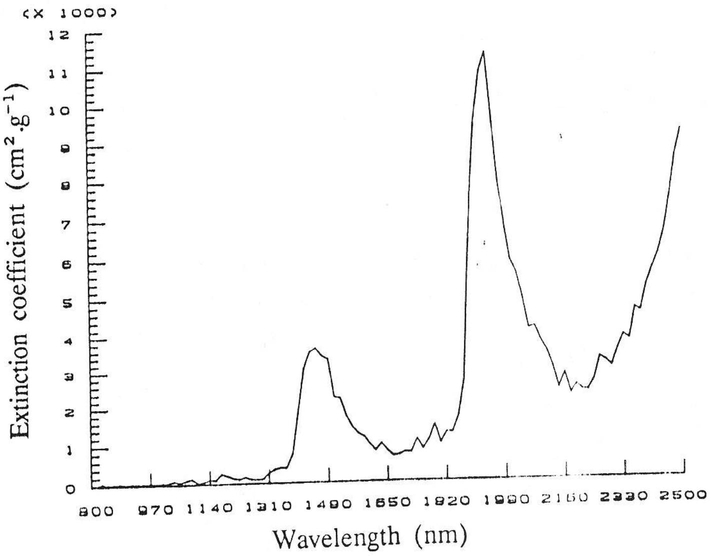

Fig.6.a Extinction coefficient spectrum of water in near and middle infrared

In the visible part, absorption is due to pigments as chlorophyll a, b, carotenoïds and brown pigments that appear during senescence. Because of the strong correlation between the concentrations of the different pigments, we cannot separate them. We have defined C_{abc} as the concentration of chlorophyll a, b, and carotenoïds, C_{br} as a brown pigments index. The resolution of the multiple linear equation $k=K_{abc}.C_{abc}+K_{br}.C_{br}+k_o$ provides a spectrum with well known absorption peaks for carotenoïds and chlorophylls (Fig.6b).

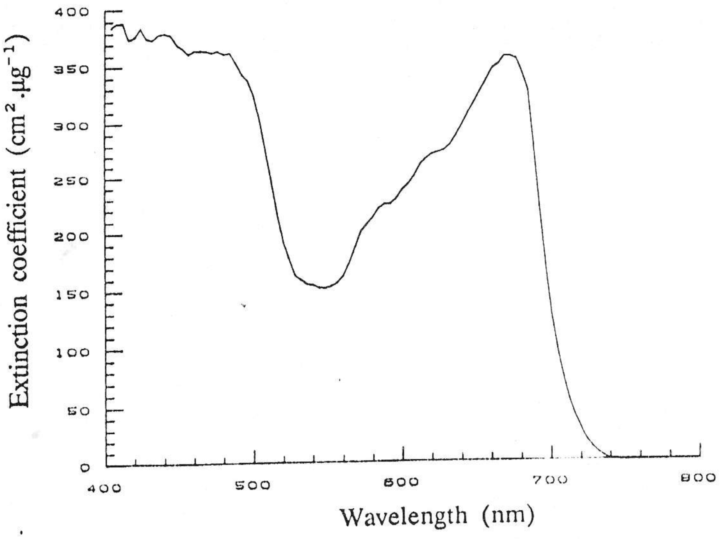

Fig.6.b Extinction coefficient spectrum of photosynthetically pigments (Chlorophyll a, chlorophyll b, carotenoïds) in visible

For brown pigments, the values regularly decrease from 400 to 1000 nm. We can notice that these pigments absorb a part of the light in the NIR region (Fig.6c).

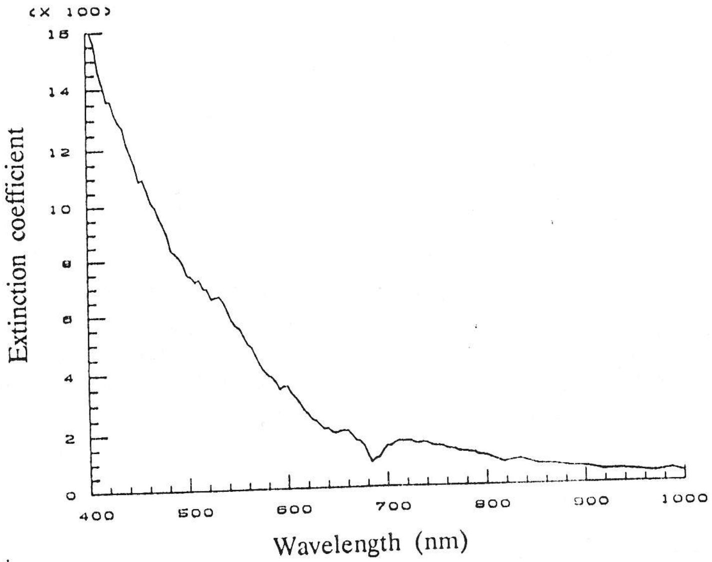

Fig.6.c Extinction coefficient spectrum of brown pigments in visible and near infrared

The difficulty in separating the photosynthetically pigments in the multiple regressions seems to be due to carotenoïds. When we measure the carotenoïds content, we may forget other accessory pigments (lutein, neoxanthin...) whose quantitative analysis is at present not accurate enough. The direct spectrophotometric measurement of this kind of pigment gives the value of total carotenoïds with a large experimental error (SESTAK Z., 1985).

CONCLUSION

We have presented a general radiative transfer model of reflectance and transmittance of a plant leaf as a function of two parameters : a structure parameter N and a concentration (pigment concentration or water content). It will be later interesting to simulate spectra of leaves and evaluate their sensitivity to these parameters. The advantage of this model is the restricted number of parameters. But some points limit its application : for example we assume a uniform distribution of water and pigments and structure inside the leaf. Further more, the high correlation between the different pigments prevent us from separating the extinction coefficients. Finally, we suppose that the angle α which represents the surface roughness is constant but, in fact, it is not the case.

When imaging spectroscopy is used for crop characterization, it increases the information content, but the way to use it is not precisely known. Reflectance and transmittance values provided by this model of leaf optical properties will give input values for canopy reflectance models. They will contribute to improve our understanding of high spectral resolution data for an efficient use.

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