REMOTE SENS. ENVIRON. 34:75–91 (1990)

PROSPECT: A Model of Leaf Optical Properties Spectra

S. Jacquemoud and F. Baret
INRA, Station de Bioclimatologie, Montfavet, France

PROSPECT is a radiative transfer model based on Allen's generalized "plate model" that represents the optical properties of plant leaves from 400 nm to 2500 nm. Scattering is described by a spectral refractive index (n) and a parameter characterizing the leaf mesophyll structure (N). Absorption is modeled using pigment concentration (C_{a+b}), water content (C_w), and the corresponding specific spectral absorption coefficients (K_{a+b} and K_w). The parameters n, K_{a+b}, and K_w have been fitted using experimental data corresponding to a wide range of plant types and status. PROSPECT has been tested successfully on independent data sets. Its inversion allows one to reconstruct, with reasonable accuracy, leaf reflectance, and transmittance features in the 400–2500 nm range by adjusting the three input variables N, C_{a+b}, and C_w.

INTRODUCTION

The optical properties of a plant canopy largely depend on the optical properties of leaves and soil background. Recent investigations using high spectral resolution measurements (Vane and Goetz, 1988) have shown that the interpretation of the spectral information obtained on plant canopies from remote sensing techniques is limited by the need of detailed information on leaf optical properties.

The interaction of electromagnetic radiation with plant leaves (reflection, transmission, absorption) depends on the chemical and physical characteristics of these leaves. The absorption is essentially a 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, carotenoids, brown pigments, and other accessory pigments) and vibrational-rotational modes within the polyatomic molecules (near infrared and middle infrared: water) (Hodanova, 1985). The refractive index discontinuities within the leaf ($n \approx 1.4$ for hydrated cell walls, $n \approx 1.33$ for water at 1 μm, and $n = 1$ for air) induce scattering (Woolley, 1971; Gausman et al., 1974). Therefore, the internal structure of the leaf controls the reflectance and the transmittance on the whole spectrum, but this appears more clearly where the absorption is low, especially in the near infrared domain.

In order to get a more accurate and exhaustive description of leaf optical properties, the development of physical models rapidly appeared as a necessity. Allen et al. (1969) explained the diffuse reflectance and transmittance of a typical compact plant leaf by the means of the "plate model"

Address correspondence to S. Jacquemoud, INRA, Station de Bioclimatologie, BP 91, 84143 Montfavet Cedex, France.
Received 21 June 1990; revised 6 September 1990.

0034-4257/90/$3.50

655 Avenue of the Americas, New York, NY 10010

specified by two optical constants: an effective index of refraction (n) and an effective coefficient of absorption (k). This model only applied to a compact leaf. Allen et al. (1970) and Gausman et al. (1970) later extended this model for N layers. They described the leaf internal structure with the void area index (VAI) parameter given by $\mathrm{VAI} = N - 1$. They showed that a monocotyledonous leaf had a VAI equal to zero and could be considered as a unique compact plate. In contrast, for dicotyledons, it increased from zero to a maximum value depending on the species and on the leaf development. This generalized "plate model" is a discrete approach to the problem. An equivalent continuous theory has been used to explain the propagation of diffuse light within a leaf. Allen and Richardson (1968) published a model of leaf reflectance and transmittance based on the Kubelka–Munk theory, which described the radiation transfer in diffuse scattering media with two parameters: the scattering and the absorption coefficients. Baret et al. (1988) simplified this model and successfully applied it to wheat leaves. More recently, Yamada and Fujimura (1988) have improved the K–M model: They considered four inhomogeneous layers (two cuticles, a palisade parenchyma, and a spongy mesophyll) each described by the K–M theory. These authors tested their model on different leaves. In the same way, Tucker and Garrat (1977) and Tucker (1980) represented the interactions between and within the leaf compartments by using a Markov chain approach. However, to solve this problem, it is necessary to have a very good description of the leaf internal structure and many other input variables. Other theories have been developed to describe the optical properties of leaves. Allen et al. (1973) and Brakke and Smith (1987) proposed a ray tracing method where the leaf was regarded as a two-dimensional optical system. Meanwhile, this technique requires a lot of computation time.

This brief review of leaf optical properties models reveals two categories of models. Descriptive models, which attempt a good but complex representation of the mechanisms involved (ray tracing, Markov approach), need a lot of parameters. Hence, they cannot be easily inverted. In contrast, invertible models such as radiative transfer models have parameters that can be inferred, with more or less difficulty, from remotely sensed measurements. Yamada and Fujimura (1990) presented their model as a nondestructive method to measure chlorophyll pigment concentration from leaf reflectance and transmittance data at three wavebands. With a simplified K–M model, Andrieu et al. (1988) also determined chlorophyll content from leaf reflectance measurements. These inversion studies are limited to the visible and near infrared domains and they only apply to the estimation of chlorophyll concentration. For remote sensing applications it is also necessary to extend the inversion procedure to the middle infrared domain and the estimation of leaf water content.

This paper presents a general radiative transfer model, PROSPECT, describing leaf optical properties from 400 nm to 2500 nm with a minimum number of parameters in order to facilitate its inversion. PROSPECT is an improved version of the generalized "plate model" by Allen et al. (1969; 1970). The refractive index as computed by Allen et al. (1969) for green maize leaves reveals some artifacts due to water and pigment features. The surface effects are not explicitly described. They also computed the absorption coefficients for different leaves, but they were not expressed as specific absorption coefficients for *in vivo* pigments and water. This study will attempt to provide optical constants from a wide range of leaf types. We shall also test the model's performance and discuss its inversibility.

THEORY

The "plate model" developed by Allen et al. (1969) considers a compact plant leaf as a transparent plate with rough plane parallel surfaces and initially assumes that the light fluxes are isotropic. However, the spectrophotometer incident light beam is parallel and generally perpendicular to the leaf blade. At microscopic scale, due to the undulating shape of the surface (Grant, 1987), the incoming beam penetrates the leaf with incident directions within a solid angle Ω. Ω is defined by a maximum incident angle α relative to the normal of the leaf plane. After its penetration inside the leaf, the light flux is assumed to be diffuse and isotropic. We have then modified Allen's initial expressions of the "plate model" in order to take into account the Ω solid angle of the incoming beam. The general formula for reflectance ρ_α and

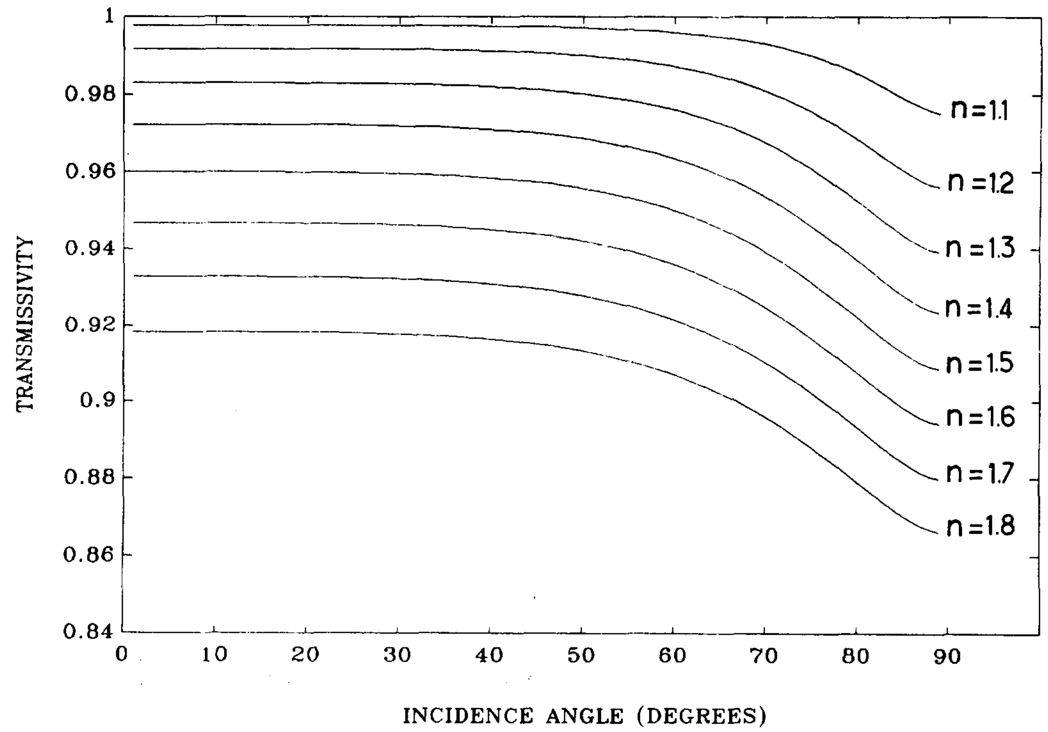


Figure 1. Average transmissivity $t_{av}(\alpha, n)$ as a function of the refractive index n and the incidence angle α.

transmittance τ_α can be written as follows for a given wavelength:

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

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

where

α = maximum incidence angle defining the solid angle Ω,

n = refractive index,

θ = transmission coefficient of the plate.

$t_{av}(\alpha, n)$ is the transmissivity of a dielectric plane surface, averaged over all directions of incidence and over all polarizations. Its expression is rather complex but it can be exactly calculated (Stern, 1964; Allen, 1973). Figure 1 shows that $t_{av}(\alpha, n)$ practically equals the transmissivity of a normal incidence for angles below 60°. For greater angles, it decreases more rapidly with increasing refractive index. From Eqs. (1) and (2) we can show that

$$\rho_\alpha = x\rho_{90} + y \quad (3)$$

$$\tau_\alpha = x\tau_{90}, \quad (4)$$

where

$$x = t_{av}(\alpha,n)/t_{av}(90,n), \quad (5)$$

$$y = x(t_{av}(90,n) - 1) + 1 - t_{av}(\alpha,n). \quad (6)$$

The "plate model" has three input parameters: a refractive index n, an incidence angle α, and a transmission coefficient θ. Unfortunately, as related by Allen, dicotyledonous and senescent leaves cannot be described as a unique compact layer and this model does not work in this case. The generalization of the "plate model" consists in stacking elementary layers. A leaf is then assumed to be composed of a pile of N homogeneous layers separated by $N-1$ air spaces. The solution of this problem has been given for many years by Stokes (1862). The discrete approach can be extended to a continuous one where N need not be an integer. As the nondiffuse character of the incident beam concerns only the top of the pile, the Stokes system has been modified by separating the first layer from the $N-1$ other ones. The first layer receives an incident beam within a solid angle Ω (incidence angle α): Let ρ_α be its reflectance and τ_α its transmittance. Inside the leaf, the light flux is assumed to be isotropic: let ρ_{90} be the reflectance and τ_{90} the corresponding transmittance of an internal elementary layer. The total reflectance and transmittance for N layers are given by

$$R_{N,\alpha} = \rho_\alpha + \frac{\tau_\alpha \tau_{90} R_{N-1,90}}{1 - \rho_{90} R_{N-1,90}}, \tag{7}$$

$$T_{N,\alpha} = \frac{\tau_\alpha T_{N-1,90}}{1 - \rho_{90} R_{N-1,90}}. \tag{8}$$

Eliminating ρ_α and τ_α by means of (3) and (4), it follows that

$$R_{N,\alpha} = x R_{N,90} + y \qquad \text{and} \qquad T_{N,\alpha} = x T_{N,90},$$

where x and y are given by Eqs. (5) and (6).

It is the key to transform our inhomogeneous system into Stokes' (1862) homogeneous system which can be put in the form

$$\frac{R_{N,90}}{b_{90}^{N} - b_{90}^{-N}} = \frac{T_{N,90}}{a_{90} - a_{90}^{-1}} = \frac{1}{a_{90} b_{90}^{N} - a_{90}^{-1} b_{90}^{-N}}, \tag{9}$$

where

$$a_{90} = \left(1 + \rho_{90}^2 - \tau_{90}^2 + \delta_{90}\right) / (2\rho_{90}),$$

$$b_{90} = \left(1 - \rho_{90}^2 + \tau_{90}^2 + \delta_{90}\right) / (2\tau_{90}),$$

$$\delta_{90} = \sqrt{\left(\tau_{90}^2 - \rho_{90}^2 - 1\right)^2 - 4\rho_{90}^2}\,.$$

The final formulation of this generalized "plate model" requires four parameters: α, n, θ, and N. In the following part, we will estimate them from our data set.

FITTING OF THE MODEL PARAMETERS

Materials and Methods

In order to have a wide range of variation of the structure, pigmentation and water content, we have chosen plant species with different types of leaves. Maize (*Zea mays*), wheat (*Triticum aestivum*), tomato (*Lycopersicon esculentum*), soybean (*Glycine max*), and sunflower (*Helianthus annuus*) were cultivated in a greenhouse. Oak (*Quercus robur*), maple (*Acer negundo*), and succulent plant (*Othonopsis cheiriifolia*) leaves were collected outdoors. We have also used maize etiolated leaves (grown in the dark) which contained carotenoids but no chlorophylls and albino maize leaves produced by treating seeds with fluridone (1-methyl-3-phenyl-5-[3-(trifluoromethyl) phenyl]-4(1H)-pyridinone) which contained no colored pigments (Maas and Dunlap, 1989). For each type of plant, five leaves were collected. We immediately measured the weight, the thickness, the water content, the specific leaf area, and the pigment concentration. Chlorophyll a, chlorophyll b, and total carotenoids were extracted in acetone 80%. Their concentration was determined according to the methodology defined by Lichtenthaler (1987). Directional-hemispherical reflectance and transmittance of the adaxial (upper) faces were measured in the laboratory using a Varian Cary 17 DI spectrophotometer equipped with an integrating sphere coated with $BaSO_4$ paint. The accuracy of the measurements was about 1%. The spectral bandwidth varied from 1 nm in the visible to 2 nm in the infrared. Spectra were scanned over the 400–800 nm wavelength interval with 4 nm steps and from 800 nm to 2500 nm with 17 nm steps. Data were corrected for the reflectance of a $BaSO_4$ reference and the geometry of the integrating sphere.

Determination of the Optical Constants of Leaf Materials

Intending to study the mesophyll structure effects, we shall first determine the refractive index spectrum and the α angle that can be assimilated to the surface roughness. Then we will be able to calculate the number N of elementary layers for each leaf. In a second step, we shall analyze the absorption processes and try to provide specific absorption coefficients for water and pigments.

Determination of a Refractive Index n and α

In order to avoid confusion between scattering and absorption phenomena which confound the computation of the refractive index value (Allen et al., 1969), it is necessary to use a compact plant leaf deprived of water and pigments. We have chosen an albino maize leaf for the 400–800 nm region and a dry (16 h at 80°C) maize leaf for the 800–2500 nm region. The albino leaf that shows minimum reflectance and maximum transmittance in the near infrared is the most compact: It will be considered as the reference layer (Breece and Holmes, 1971). We had to estimate the elementary layer reflectance and transmittance of the dry maize leaf because it was not so compact. For this purpose, we have inverted the Stokes system at 796 nm (minimum absorption) using a procedure proposed by Allen et al. (1970).

The "plate model" applies to this homogeneous elementary layer (reflectance $\rho_e = R_{1,\alpha}$, transmittance $\tau_e = T_{1,\alpha}$). Considering isotropic incident light ($\alpha = 90°$) leads to an average reflectivity $r_{av}(\alpha, n) = 1 - t_{av}(\alpha, n)$, which is greater than the lowest measured leaf reflectance corresponding to strong absorption domains! Therefore, the α parameter has been adjusted to the lowest value of elementary reflectance in order to have $r_{av}(\alpha, n) < \rho$. For simplification, we have considered that in the strong absorption domains, the elementary reflectance was very close to the actual leaf reflectance: This assumption has been verified *a posteriori* because the inversion of the Stokes system has little effect on very low values of reflectance. Although α depends on the geometry of the reflecting surface and normally varies from one plant to another, it has been set to the optimum value $\alpha = 59°$ in this study.

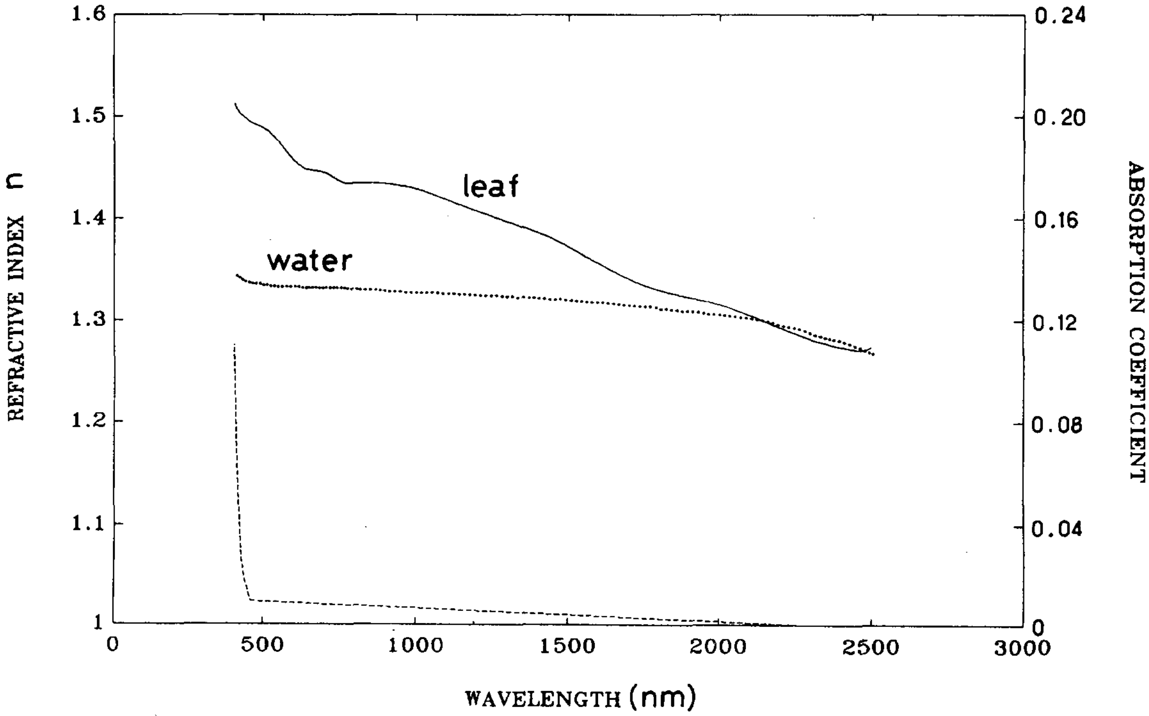
Using previous values of α, ρ_e, and τ_e, and eliminating θ_e between Eqs. (1) and (2), we can compute the refractive index n by solving

$$\left[\tau_e^2 - \left[\rho_e - 1 + t_{av}(59, n)\right]^2\right]\left[n^2 - t_{av}(90, n)\right] - t_{av}(90, n)\,t_{av}(59, n)\left[\rho_e - 1 + t_{av}(59, n)\right] = 0. \tag{10}$$

The adjusted refractive index of mesophyll interface material is close to 1.4. It regularly decreases from 400 to 2500 nm (Fig. 2) like the refractive index of pure liquid water (Palmer and Williams, 1974). These experimental data are in agreement with the literature (Gausman et al., 1974; Woolley, 1975; Vanderbilt and Grant, 1986).

We will now look for the absorption characteristics of leaf materials with our data set. Unfortunately, most of the leaves cannot be considered as a compact layer. Therefore, we will first compute the equivalent number of layers (N) for each plant type in order to get the elementary layer reflectance ($R_{1,59}$) and transmittance ($T_{1,59}$).

Figure 2. Refractive indexes n of leaf material (——) and water (· · ·) (from Palmer and Williams, 1974), and absorption coefficient spectrum k_e of the albino and dry maize leaf (---).



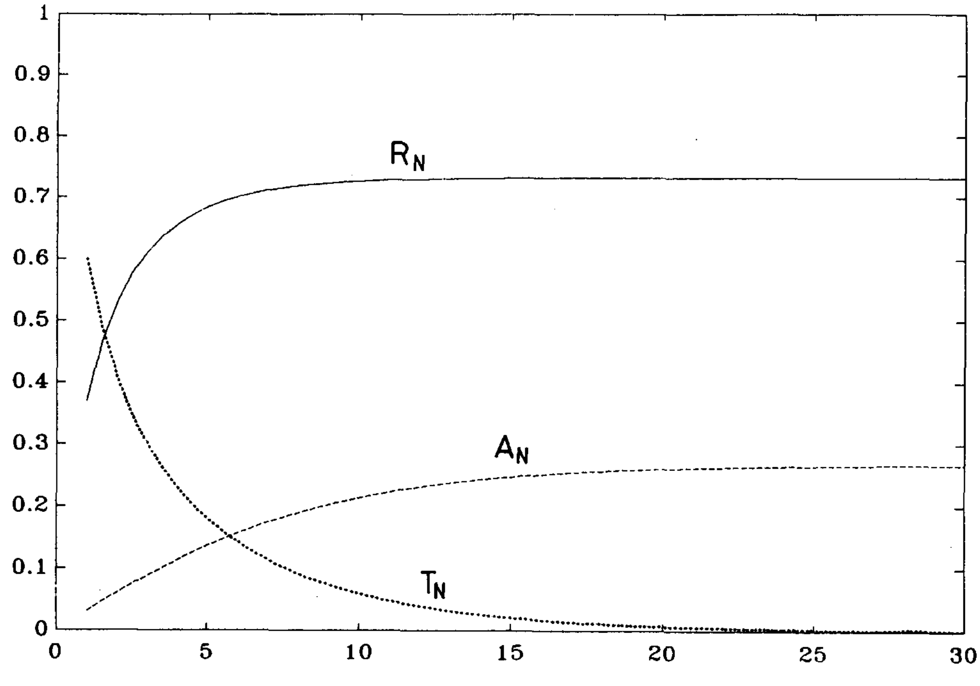


Figure 3. Variations of total reflectance R_N, transmittance T_N, and absorptance A_N for different values of N.

Determination of the Structure Parameter N

For each plant type, we have adjusted the N parameter at the wavelength where the absorptance is minimum (near infrared) by minimizing $(R - R_{N,59})^2 + (T - T_{N,59})^2$, where R and T are experimental data and $R_{N,59}$ and $T_{N,59}$ are theoretical data. Figure 3 demonstrates the interest of using simultaneously the reflectance and the transmittance of the leaf rather than only the reflectance: The transmittance is more sensitive to variation of N than the reflectance. As an important result, we can notice that both reach asymptotical limits. In the abstract, N relates to the cellular arrangement within the leaf. N ranging between 1 (albino maize leaf) and 1.5 corresponds to monocotyledons with compact mesophyll; Dicotyledons, characterized by a spongy parenchyma with air cavities on the abaxial face, have N values between 1.5 and 2.5. N values greater than 2.5 represent senescent leaves with a disorganized internal structure. Therefore, it may be used for separating or identifying vegetation types.

This parameter is well correlated with the specific leaf area (SLA: leaf area per unit leaf dry weight), which allows the physiologists to transform leaf biomass production into leaf area in most growth models. Assuming that the cell walls have a constant weight per unit area, we can see that an increase of the SLA corresponds to a decrease of the number of cell-wall interfaces inside the leaf and a decrease of N. We have observed an hyperbolic relationship between the SLA and N calculated for all the leaves (Fig. 4).

The determination of the structure parameter N allows us to invert the Stokes model using measured reflectance and transmittance values in order to calculate the equivalent reflectance and transmittance corresponding to a compact leaf layer. We can now estimate the specific absorption characteristics of leaf components.

Specific Absorption Spectra of Pigments and Water

The "plate model" provides a transmission coefficient θ, which is related to the absorption coefficient k through the following equation (Allen et al., 1969):

$$\theta - (1-k)e^{-k} - k^2\int_k^{\infty} x^{-1}e^{-x}\,dx = 0. \quad (11)$$

The spectral absorption coefficient $k(\lambda)$ can be written in the form

$$k(\lambda) = \sum K_i(\lambda)C_i \quad (12)$$

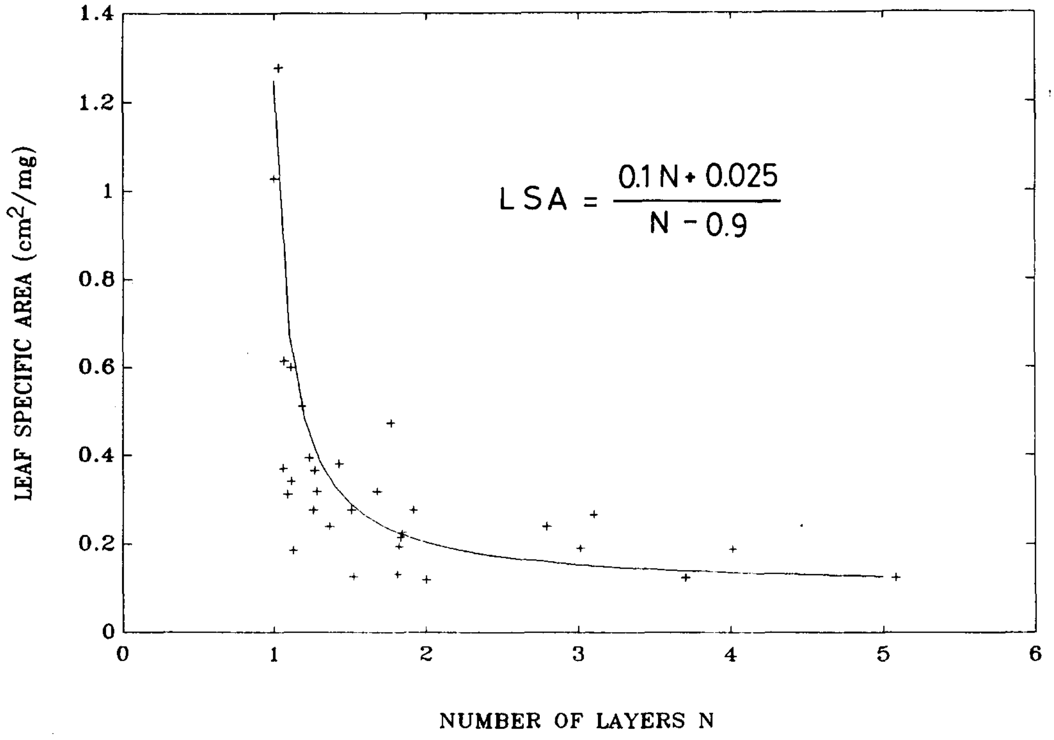


Figure 4. Relationship between number of layers N and leaf specific area.

where λ is the wavelength, $K_i(\lambda)$ is the spectral specific absorption coefficient relative to the leaf component i, and C_i is the leaf component i content per unit leaf area. In the case of our elementary albino and dry flat leaves, the C_i equal zero while the absorptance is different from zero. So we will take it into account by adding a $k_e(\lambda)$ term to Eq. (12):

$$k(\lambda) = \sum K_i(\lambda)C_i + k_e(\lambda). \qquad (13)$$

$k_e(\lambda)$ has been calculated by minimizing $(\rho_e - \rho_{59})^2 + (\tau_e - \tau_{59})^2$, where ρ_e and τ_e are the reflectance and transmittance values of our elementary albino and dry layer and ρ_{59} and τ_{59} the simulated values. Figure 2 shows that k_e decreases sharply until 450 nm and reaches a plateau close to zero. It seems that nonpigment cellular constituents such as phenolics, nucleic acids, and proteins are significative potential light receptors (Maas and Dunlap, 1989). Some of these photoreceptors may protect the leaf from light damage when approaching the ultraviolet. As the absorption features of water and pigments are clearly spectrally separated, we studied independently pigments in the 400–800 domain and water in the 800–2500 domain.

In the spectral range 800–2500 nm, absorption by water molecules almost completely masks the effects of cellulose, sugar, proteins, and lignin (Peterson et al., 1988). So we can write

$$k(\lambda) = K_w(\lambda)C_w + k_e(\lambda), \qquad (14)$$

where

K_w = water specific absorption coefficient (cm^{-1}),

C_w = equivalent water thickness (cm).

We determine the $k(\lambda)$ parameter using the same procedure as for the k_e evaluation. Then, the slope of the linear regression between $k(\lambda)$ and C_w with a fixed intercept $k_e(\lambda)$ gives the $K_w(\lambda)$ values. Figure 5 shows good agreement with the fundamental constants published for pure liquid water (Curcio and Petty, 1951). It confirms the choice of Tucker and Garrat (1977): These authors have used in their model Curcio and Petty's results, assuming that the differences existing between these data and the *in vivo* coefficients for the water in leaves were slight.

In the visible part, absorption is due to pigments such as chlorophyll a, b, carotenoids, and brown pigments (tannins) that appear during senescence. As there is not yet any method for determining the concentration of brown pigments,

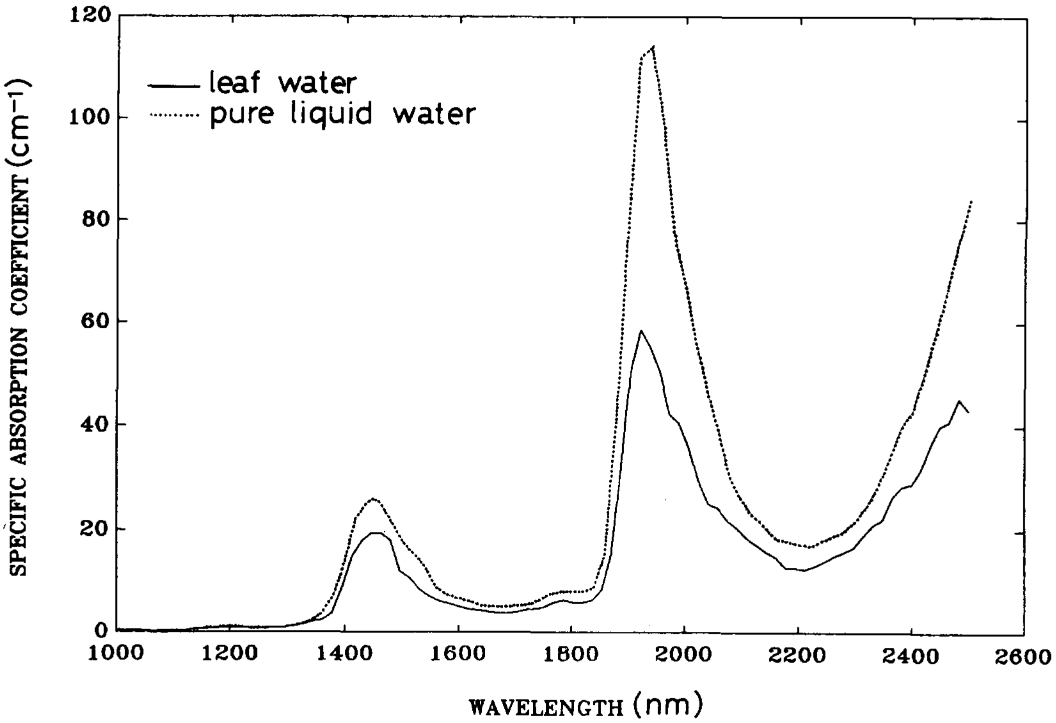
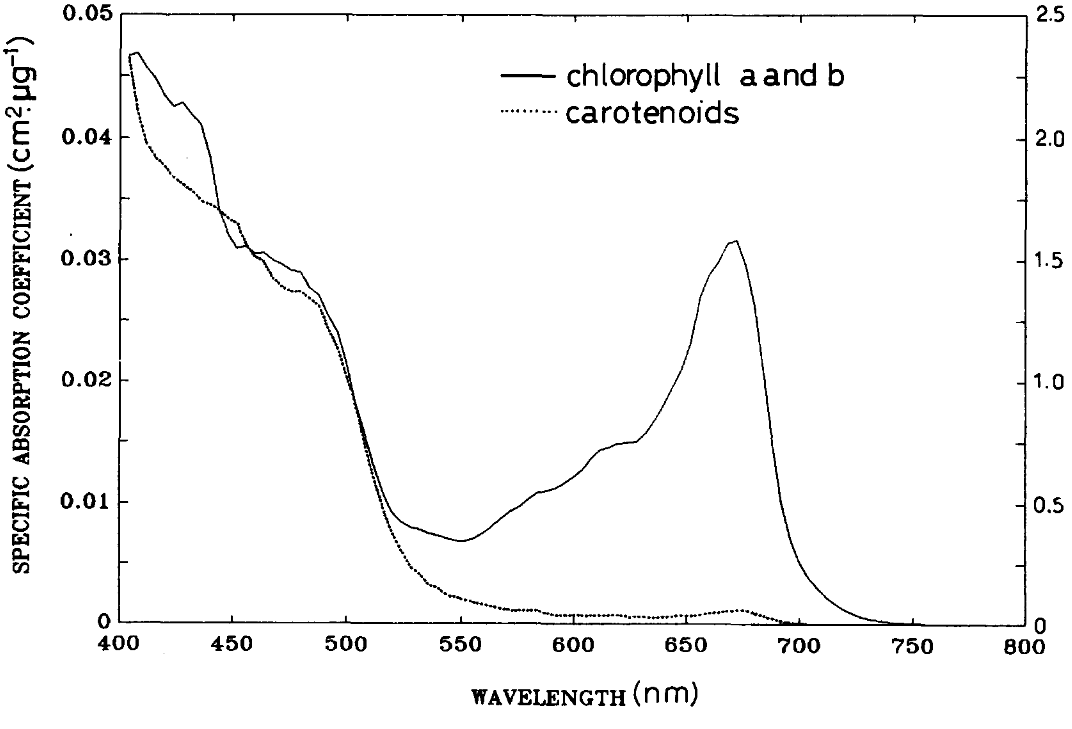


Figure 5. Specific absorption coefficient spectrum of *in vivo* leaf water K_w (——) compared with absorption coefficient for pure liquid water (· · ·) at 20°C (from Curcio and Petty, 1951).

Figure 6. Specific absorption coefficient spectrum of *in vivo* carotenoids K_{x+c} (right scale) (· · ·) and *in vivo* chlorophyll a+b k_{a+b} (left scale) (——).



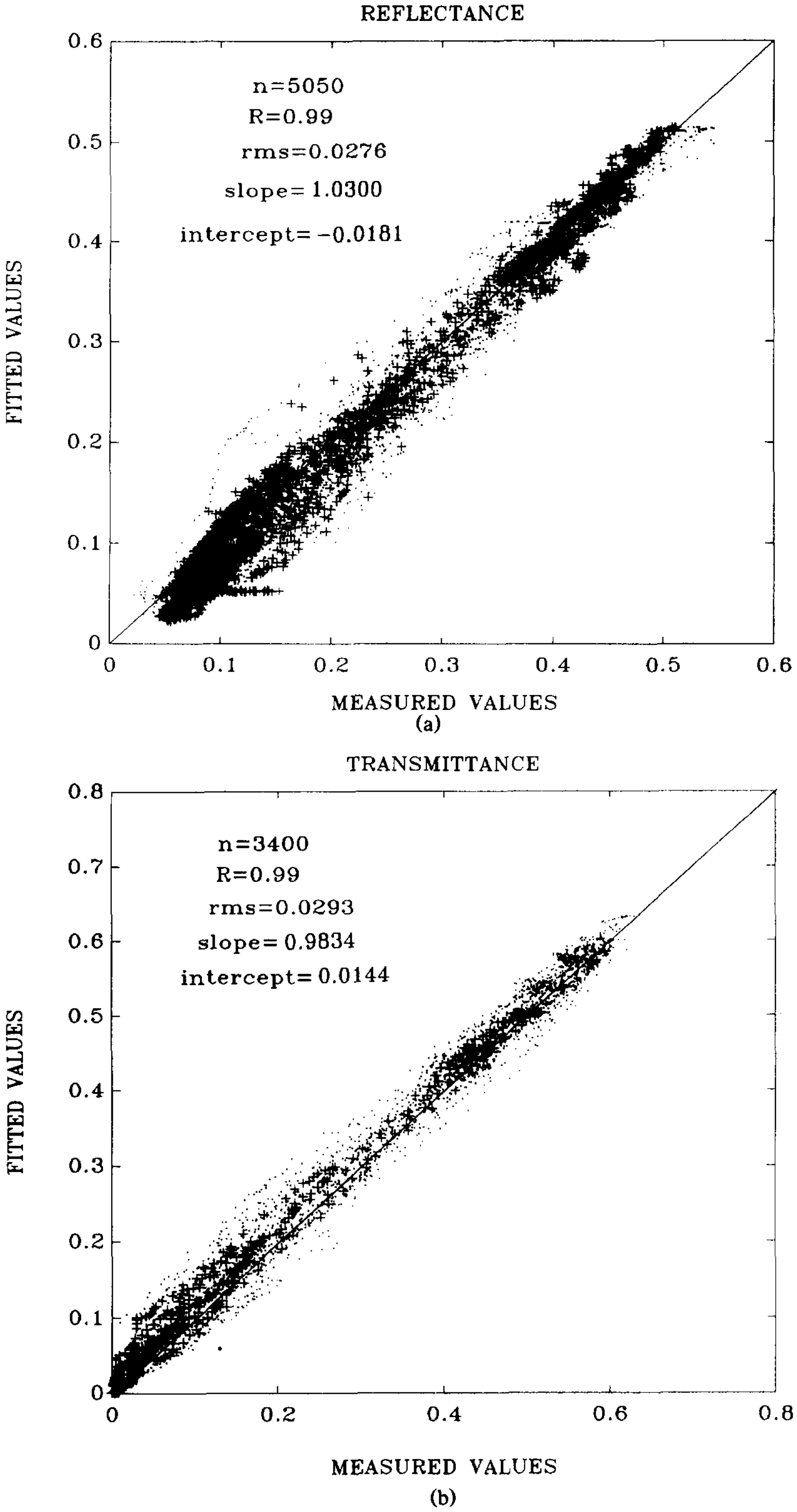


Figure 7. Comparison between simulated and measured reflectance (a) and transmittance (b). Data correspond to several experiments: points from Jacquemoud and Baret (1990); crosses from Andrieu et al. (1988) and Malthus et al. (1989).

senescent leaves have been moved away from this study. Furthermore, because of the strong correlation existing between the concentrations of the photosynthetic pigments (≈ 90%), the other leaves generally cannot be separated by classical analysis.

Nevertheless, in the case of two etiolated leaves for which chlorophyll concentration is very low, we have adjusted the total carotenoids (xanthophyll plus carotenes) specific absorption K_{x+c} spectrum using the same procedure as previously described for K_w. Figure 6 agrees with published curves (Lichtenthaler, 1987) with absorption shoulders at 450 and 480 nm. For the other leaves, we have considered the chlorophyll a and b together. The corresponding specific absorption coefficient K_{a+b} displays classical features (Fig. 6) with some spectral shifts of the principal absorption peaks compared to *in vitro* (in solvents) chlorophyll observations (Lichtenthaler, 1987). We can notice that K_{a+b} implicitly take into account carotenoid effects.

There is difficulty in extracting and separating the photosynthetical pigments for different reasons: At first, when we measure the carotenoid content, we may forget other accessory pigments (lutein, neoxanthin, etc.), the quantitative analysis of which is at present not accurate enough. The spectrophotometric measurement of this kind of pigment gives global values with a large experimental error (Sestak, 1985). Secondly, structural alterations of the chlorophyll molecules may result from the extraction solvent (acetone 80% in our case) and lead to wrong measures of concentration (Tucker and Garratt, 1977).

The spectral refractive index, specific absorption of water, and pigments representing the optical properties of leaf materials will be considered as constant parameters. Therefore, we can now test the applicability and accuracy of PROSPECT.

VALIDATION OF THE PROSPECT MODEL

The validation has been carried out with four data sets including our experiment described in a previous section and three external data sets corresponding to green wheat leaves (Andrieu et al., 1988) and sugar beet leaves (Malthus et al., 1989). Reflectance and sometimes transmittance measurements are available for each leaf, partially accompanied by biological characteristics such as pigment concentration or water content. These data sets represent a wide range of internal structure, pigment concentration, and water content.

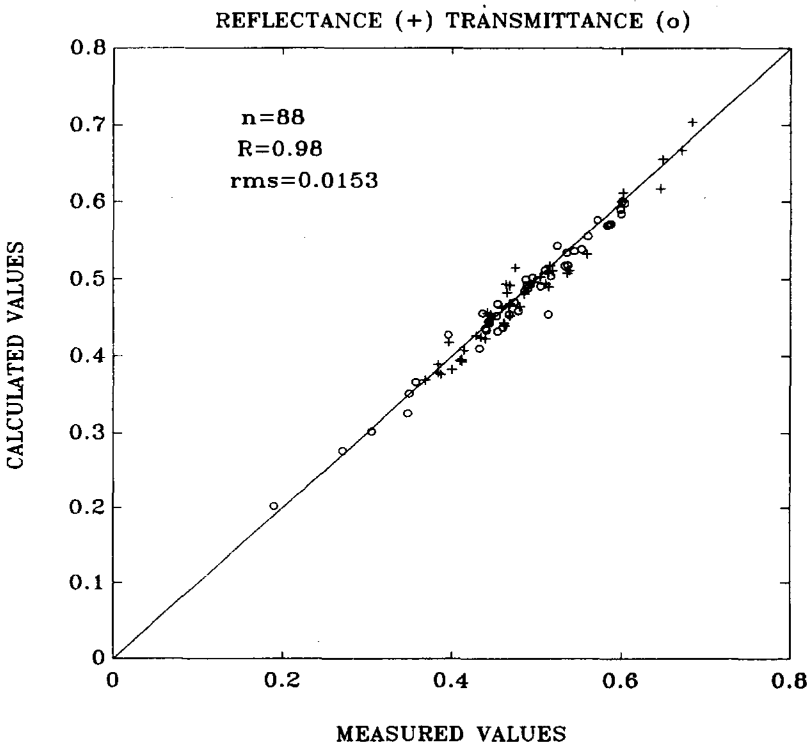
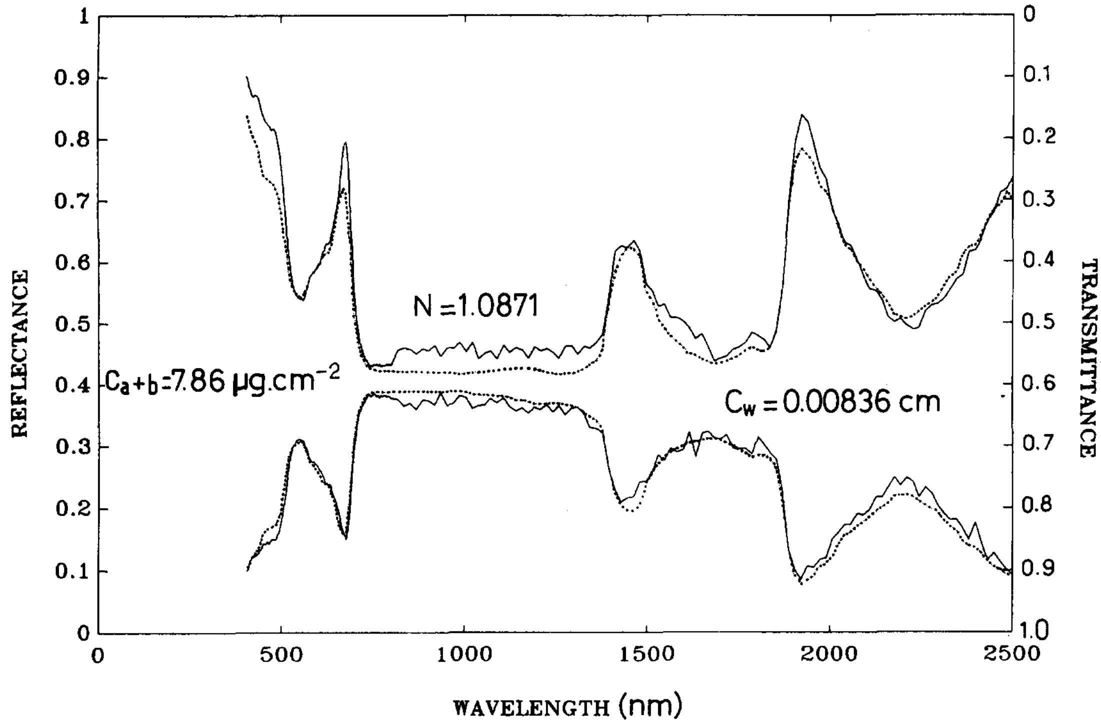


Figure 8. Comparison between reflectance (×) and transmittance (o) data simulated [Eq. (7)] and measured (2×44 = 88 data).

(a) YELLOWING MAIZE



(b) GREEN SOYBEAN

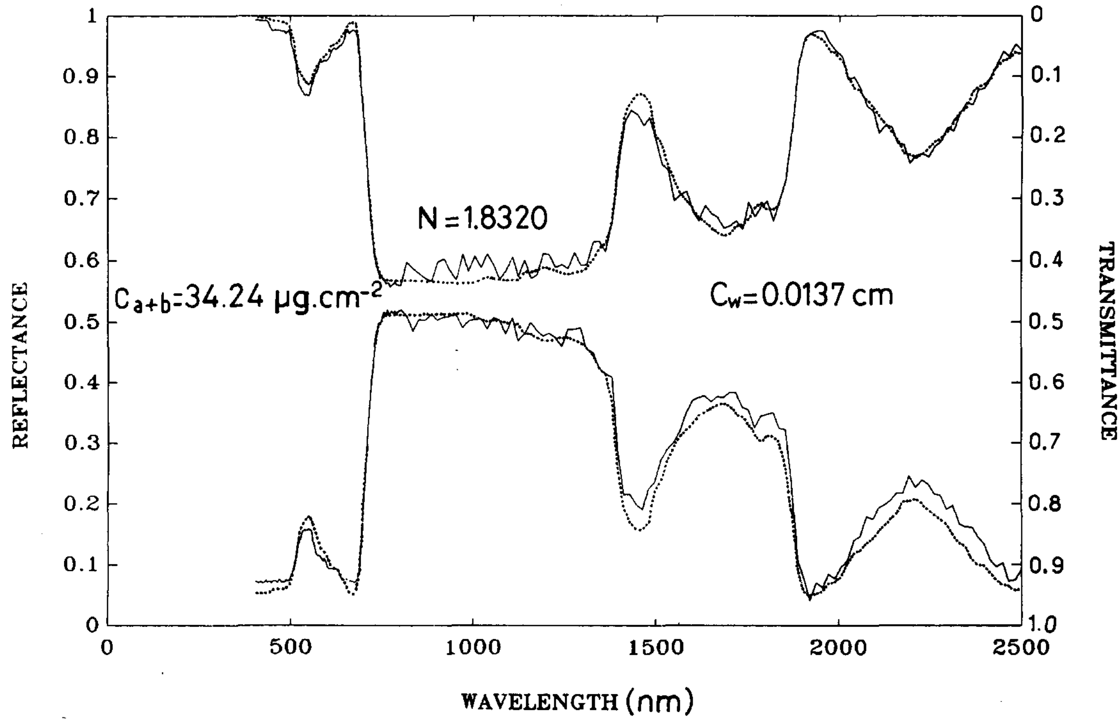


Figure 9. Comparison of the spectral reflectance and transmittance modeled (· · ·) and measured (——) for (a) yellowing maize and (b) green soybean.

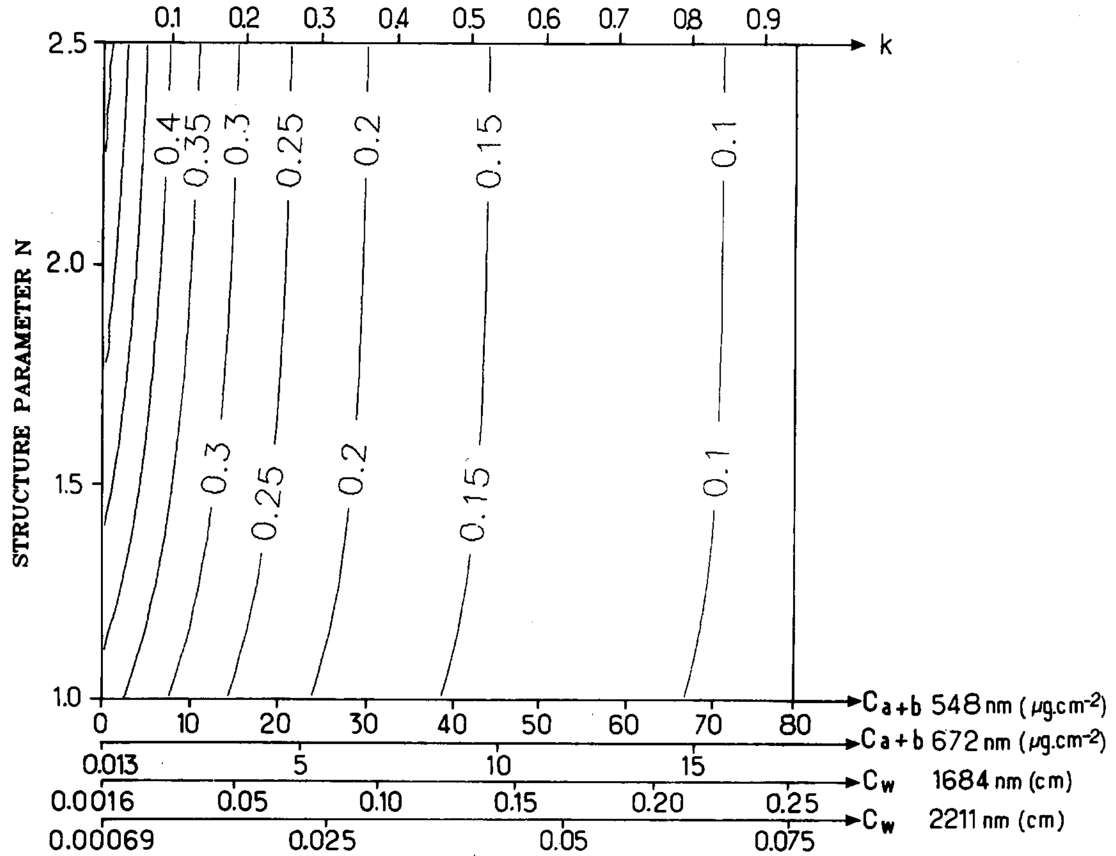
The linear regression analysis between simulated and measured values provides a correlation coefficient superior to 99% for both reflectance and transmittance. Figures 7a and 7b do not show any significant difference between the data set on which PROSPECT has been tested and the independent ones. Both exhibit root mean squares lower than 0.03. Prediction of the spectral optical properties by the model does not vary significantly in accuracy with wavelength, except in the visible region where there is a trend for the calculated data to underestimate the lowest measured reflectances (Fig. 7a). This problem may be due to the difficulty in separating the differing leaf pigments. But the assumption of a uniform distribution of the absorbing materials inside the leaf, and the simplistic way of describing the surface roughness may also be causes. The good performance of PROSPECT for high reflectance and transmittance values strengthens these observations. The transmittance for which dynamics are greater is well simulated at every wavelength (fig. 7b).

The comparison between measured and calculated leaf reflectance and transmittance values at the minimum absorption wavelength (Fig. 8) leads to a lower root mean square (rms = 0.0153, 2×44 = 88 data points). It indicates that the structure parameter N gives a good representation of the leaf internal structure. Senescent leaves characterized by a disorganized mesophyll even agree (low reflectance and high transmittance values). The results confirm the validity of the structure model and the inversion procedure of the Stokes system. This generalization of Allen's works, obtained from model inversion on both reflectance and transmittance data, is necessary to have a correct description of the optical properties in the absorption domains.

Finally, PROSPECT allows one to compute with only three input variables the 400–2500 nm

Figure 10. Reflectance (a) and transmittance (b) levels for different values of N and C (chlorophyll concentration or water content) at different wavelengths.

(a) REFLECTANCE



reflectance and transmittance spectra of very differing leaves. For example, the mesophyll structural differences between monocotyledons and dicotyledons are accurately described by the *N* parameter (Fig. 9). Absorption due to pigments or water is correctly simulated with the two corresponding contents (C_{a+b} and C_w). According to this approach, model inversion is possible even if some small discrepancies remain.

MODEL INVERSION

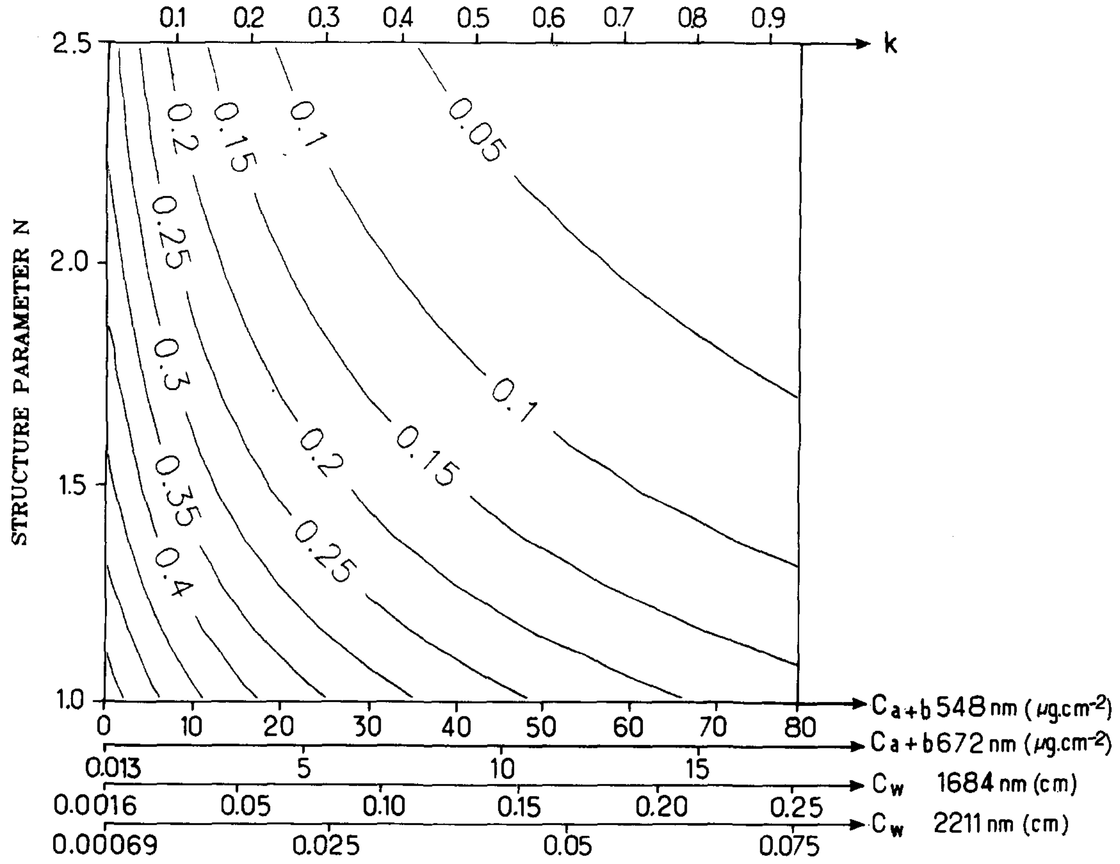
Based on the good prediction capacity of the model, we can now invert it to estimate leaf characteristics. First, a sensitivity analysis which simulates leaf spectra using a wide range of input parameters, will give us useful information for the inversion procedure.

Sensitivity Analysis

Simulating leaf spectra allows us to test the relative influence of each of the input parameters that control the spectral response. As discussed earlier [see Eq. (12)], absorption is determined by an absorption coefficient *k*, which is the product of a specific absorption coefficient (wavelength-dependent but independent of plant leaf) by the pigment concentration (C_{a+b}) or water content (C_w) which only depends on the physiological status of the plant. We prefer to use the concept of absorption coefficient rather than the concentration of absorbing material for a particular wavelength, in order to give more generality to the sensitivity analysis. Figures 10a and 10b, respectively, show the variations of the leaf reflectance and transmittance as a function of the structure parameter (N) and the absorption coefficient (k). As a general property, the transmittance is more sensitive to the model parameters than the reflectance. For a given structure parameter *N*, the reflectance and the transmittance of a leaf vary strongly when the absorption coefficient is low. They approach a limit for high absorptions. For low values of absorption coefficient, the reflectance and the transmittance will be the more sensitive to the *N* parameter. For high values of

Figure 10. Continued.

(b) TRANSMITTANCE



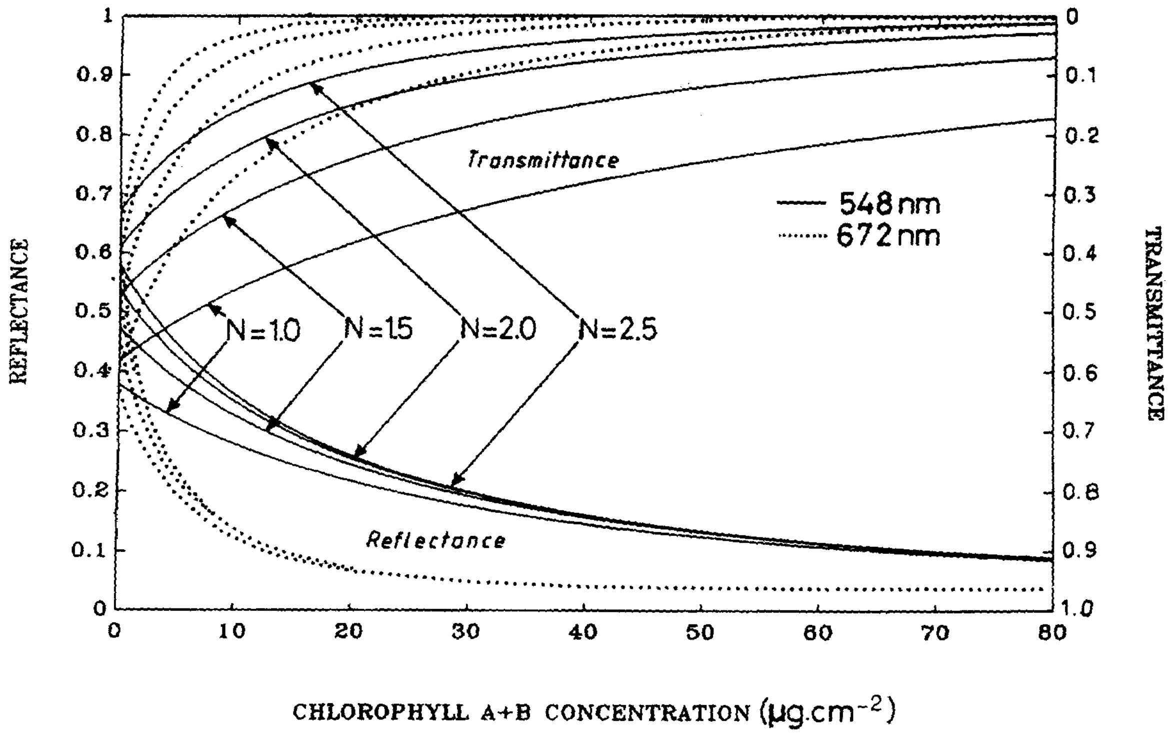


Figure 11. Variation of leaf reflectance and transmittance as a function of chlorophyll a + b concentration at different wavelengths and for different mesophyll structures: (——) 548 nm; (· · ·) 672 nm.

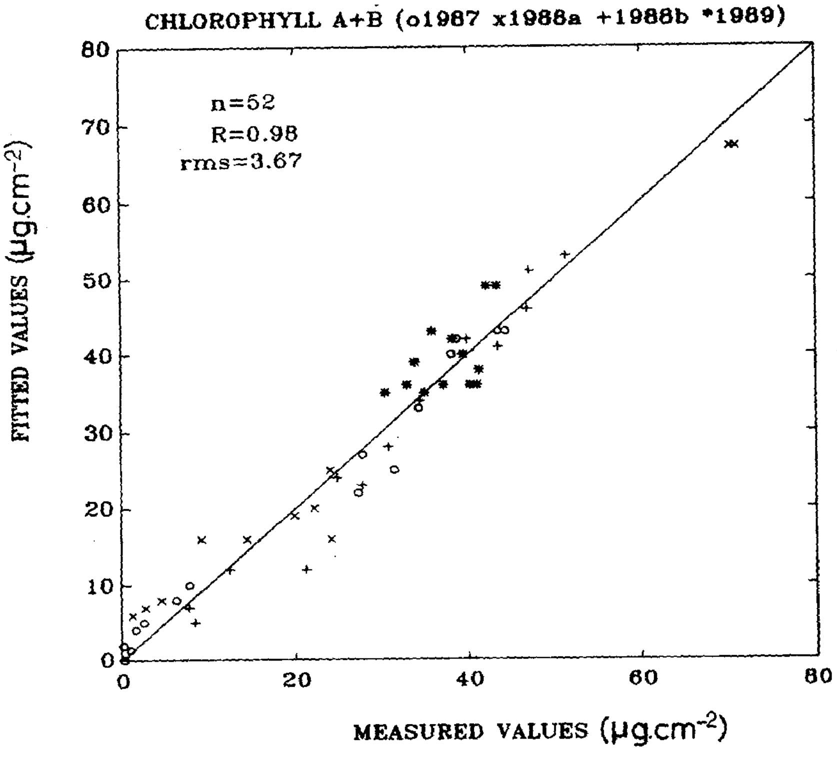


Figure 12. Estimation of leaf chlorophyll a + b concentration for four different data sets [Andrieu et al., 1987 (O); 1988 (x); Jacquemoud and Baret (+); Malthus et al., 1989 (*)].

absorption coefficient, leaf optical properties are relatively insensitive to the structure parameter particularly in the case of reflectance. Consequently, model inversion for the *N* parameter is more efficient in the near-infrared domain. Model inversion for pigment concentration and water content is more complex because the choice of the optimum wavelength depends on the level of contents. As seen in Figure 11, for low concentrations, the sensitivity is maximum when the absorption is maximum, i.e., the blue (450 nm) and red (672 nm) wavebands for chlorophyll and water absorption bands (1450 nm, 1950 nm, and 2500 nm). For high pigment concentrations, the inversion is more efficient for low absorption wavebands, i.e., the green (548 nm) and the transition between red and near infrared (red edge) for pigments, around 1684 nm and 2211 nm for water. If we have no information about the chlorophyll and water content, it would be more reliable to choose a set of particular wavelengths corresponding to the larger range of variation of the specific absorption coefficient. This situation is the case for the sharp absorption transitions encountered in the red edge region and the second water absorption peak between 1800 nm and 1950 nm. These simulation studies are useful because they indicate the inversion procedure that will be developed in the following section.

Model Inversion

Instead of choosing a particular wavelength for this operation, we have decided to find the parameter C which minimizes Δ^2 [Eq. (15)] on the whole spectrum. Because of the nonlinearity of the model, the inverse problem is numerically solved to determine the best value of water content (middle infrared) or pigments concentration (visible):

$$\Delta^2 = \sum_{\lambda} \left\{ [R_{\mathrm{mes}}(\lambda) - R_{\mathrm{mod}}(\lambda, C)]^2 + [T_{\mathrm{mes}}(\lambda) - T_{\mathrm{mod}}(\lambda, C)]^2 \right\} \quad (15)$$

where R_{mes} and T_{mes} are the experimental data, R_{mod} and T_{mod} the simulated data for a pigment concentration or a water content defined by C. We have achieved the inversion procedure on our data set and on the three external data sets for which leaf biological measurements were available. Note that Δ^2 can be calculated with the first term of Eq. (15) when we have only reflectance values. Figures 12 and 13 show that the estimates of C_w and C_{a+b} are in good agreement with the measured data. There is no systematic bias and the accuracy

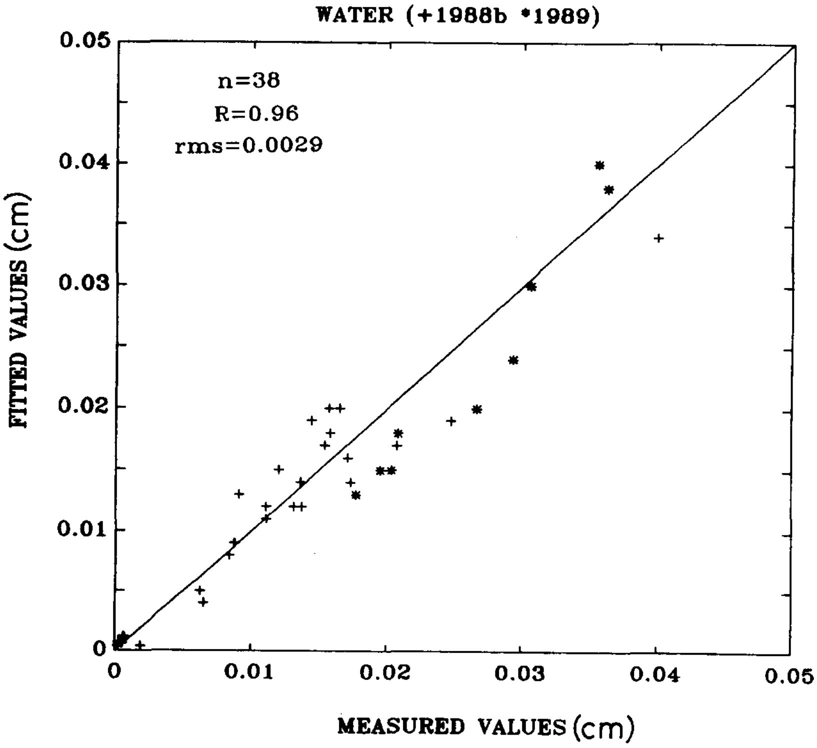


Figure 13. Estimation of leaf water content for two different data sets [Jacquemoud and Baret, (+); Malthus et al., 1989 (*)].

of the C_{a+b} or C_w prediction does not depend on the concentration level. The root mean square for chlorophyll concentration (rms = 3.669 μg cm^{-2}) is lower than that reported for the Yamada and Fujimura's (1990) multilayer model. This can be due to our inversion technique performed for the whole reflectance and transmittance spectra. Such a method can be proposed as a non destructive *in situ* measure of leaf biological parameters.

Spectra reconstruction from fitted values C_{a+b}, C_w, and N is another way to test the quality of PROSPECT. For this purpose, all the available spectra have been inverted in order to infer the three previous input variables. Then, these fitted variables have been used to simulate the corresponding reflectance and transmittance spectra. The comparison between actual and reconstructed spectra lead to high correlation coefficients (R^2 = 0.99) and low values of the root mean square ($n = 8657$ data and rms = 0.0262 for the reflectance; n = 5200 data and rms = 0.0274 for the transmittance). These results indicate the capability of PROSPECT to accurately synthesize the whole leaf spectra using only three parameters (N, C_{a+b}, and C_w) for different kinds of nonsenescent plant leaves.

CONCLUSIONS

In this work, we have developed a general radiative transfer model of reflectance and transmittance of a plant leaf, PROSPECT, as a function of three parameters: a structure parameter N, a pigment concentration, and a water content. We have provided the refractive index spectra, the water, and photosynthetic pigments specific absorption coefficients spectra. These results are in good agreement with the literature. Its simplicity makes it a good tool to elucidate the physical and physiological processes which control the characteristics observed in leaf spectra. It allows us to develop efficient algorithms in order to extract information from remotely sensed measurements. However, some of the assumptions limit the accuracy of the model. For example, we assume a uniform distribution of water and pigments and structure inside the leaf. Furthermore, the high correlation between the different pigments prevents us from separating the individual specific absorption coefficients. Finally, we assume that the α angle that represents the surface roughness is constant, which in fact is not exactly the case. Surface features that are very complex merit more work.

When imaging spectroscopy is used for crop characterization, it increases the information content, but the way to extract canopy characteristics is not precisely known. The inversion procedure is a way to derive leaf parameters from *in situ* and nondestructive optical measurements. Furthermore, the important raw leaf spectral information can be accounted for by only three parameters. The advantage of such a parameterization may be realized when using models that require reflectance and transmittance spectra as input parameters. PROSPECT should contribute to improve our understanding of high spectral resolution data for an efficient use.

This study was in part supported by a grant from "ATP Télédétection Spatiale 1990" with a financial contribution from CNES, CNRS, INRA, and IFREMER. Special thanks must be given to T. Malthus (University of Nottingham, U.K.), who provided external data sets, and to J. Nicolas, M. Tacchini, and P. Varoquaux (Station de Technologie, INRA Montfavet, France) for their help in determining pigment concentrations.

REFERENCES

Allen, W. A. (1973), Transmission of isotropic light across a dielectric surface in two and three dimensions, *J. Opt. Soc. Am.* 63(6):664–666.

Allen, W. A., and Richardson, A. J. (1968), Interaction of light with a plant canopy, *J. Opt. Soc. Am.* 58(8):1023–1028.

Allen, W. A., Gausman, H. W., Richardson, A. J., and Thomas, J. R. (1969), Interaction of isotropic light with a compact plant leaf, *J. Opt. Soc. Am.* 59(10):1376–1379.

Allen, W. A., Gausman, H. W., and Richardson, A. J. (1970), Mean effective optical constants of cotton leaves, *J. Opt. Soc. Am.* 60(4):542–547.

Allen, W. A., Gausman, H. W., and Richardson, A. J. (1973), Willstätter–Stoll theory of leaf reflectance evaluated by ray tracing, *Appl. Opt.* 12(10):2448–2453.

Andrieu, B., Baret, F., Schellberg, J., and Rinderle, U. (1988), Estimation de spectres de feuilles à partir de mesures dans les bandes spectrales larges, in *Proc. 4th Int. Coll. on Spectral Signatures of Objects in Remote Sensing*, Aussois, France, 18–22 January 1988, ESA SP-287, pp. 351–356.

Baret, F., Andrieu, B., and Guyot, G. (1988), A simple model for leaf optical properties in visible and near infrared: application to the analysis of spectral shifts determinism, in *Applications of Chlorophyll Fluorescence* (H. K. Lichtenthaler, Ed.), Kluwer Academic, pp. 345–351.

Brakke, T. W., and Smith, J. A. (1987), A ray tracing model for leaf bidirectional scattering studies, in *Proc. Int. Geosci. and Remote Sens. Symp.* (IGARSS '87), Ann Arbor, MI, 18–21 May 1987, pp. 643–648.

Breece, H. T., and Holmes, R. A. (1971), Bidirectional scattering characteristics of healthy green soybean and corn leaves in vivo, *Appl. Opt.* 10(1):119–127.

Curcio, J. A., and Petty, C. C. (1951), Extinction coefficients for pure liquid water, *J. Opt. Soc. Am.* 41:302–304.

Gausman, H. W., Allen, W. A., Cardenas, R., and Richardson, A. J. (1970), Relation of light reflectance to histological and physical evaluation of cotton leaf maturity, *Appl. Opt.* 9(3):545–552.

Gausman, H. W., Allen, W. A., and Escobar, D. C. (1974), Refractive index of plant cell walls, *Appl. Opt.* 13(1):109–111.

Grant, L. (1987), Diffuse and specular characteristics of leaf reflectance, *Remote Sens. Environ.* 22:309–322.

Hodanova, D. (1985), Leaf optical properties, in *Photosynthesis during Leaf Development* (Zdenek Sesták, Ed.), Academia Praha, Prague.

Lichtenthaler, H. K. (1987), Chlorophylls and carotenoids: pigments of photosynthetic biomembranes, *Methods Enzymol.* 148:350–382.

Lichtenthaler, H. K., and Wellburn, A. R. (1983), Determination of total carotenoids and chlorophylls a and b of leaf extracts in different solvents, *Biochem. Soc. Trans.* 603:591–592.

Maas, S. J., and Dunlap, J. R. (1989), Reflectance, transmittance, and absorptance of light by normal, etiolated, and albino corn leaves, *Agron. J.* 81:105–110.

Malthus, T., Andrieu, B., Baret, F., Danson, M., Jaggard, K., and Steven, M. (1989), Sugar-beet experiment and database, unpublished works.

Palmer, K. F., and Williams, D. (1974), Optical properties of water on the near infrared, *J. Opt. Soc. Am.* 64(8):1107–1110.

Peterson, D. L., Aber, J. D., Matson, P. A., Card, D. H., Swanberg, N., Wessman, C., and Spanner, M. (1988), Remote sensing of forest canopy and leaf biochemical contents, *Remote Sens. Environ.* 24:85–108.

Sestak, Z. (1985). Chlorophylls and carotenoids during leaf ontogeny, in *Photosynthesis during Leaf Development* (Zdenek Sesták, Ed.) Academia Praha, Prague.

Stern, F. (1964), Transmission of isotropic radiation across an interface between two dielectrics, *Appl. Opt.* 3(1):111–113.

Stokes, G. G. (1862), On the intensity of the light reflected from or transmitted through a pile of plates, *Proc. Roy. Soc. Lond.* 11:545–556 (30 Nov. 1860 to 27 Feb. 1862).

Tucker, C. J. (1980), Remote sensing of leaf water content in the near infrared, *Remote Sens. Environ.* 10:23–32.

Tucker, C. J., and Garratt, M. W. (1977), Leaf optical system modelled as a stochastic process, *Appl. Opt.* 16(3):635–642.

Vanderbilt, V. C., and Grant, L. (1986), Polarization photometer to measure bidirectional reflectance factor R(55°, 0°; 55°, 180°) of leaves, *Opt. Eng.* 25(4):566–571.

Vane, G., and Goetz, A. F. H. (1988) Terrestrial imaging spectroscopy, *Remote Sens. Environ.* 24:1–29.

Woolley, J. T. (1971), Reflectance and transmittance of light by leaves, *Plant Physiol.* 47:656–662.

Woolley, J. T. (1975), Refractive index of soybean leaf cell walls, *Plant Physiol.* 55:172–174.

Yamada, N., and Fujimura, S. (1988), A mathematical model of reflectance and transmittance of plant leaves as a function of chlorophyll pigment content, in *Proc. Int. Geosci. and Remote Sens. Symp.* (IGARSS '88), Edinburgh, Scotland, 13–16 Sep. 1988, pp. 833–834.

Yamada, N., and Fujimura, S. (1990), Nondestructive measurement of chlorophyll pigment content in plant leaves from three-colour reflectance and transmittance, *Appl. Opt.*, forthcoming.