A LEAF OPTICAL PROPERTIES MODEL ACCOUNTING FOR DIFFERENCES BETWEEN THE TWO FACES

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Theme: Physical modeling in remote sensing

ABSTRACT:

Modeling radiative transfer in canopies allows efficient use of remote sensing observations to quantify vegetation state variables and functioning. Canopy radiative transfer models use requires accurate description of leaf optical properties. Although widely used, the PROSPECT leaf optical properties model is based on simplifying assumptions that limit its performances. One of these assumptions is that scattering and absorbing materials are evenly distributed in the leaf thickness, leading to the same optical properties for both faces. However, plants have developed particular adaptations resulting sometimes in strong differences in the properties of each faces, in relation to surface characteristics as well as leaf internal structure and distribution of chlorophyll and water. The objective of this paper is to develop a new model accounting for the difference between leaf upper and lower faces.

The QSPECT model is an improved version of PROSPECT where the leaf considered made of four layers corresponding to the upper and lower epidermis, the palisade and spongy mesophylls. This advanced model requires four additional parameters describing the distribution of main scattering and absorbing materials. Results acquired over few reflectance and transmittance measurements show that QSPECT is able to describe accurately the typical differences observed between upper and lower leaf faces. Of particular importance are the surface reflectivities as well as chlorophyll content distribution

Introduction

Leaf optical properties are key input variables to understand and model radiative transfer in canopies. Radiative transfer models are very useful for exploiting remote sensing observations and transform the signal collected onboard satellite into surface characteristics such as leaf area index or chlorophyll content. Several leaf optical properties models heave been proposed in the past as listed in a recent review (Jacquemoud et al., 2001). They allow to simulate leaf reflectance and transmittance from a limited set of state variables describing the content of absorbing materials such as chlorophyll, water or dry matter, and the scattering occurring at the interfaces between materials with difference in refraction index value. Most leaf optical properties models assume the leaf as an homogeneous layer with evenly distributed absorbing and scattering materials. As a consequence, reflectance and transmittance of both faces are the same. However, leaves have to ensure a number of functions under very wide environment conditions. They have therefore adapted their structure to better answer these challenges.

A typical dicotyledon leaf section shows the palisade and spongy mesophyll tissue layers, bounded by two layers of epidermal cells as illustrated in Figure 1. The epidermis is made up of a single layer of colorless cells, with few if any chloroplasts. Its main role is to protect the inner layers form the outside environment, contributes to maintain leaf port, while controlling exchanges of gas and radiation with the cuticle (waxy, crystallized), its roughness, and the possible presence of hairs and their characteristics (length, density, shapes). Palisade cells are elongated, generally densely packed, and arranged in one to several layers. They contain the largest proportion of chloroplasts where most of photosynthesis is taking place. The spongy mesophyll is made up of highly lobed irregularly shaped cells of variable size, separated by large intercellular air-filled spaces that facilitate the circulation of gases inside the leaf. As a consequence, the small amount of absorbing material in the spongy mesophyll and the high number of discontinuities in the refraction index values, a large fraction of light incoming from the palisade mesophyll is scattered back, increasing light absorption efficiency by chloroplasts (Raven et al., 1996).

Because of the particular organization of leaves, important differences may be observed between the optical properties of upper and lower faces particularly in spectral domains where stronger absorption occurs: in the visible domain characterized by chlorophyll pigment absorption, reflectance of upper faces is generally lower than that of lower faces where more scattering occurs. Transmittance and reflectance in the near infrared domain are generally less affected. Plants will exploit these differences in leaf optical properties between faces to better suit environmental conditions. This is reported for olive trees that have leaves with more reflective lower faces. In case of

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severe water stress, olive trees orientate their leaves in a more erectophile way, exposing the lower faces towards the incoming light which reduces the amount of radiation absorbed by the canopy, hence transpiration and photosynthesis. Apart from the effect of differences between faces on canopy functioning, impact is also expected on canopy reflectance. This may induce additional uncertainties in remote sensing retrieval of some key biophysical variables such as leaf area index (LAI) or chlorophyll content.

This study will attempt to document differences between leaf optical properties faces: as a matter of fact, although differences between optical properties of the two faces are known qualitatively, very little studies documented their magnitude. More precisely, the objective of this study is to develop a leaf optical properties model that explicitly accounts for inhomogeneity in the leaf and describes the corresponding differences in leaf reflectance of both faces. The modeling will be based on the PROSPECT model proposed by Jacquemoud and Baret (1990). This model offers the advantage to be relatively simple with a limited number of variables allowing to use it in a more operational way. PROSPECT was already validated several times with relatively good performances although not describing the effects due to inhomogeneous leaf structure (Jacquemoud and Baret, 1990).

In this study, measurements of leaf optical properties are acquired to quantify the possible differences between upper and lower faces. Then, the PROSPECT model is adapted to account for the layer structure description according to Figure1. It will be named hereafter "QSPECT". A sensitivity analysis is conducted, with emphasis on the variables that drive the differences between both faces. Finally, some validation elements are presented and discussed.
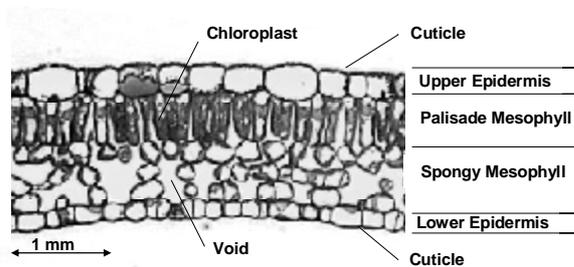

Figure 1. Structure of a typical dicotyledon leaf. Chloroplasts are drawn in one cell only of both palisade and spongy tissues.

MATERIALS AND METHODS

Measurements were made during spring 2006. Six species of leaves were selected, describing large variability of properties between upper and mower faces: Tilia, Medlar (*Mespilus*), banana (*Musa*), Sage (*Salvia officinalis*), Ivy (*Hedera*) and Maple (*Aceraceae*).

Four leaves for each species were selected with similar visual aspects. Reflectance and transmittance of leaves were measured at three distinct locations over each of the 4 leaves, trying to avoid the larger veins when observed.

Reflectance and transmittance measurements were achieved using an ASD Fieldspec spectrophotometer (Rollin E. M. and al., 1996), with a 1 nm sampling interval from 400 to 2400 nm. Its spectral resolution varies from 1 nm in the shorter wavelengths, up to about 2 nm for the longer ones. A Li-Cor 1800-12 (Verney C. A., 2002) integrating sphere was used to get directional/hemispherical reflectance and transmittance values. The incoming light arrived almost normally to the leaf sample. The original Li-Cor lamp system was replaced by a lamp powered by a large battery ensuring steady input electric characteristics during a time period used for single measurements (few minutes) and bracketed by measurements made over reference targets. The infrared filter placed on front of the original light was removed as well. The bare fiber optic (25° field of view) was looking the integrative sphere wall. To reduce possible stray-light, the experiment was conducted in a darkroom. Reflectance (spectralon) and transmittance (Teflon sheet) target references with precisely known directional hemispherical reflectance, R_{ref} (transmittance, T_{ref}) values were used to get absolute directional hemispherical reflectance or transmittance values of the sample.

The measurement protocol consisted in three consecutive measurement steps for each individual leaf sample:

1. Reflectance S_{rref}^{start} (transmittance, S_{tref}^{start}) signal of the reference were first acquired.
2. Then, reflectance, S_{rleaf} (transmittance, S_{tleaf}) of the sample were measured at three different locations on the leaf sample.
3. Finally, references were again acquired (S_{rref}^{end}, S_{tref}^{end}) to account for possible variation during the sample measurement.

Absolute values of reflectance (R^i) and Transmittance (T^i) of leaf samples i were computed as:

$$R^i = R_{ref} \frac{2 \cdot S_{rmes}^i}{(S_{rmes}^{start} + S_{rmes}^{end})}$$

$$T^i = T_{ref} \frac{2 \cdot S_{tmes}^i}{(S_{tmes}^{start} + S_{tmes}^{end})} \tag{1}$$

The sequence for reflectance and transmittance of both faces for the four leaves, took about 30 minutes in total. Absolute values of reflectance (and transmittance) were finally averaged over the four leaves and the three locations.

Uncertainties were characterized by RMSE values over the 4 replicates times 3 locations. Reflectance and transmittance on both faces have about the same uncertainties which do not vary much with wavelength except above 2000 nm where instrumental noise is dominant. For wavelengths beyond 2000nm, the mode of RMSE values is close to 0.015 (Figure 3). It is mainly explained by differences between leaves and locations, the instrumental noise being marginal (lower than 0.001) in this wavelength domain.
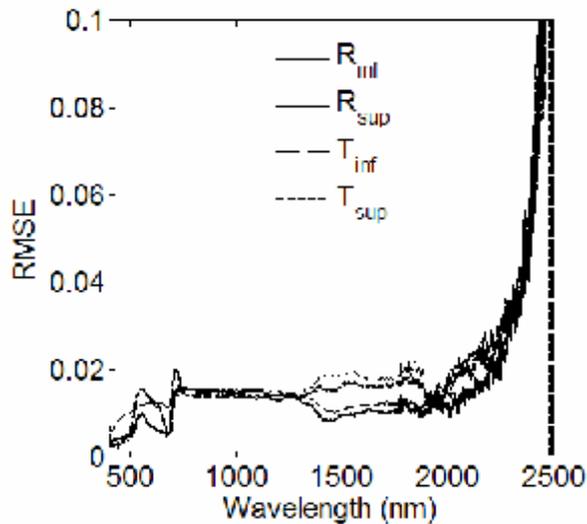
Figure 2. Inspection of the distribution of the uncertainties computed between the 12 replicates (3 locations time 4 leaves)
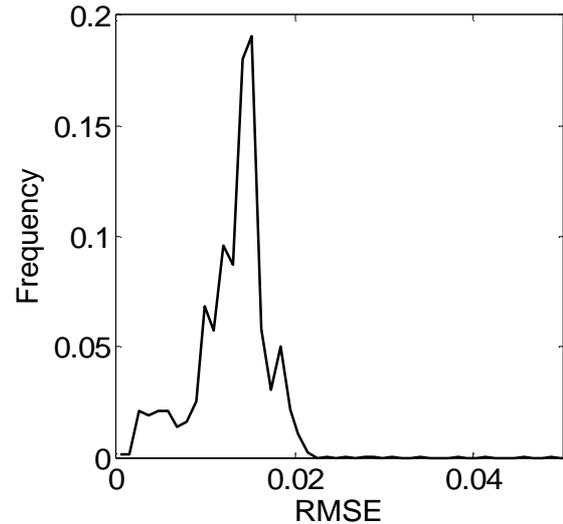

Figure 3. Histogram of the RMSE values computed for each wavelength between the 12 replicates of measurements for reflectance or transmittance of the two faces.

EXPERIMENTAL EVIDENCE OF DIFFERENCES BETWEEN FACES

Reflectance and transmittance spectra show very classical features, with low values in the visible because of chlorophyll pigment absorption, large values in the near infrared due of intense volume scattering and very low absorption, and intermediate situation in the short wave infrared dominated by water absorption features (Figure 4). Note that the absorptance (1-Reflectance-Transmittance) may be very small in the near infrared as observed for Tilia (Figure 4 right,).

Measurements show that tilia and medlar leaves exhibit large differences between both faces, while Ivy, Musa and Sage show smaller differences and the young Maple leaves show almost similar properties on both faces.

Differences between upper and lower faces show regularities with however, variation in magnitude among leaf types and spectral domains (Figure 5). In the visible domain, upper faces reflect significantly less while transmitting about the same, therefore absorbing more light than the lower faces. Conversely, in the near infrared domain, upper faces reflect more, transmit less and absorb slightly more than lower faces. In the short wave infrared domain, upper leaves transmit less, absorb more, and generally reflect less than lower faces although two leaves are reflecting slightly more.
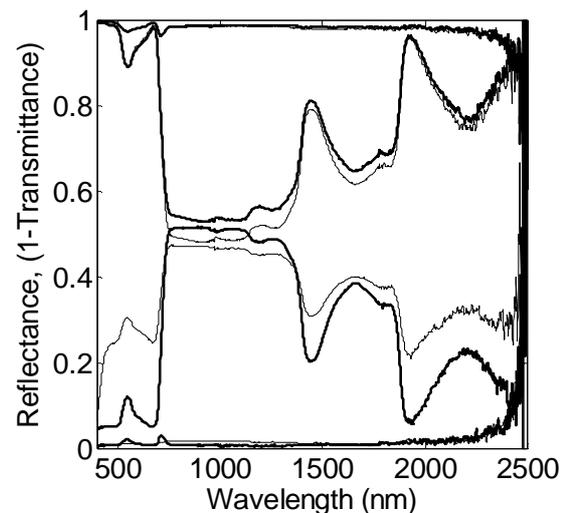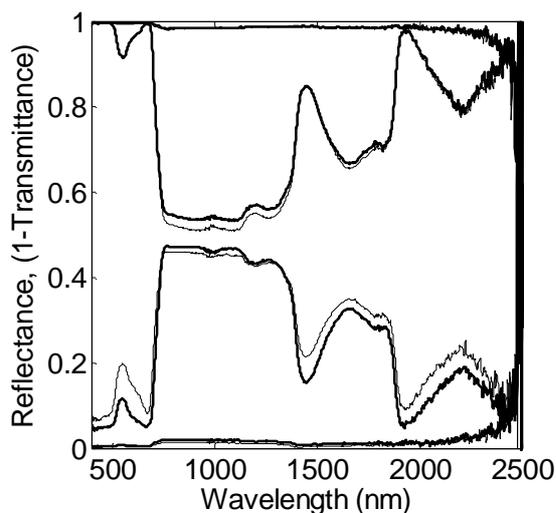

Figure 4. Sample leaf reflectance and transmittance (displayed here as 1-transmittance) measured over Ivy (left) and Tilia (right) leaves. Upper (lower) faces are represented by a thick (thin) lines. The corresponding uncertainties (RMSE values) are shown for reflectance (at the bottom) and transmittance (1-RMSE) at the top for upper (bold) and lower (thin) faces
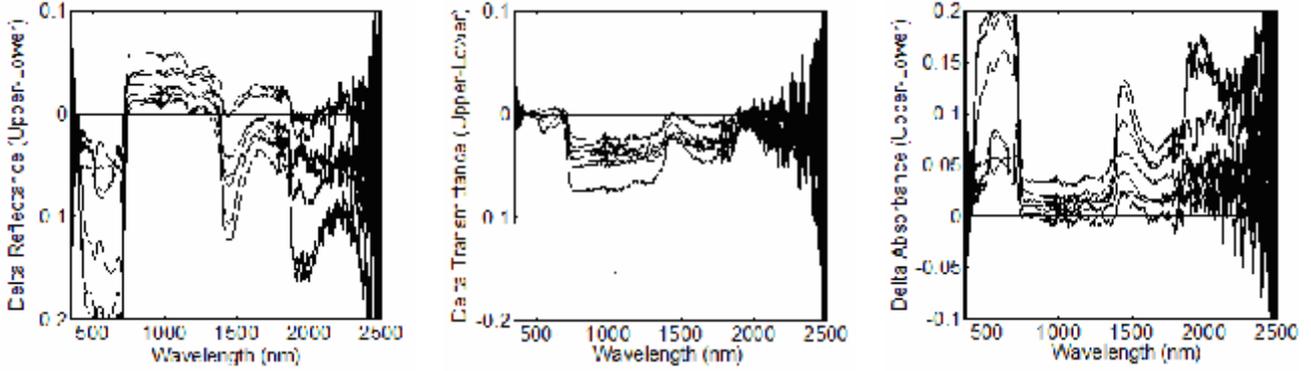
Figure 5. Differences (Delta) in Reflectance (left), Transmittance (centre), and Absorptance (right) between the Upper and Lower faces of the 7 leaves considered.

These observations could be explained qualitatively by considering the leaf as made of two layers: an upper layer made of the upper epidermis on top of the palisade mesomphyll, and a lower layer made of the spongy mesophyll on top of the lower epidermis (Figure 6). Reflectance and transmittance of this system of two layers may be described simply by considering the multiple scattering between the 2 layers. For elementary fluxes, small letters are used (r, t) while capital letters are reserved for the net fluxes created by the 2 layers (R_{12}, T_{12}). Subscripts correspond to layer number ($_1$, $_2$). The superscript arrows correspond to the direction of the incident flux considered ($^\downarrow$, $^\uparrow$). Reflectance of the upper (lower) face generated by a flux impinging on it, $R_{12}^\downarrow$ ($R_{12}^\uparrow$), writes:

$$R_{12}^{\downarrow} = r_1^{\downarrow} + \frac{r_2^{\downarrow} t_1^{\downarrow} t_1^{\uparrow}}{1 - r_2^{\downarrow} r_1^{\uparrow}}$$

$$R_{12}^{\uparrow} = r_2^{\uparrow} + \frac{r_1^{\uparrow} t_2^{\downarrow} t_2^{\uparrow}}{1 - r_2^{\downarrow} r_1^{\uparrow}} \qquad (2)$$

Similarly, transmittance of the upper (lower) face generated by a flux impinging on the face opposite to it, $T^\downarrow$ ($T^\uparrow$), writes:

$$T_{12}^{\uparrow} = \frac{t_2^{\uparrow} t_1^{\uparrow}}{1 - r_2^{\downarrow} r_1^{\uparrow}}$$

$$T_{12}^{\downarrow} = \frac{t_1^{\downarrow} t_2^{\downarrow}}{1 - r_2^{\downarrow} r_1^{\uparrow}} \qquad (3)$$

The first layer contains most of the chlorophyll with very strong radiation absorption. Transmittance of this layer are very small ($t_1^{\downarrow} \approx t_1^{\uparrow} \approx 0$) and leaf reflectance can be approximated as the reflectance value of the first layer ($R_{12}^{\downarrow} \approx r_1^{\downarrow}$). In addition, the stronger chlorophyll content in the first layer corresponds to a lower layer reflectance than that of layer 2 ($r_1^{\downarrow} << r_2^{\downarrow}$). This proves that the upper face leaf reflectance is expected to be smaller than that of the lower face ($R_{12}^{\downarrow} < R_{12}^{\uparrow}$).

In the near infrared, the smaller transmittance and the larger reflectance values of the upper as compared to those of the lower face may be explained by the is more surprising and was not expected if the reciprocity of light traveling is verified. However, the observed differences in transmittance between the two faces may probably be explained by the directionality of the incident radiation (directional flux normal to the leaf) and the hemispherical nature of the transmitted flux measured. This will be investigated more deeply later.
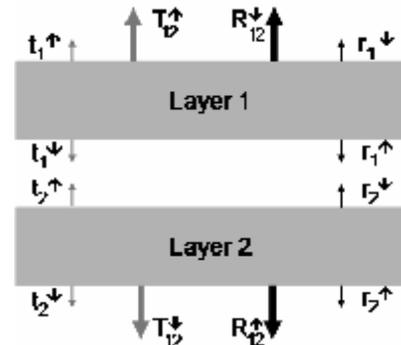

Figure 6. Schema describing the fluxes considered for a 2 layer system.

Resulting from these observations, it appears that leaf absorptance is higher over the whole spectral domain when incident light penetrates from leaf upper face as compared to leaf lower face.

MODELING DIFFERENCES BETWEEN FACES

PROSPECT model (Jacquemoud and Baret, 1990) describes the scattering by the refractive index (n) of bulk leaf material and by a parameter characterizing leaf mesophyll structure (N). Absorption was modeled using a uniform distribution of absorbing materials such as chlorophyll, water and dry matter. Total absorption is the sum of the contribution of each absorbing material, itself computed as the product between the content in expressed in mass per unit leaf area (*Cab*, *Cw* and *Cm* respectively for chlorophyll, water and dry matter) and the corresponding specific absorption coefficients (respectively

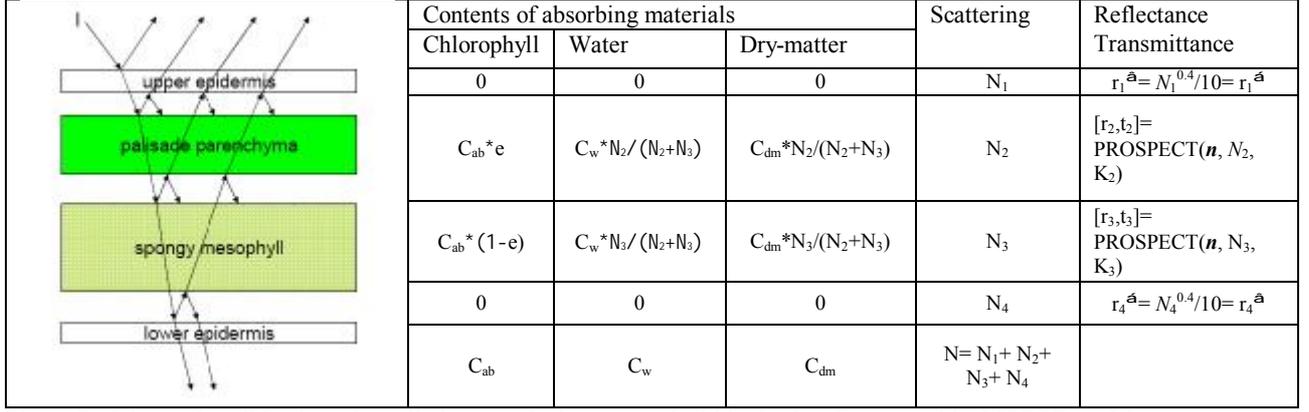| Contents of absorbing materials			Scattering	Reflectance Transmittance
Chlorophyll	Water	Dry-matter		
0	0	0	N_1	$r_1^{\downarrow}= N_1^{0.4}/10= r_1^{\uparrow}$
$C_{ab}*e$	$C_w*N_2/(N_2+N_3)$	$C_{dm}*N_2/(N_2+N_3)$	N_2	$[r_2,t_2]=$ PROSPECT(n, N_2, K_2)
$C_{ab}*(1-e)$	$C_w*N_3/(N_2+N_3)$	$C_{dm}*N_3/(N_2+N_3)$	N_3	$[r_3,t_3]=$ PROSPECT(n, N_3, K_3)
0	0	0	N_4	$r_4^{\downarrow}= N_4^{0.4}/10= r_4^{\uparrow}$
C_{ab}	C_w	C_{dm}	$N= N_1+ N_2+ N_3+ N_4$	

Figure 7. Scheme describing how the radiative transfer is computed within the four layers used in QSPECT model.

Kab, *Kw* and *Km*). The interaction with leaf surface is very simply described by computing the transmissivity and reflectivity of the first interface characterized by a refraction index *n* and an impinging radiation coming from a solid angle α.

The main adaptations of PROSPECT proposed within QSPECT consider the leaf as organized into four layers: two epidermis, palisade parenchyma and spongy mesophyll. Reflectance and transmittance values of each of the four layers are calculated using the PROSPECT model according to the scheme described in Figure 7. In the following, indices (1), (2), (3) and (4) refer to each layer according to Figure 7.

Epidermis layers are very thin with a small structure index N <0.01 and assumed having no absorption. Therefore $r_1^{\downarrow}= r_1^{\uparrow}$ and $t_1^{\downarrow}= t_1^{\uparrow}=1- r_1^{\downarrow}$. Similarly, $r_4^{\downarrow}= r_4^{\uparrow}$ and $t_4^{\downarrow}= t_4^{\uparrow}=1- r_4^{\downarrow}$. Since the PROSPECT model isn't applicable for such small values of N, an approximation was proposed offering a solution of continuity between reflectances computed between $N=0$ and $N= 0.01$: $r = aN^b$ where $a=1/10$, $b=0.4$, for all wavelengths since the refractive index does not vary much with wavelength, hence layer reflectance and transmittance.

Palisade and spongy mesophyll are characterized respectively with N_2 and N_3 structure parameters. However, parameter $p = N_2/(N_2 + N_3)$ was preferred to better denote the gradient in scattering properties. Total chlorophyll content, C_{ab}, is distributed in the two mesophyll layers using parameter e computed as the ratio between chlorophyll concentration of the palisade mesophyll and the total chlorophyll content. Water and dry matter are assumed distributed proportionally to the N parameter in the palisade and spongy mesophyll layers.

The radiative transfer between each of these layers may be described by the following set of equations, where reflectances and transmittances of upper and lower faces of each layer $i=1$, 2, 3, 4 are represented by $r_i^{\downarrow}$, $t_i^{\downarrow}$, $r_i^{\uparrow}$ and $t_i^{\uparrow}$. Reflectance and transmittance made of layers 1 and 2 are noted $R_{12}^{\downarrow}$, $T_{12}^{\downarrow}$, $R_{12}^{\uparrow}$ and $T_{12}^{\uparrow}$ and computed from equations (2) and (3). For 3 layers: $R_{123}^{\downarrow}$, $T_{123}^{\downarrow}$, $R_{123}^{\uparrow}$ and $T_{123}^{\uparrow}$ are computed according to:

$$R_{123}^{\downarrow} = R_{12}^{\downarrow} + \frac{T_{12}^{\downarrow}r_3^{\downarrow}T_{12}^{\uparrow}}{1-r_3^{\downarrow}R_{12}^{\uparrow}} ; \quad T_{123}^{\downarrow} = \frac{T_{12}^{\downarrow}t_3^{\downarrow}}{1-r_3^{\downarrow}R_{12}^{\uparrow}} \qquad (4)$$

$$R_{123}^{\uparrow} = r_3^{\uparrow} + \frac{t_3^{\uparrow}R_{12}^{\uparrow}t_3^{\downarrow}}{1-r_3^{\downarrow}R_{12}^{\uparrow}} ; \quad T_{123}^{\uparrow} = \frac{t_3^{\uparrow}T_{12}^{\uparrow}}{1-r_3^{\downarrow}R_{12}^{\uparrow}} \qquad (5)$$

Finally, leaf total reflectance and transmittance noted $R^{\downarrow}$, $T^{\downarrow}$, $R^{\uparrow}$ and $T^{\uparrow}$ of upper face and lower faces for four layer system are given by:

$$R^{\downarrow} = R_{123}^{\downarrow} + \frac{T_{123}^{\downarrow}r_4^{\downarrow}T_{123}^{\uparrow}}{1-r_4^{\downarrow}R_{123}^{\uparrow}} ; \quad T^{\downarrow} = \frac{T_{123}^{\downarrow}t_4^{\downarrow}}{1-r_4^{\downarrow}R_{123}^{\uparrow}} \qquad (6)$$

$$R^{\uparrow} = r_4^{\uparrow} + \frac{t_4^{\uparrow}R_{123}^{\uparrow}t_4^{\downarrow}}{1-r_4^{\downarrow}R_{123}^{\uparrow}} ; \quad T^{\uparrow} = \frac{t_4^{\uparrow}T_{123}^{\uparrow}}{1-r_4^{\downarrow}R_{123}^{\uparrow}} \qquad (7)$$

Consistency of the computation of reflectance and transmittance for the two faces was checked in the case of homogeneous chlorophyll distribution and reflectivity of the first interface computed according to the original PROSPECT model. As expected, QSPECT simulations are equal to thos of PROSPECT in thisvery particular case. When using typical values for the parameters, QSPECT model simulations shows differences of leaf reflectances between the two faces in the visible domain. In the near infrared and short wave infrared domains, no differences are observed both in reflectance and transmittance values as expected according to QSPECT model assumptions (Figure 8).
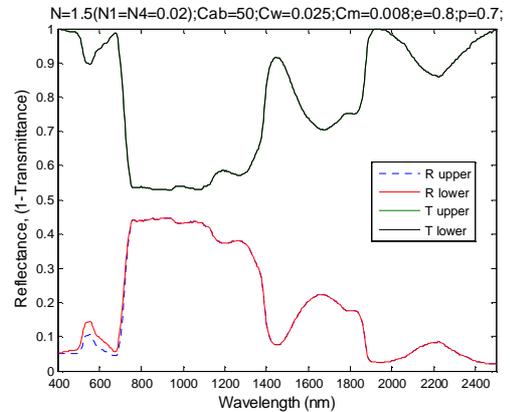

Figure 8. Reflectance and transmittance spectra of upper and lower face calculated with model QSPECT

leaf	N	$C_{ab}+C_\beta$ ($\mu g/cm^2$)	Cm (g/cm^2)	e	p	N_1	N_4
Ivy	1.5	49 (51)[*]	0.0047	0.88	0.70	0.001	0.005
Maple(young)	1.01	18 (18)	0.0006	0.64	0.52	0.001	0.001
Tilia	1.56	44 (48)	0.0008	0.96	0.58	0.001	0.004
Medlar	1.39	34 (37)	0.0006	0.95	0.66	0.001	0.006
Musa	1.10	49 (50)	0.0007	0.96	0.79	0.001	0.003
Sage	1.19	42 (40)	0.0013	0.97	0.85	0.001	0.001

Table 1. Coefficient of Determination Obtained for the Estimation of chlorophyll, dry matter, parameter e, p and N1, N4 calculated with QSPECT.
Note:* the numbers within brackets are estimated by PROSPECT Model.

As compared to the initial PROSPECT model, description of differences between faces is achieved at the expense of 4 additional parameters that do not vary with wavelength: N_1, N_4, e and p. In the following section we will investigate the effect of these parameters on leaf optical properties.

SENSITIVITY ANALYSIS

Simulations will be restricted to the visible up to the beginning of near infrared domain since no differences are expected in the near and shortwave infrared domains accordingly to QSPECT model assumptions. The sensitivity analysis will be achieved over a typical leaf with Cab=50, Cw=0.025, Cdm=0.008, N=1.5, N_1=0.01, N_4=0.02, e=0.8, p=0.7. Reflectance of the upper leaf will be shown.

Figure 9 illustrates several new parameters affect the reflectance. The parameter e has greater influence in VIS, others parameters have also enough influence toward the reflectance.

VALIDATION

Validation of QSPECT was carried out over the data sets measured previously and including six types of leaves. It consisted in estimating the model parameters symbolized by the vector X by minimizing the following merit function:

$$F(X) = \sum_2 \sum_l \left(\frac{(r_{mod}(l) - r_{mes}(l))^2}{s_r} + \frac{(t_{mod}(l) - t_{mes}(l))^2}{s_t} \right)$$

Where 2 represent the upper face and lower face, l is the wavelength, r_{mes} and r_{mod} are respectively the measured and modeled reflectances, t_{mes} and t_{mod} are respectively the measured and modeled transmittances, s_r and s_t are the variances of the measured reflectances et transmittances. Inversions were performed using a routine fminsearch.M in Matlab. In Table 1 we show the coefficients of determination for each biochemical.

We notice that the parameter e and p are greater than 0.5, this result verifies that the chlorophyll is more concentrated in the upper part or in the palisade parenchyma, and the palisade parenchyma has more complex structure and more cellular component.

Figures 11 and 12 do not show any significant difference between measured and calculated ones. It exhibits root mean squares lower than 0.02, indicating good spectrum reconstruction.

These results indicate that QSPECT model is capable of being applied to different type leaves. It can describe the chlorophyll gradient and the distribution of cellular component inside leaf. Relative to model PROSPECT (Figure 13), it can accurately simulate the spectral of two faces.

CONCLUSION

This paper concerns leaf optical properties and their modeling, and provides a new model which are used to accurately simulate the different spectral of upper and lower leaf faces and estimate biochemical contents. There are still many improved aspect and further work should ulteriorly consider the effect of leaf surface which has an important role in optical properties of plant canopy.
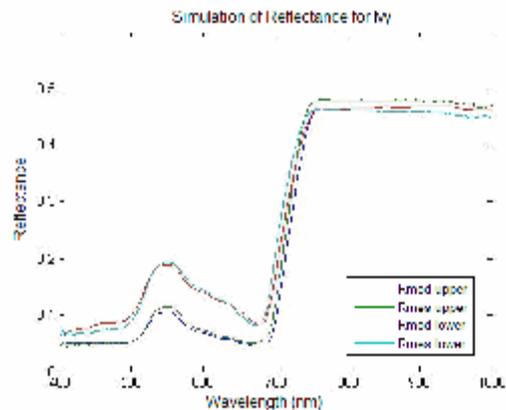

Figure 10. Comparison of the spectral reflectance and transmittance modeled and measured for Ivy By Model QSPECT.
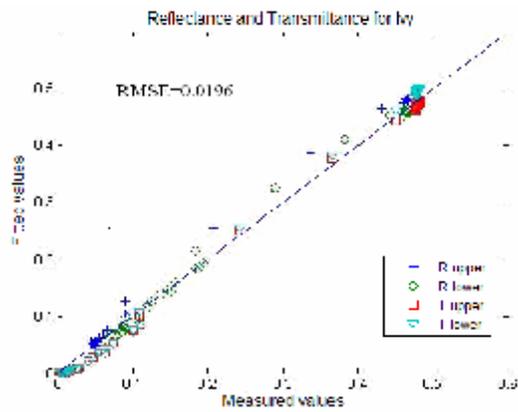
Figure 12. Comparison between simulated and measured reflectance and transmittance for Ivy.
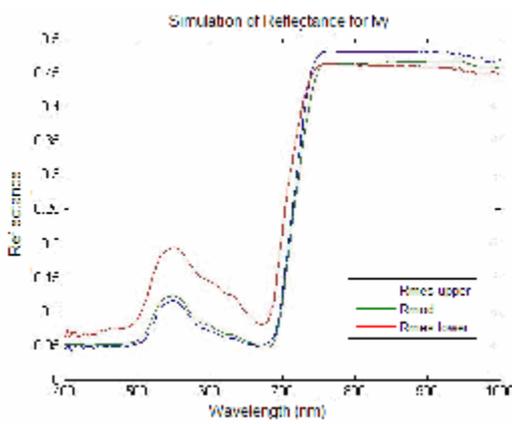

Figure 13. Comparison of the spectral reflectance and transmittance modeled and measured for Ivy by Model PROSPECT.

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