1. INTRODUCTION

The remote estimation of leaf biochemical content from spaceborne platforms has been the subject of many studies aimed at better understanding of terrestrial ecosystem functioning. The major ecological processes involved in exchange of matter and energy, like photosynthesis, primary production, evapotranspiration, respiration, and decomposition can be related to plant properties e.g., chlorophyll, water, protein, cellulose and lignin contents (Peterson, 1991). As leaves represent the most important plant surfaces interacting with solar energy, a top priority has been to relate optical properties to biochemical constituents. Two different approaches have been considered: first, statistical correlations between the leaf reflectance (or transmittance) and biochemical content, and second, physically based models of leaf scattering and absorption developed using the laws of optics. Recently reviewed by Verdebout et al. (1994), the development of models of leaf optical properties has resulted in better understanding of the interaction of light with plant leaves.

Present radiative transfer models mainly use chlorophyll and/or water contents as input parameters to calculate leaf reflectance or (Jacquemoud and Baret, 1990; Fukshansky et al., 1991; Yamada and Fujimura, 1991; Martinez v. Remisowsky et al., 1992). Inversion of these models allows to retrieve these constituents from spectrophotometric measurements. Conel et al. (1993) recently proposed a two-stream Kubelka-Munk model to analyse the influence of protein, cellulose, lignin, and starch on leaf reflectance, but in fact, the estimation of leaf biochemistry from remote sensing is still an open question. In order to clarify it, a laboratory experiment associating visible/infrared spectra of plant leaves both with physical measurements and biochemical analyses was conducted at the Joint Research Centre during the summer of 1993. This unique data set has been used to upgrade the PROSPECT model (Jacquemoud and Baret, 1990) by including leaf biochemistry.

2. THE EXPERIMENT

The LOPEX (Leaf Optical Properties Experiment) is detailed in Jacquemoud et al. (1994); it consists of a wide range of variation in leaf internal structure, pigments, water, and biochemistry contents. In total, about 70 leaf samples representing 50 woody and herbaceous species were obtained from trees and crops near the Joint Research Centre in Italy. The hemispherical reflectance (R), transmittance (T), and infinite reflectance (R∞) of fresh and dry leaves were measured using a Perkin Elmer Lambda 19 spectrophotometer over the 400-2500 nm wavelength interval.

Many physical and biological measurements were performed on leaf samples: blade thickness, specific leaf area (SLA = dry weight per unit leaf area), equivalent water thickness (EWT = water mass per unit leaf area), photosynthetic pigments (chlorophyll a, b, and total carotenoids), biochemical components (total proteins, cellulose, lignin, and starch), and finally elementary composition (C, H, O, N). Table 1 gives descriptive statistics and illustrates the range in leaf biophysical characteristics. Good relationships among some biochemicals were established, including leaf thickness.
<table>
<thead>
<tr>
<th>thickness (μm)</th>
<th>range</th>
<th>mean</th>
<th>std</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLA (cm².g⁻¹)</td>
<td>73.9 - 535.3</td>
<td>224.6</td>
<td>93.4</td>
</tr>
<tr>
<td>EWT (g.cm⁻²)</td>
<td>0.0046 - 0.0405</td>
<td>0.0115</td>
<td>0.0067</td>
</tr>
<tr>
<td>Chl. a (μg.cm⁻²)</td>
<td>12.8 - 64.2</td>
<td>36.9</td>
<td>11.4</td>
</tr>
<tr>
<td>Chl. b (μg.cm⁻²)</td>
<td>3.7 - 21.3</td>
<td>11.7</td>
<td>3.8</td>
</tr>
<tr>
<td>Carot. (μg.cm⁻²)</td>
<td>3.7 - 19.4</td>
<td>10.5</td>
<td>3.6</td>
</tr>
<tr>
<td>Proteins (% MS)</td>
<td>7.4 - 36.7</td>
<td>20.0</td>
<td>7.0</td>
</tr>
<tr>
<td>Cellulose (% MS)</td>
<td>9.1 - 37.2</td>
<td>19.7</td>
<td>6.4</td>
</tr>
<tr>
<td>Lignin (% MS)</td>
<td>1.1 - 27.5</td>
<td>10.2</td>
<td>6.5</td>
</tr>
<tr>
<td>Starch (% MS)</td>
<td>0.0 - 10.0</td>
<td>1.9</td>
<td>2.1</td>
</tr>
<tr>
<td>Carbon (% MS)</td>
<td>38.5 - 52.3</td>
<td>47.1</td>
<td>2.9</td>
</tr>
<tr>
<td>Nitrogen (% MS)</td>
<td>1.2 - 5.9</td>
<td>3.4</td>
<td>1.1</td>
</tr>
</tbody>
</table>

Table 1. Leaf biophysical measurements.

The strongest relationships were obtained between nitrogen and proteins, and between carbon and cellulose + lignin (Figure 1). This equivalence is very important because the C/N ratio which drives the decomposition rates of forest litter, affecting nutrient cycling and trace gas fluxes, can be replaced by the cellulose + lignin over protein ratio.

3. CONSTRUCTION OF THE MODEL

PROSPECT is a radiative transfer model which calculates the leaf spectral reflectance and transmittance from 400 to 2500 nm. Scattering is described by the refractive index (n) of leaf materials and by a parameter characterizing the leaf mesophyll structure (N). Absorption is modeled using pigment concentration (Cab), water depth (Cw ↔ EWT), and the corresponding specific absorption coefficients (Kab and Kw).

Modeling absorption processes implies that the effects of mesophyll structure in the NIR (780-920 nm) are accounted for. The reflectance and transmittance levels in the NIR are driven by the parameter N, number of stacked elementary layers. In the basic version of PROSPECT, the absorption by one elementary layer was small and was assumed to be constant (ko=0.0134). The origin of this absorption is uncertain but it cannot be attributed to either chlorophyll or water. Hypothesizing that NIR radiation is absorbed by the cell walls, then leaf optical properties must be explained by the N parameter and the absorption coefficient ko of the elementary layer. Neglecting the contributions of water and starch which are very small, ko can be written both as a function of N and the protein and cellulose+lignin concentrations expressed in g.cm⁻².

\[
k_o = \frac{k_1 \cdot \text{[protein]} + k_2 \cdot \text{[cellulose + lignin]}}{N}
\]
The N parameter has been adjusted for each leaf while a global value for the two specific absorption coefficients was determined (k1=12.10 and k2=6.92). In that way, leaf reflectance and transmittance in the NIR are well modeled with a root mean square error \( rmse = 0.0243 \). The \( k_0 \) values range from 0.0050 to 0.0275 with an average of 0.0135 which is very close to the constant provided by Jacquemond and Baret (1990); in consequence, if leaf biochemistry is unknown, the coefficient \( k_0=0.0135 \) can be used with reasonable results (\( rmse=0.0250 \)).

The wavelength independent mesophyll structure parameter N is used to invert the Stokes equations: using measured reflectance and transmittance, the compact layer is easily calculated, permitting the determination of a spectral absorption coefficient \( k_0(\lambda) \). If the assumption is made that the leaf is a homogeneous mixture of biochemical components, the absorption coefficient can be written as:

\[
k_0(\lambda) = k_1(\lambda)[\text{protein}]+k_2(\lambda)[\text{cellulose + lignin}]+k_3(\lambda)[\text{water}]+k_4(\lambda)[\text{pigments}]
\]

where \( \lambda \) is the wavelength, \( k_1(\lambda)...k_4(\lambda) \) are respectively the specific absorption coefficients for protein, cellulose+lignin, water, and photosynthetic pigments (chlorophyll a+b and total carotenoids). \( k_e(\lambda) \) explains the non-zero absorption of an albino leaf under 500 nm. Assuming that the specific absorption coefficients are known, one can predict the constituent concentrations and compare them with measured ones. For various reasons, this method is difficult to apply so another strategy was adopted: using the absorption coefficients \( k_0(\lambda) \) and the measured concentrations, we deduced the specific absorption coefficients of leaf biochemical components.

![Figure 2](image-url)

**Figure 2.** Specific absorption coefficients of a) photosynthetic pigments [the dotted points correspond to pigments in acetone, Lichtenthaler, 1987] b) water [the dotted points correspond to pure liquid water, Curcio and Petty, 1951] c) protein [the dotted points correspond to pure powdered material, Wessman, 1990] d) cellulose+lignin [the dotted points correspond to pure powdered material, Wessman, 1990].
Figure 2 shows that $k_3(\lambda)$ agrees very well with the fundamental constants published for pure liquid water. For pigments, the specific absorption coefficient $k_4(\lambda)$ displays classical features with some spectral shifts of the principal absorption peaks compared to \textit{in vitro} observations. Results are less convincing for protein and cellulose+lignin: in particular, absorption peaks for protein are not well represented. Cellulose+lignin is better reproduced with some characteristic spectral features.

4. VALIDATION

Before a model can be used with confidence it must be validated. We tested our model in direct mode, by simulating reflectance and transmittance of 63 fresh leaves using the measured concentrations of pigments, water, protein, cellulose+lignin, and the estimated values of the mesophyll structure parameter $N$; the spectral $\text{rmse}$ is low ($<0.02$) except in the absorption peaks of the visible where it equals 0.03. The transmittance, which is generally more sensitive to the model parameters than the reflectance, is surprisingly better simulated. The validation was carried out with the same data set. In Figure 3 the values provided by the model inversion are plotted against measured values: the high correlation for pigments and water shows that the procedure is successful in retrieving major leaf components whose effects predominate. Concerning minor ones, we notice that there is no sensitivity for protein but that cellulose+lignin is well estimated. In terms of reflectance and transmittance reconstruction, the very low spectral $\text{rmse}$ ($<0.01$) demonstrates the capability of this new version of the PROSPECT model to accurately synthesize the whole leaf spectrum for widely different kinds of plant leaves using only 5 parameters.

5. CONCLUSION

In spite of the difficulties to derive specific absorption spectra in agreement with the literature, these results are very promising. It indicates that water does not obstruct all of the signal in the SWIR and that leaf biochemistry is potentially attainable from remote sensing data. The extension of the PROSPECT model to important constituents other than chlorophyll or water, i.e. proteins and cellulose+lignin, should help us to understand their specific effects on the radiometric signal. Finally, the search for the best specific absorption curves is certainly not ended.
REFERENCES


