APPLICATION OF A TWO-STREAM RADIATIVE TRANSFER MODEL FOR LEAF LIGNIN AND CELLULOSE CONCENTRATIONS FROM SPECTRAL REFLECTANCE MEASUREMENTS (PART 1)

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1. **Introduction.** Lignin and nitrogen contents of leaves constitute the primary rate-limiting parameters for the decomposition of forest litter, and are determinants of nutrient- and carbon-cycling rates in forest ecosystems (Melillo et al., 1982). Wessman et al. (1988a) developed empirical multivariate relationships between forest canopy lignin amount and the (first-difference) AIS spectral response in three bands spread over the wavelength interval 1256-1555 nm. Wessman et al. (1988b) and McLellan et al. (1991) developed similar regression relationships from laboratory reflectance measurements on dried samples prepared in a standard fashion. They used four to six infrared bands for analysis of nitrogen, lignin and cellulose content of foliage in forest and prairie species. In the present article (Parts 1 and 2) the feasibility of compositional determinations is explored using positions of composite absorption bands that originate from mixtures of lignin, cellulose, and possibly other chemical constituents in the spectral reflectance of green leaves. To carry out this program, we employ full-spectral-resolution single-leaf diffuse reflectance measurements made with a laboratory spectrometer and integrating sphere. The leaf and other chemical reflectance data compiled by Elvidge (1990) have also been utilized extensively.

2. **Model.** The spectra of fresh leaves contain strong liquid water absorptions that may mask nearly completely the spectral signatures of other leaf chemical constituents (e.g., Elvidge, 1990). A background liquid leaf water reflectance spectrum is required to remove the effects of liquid water. Previously, such a background spectrum was estimated using mixtures of glass beads and liquid water (Goetz et al. 1990). In the present work on the other hand, the so-called Kubelka-Munk (KM) theory of radiative transfer (Wendlandt and Hecht, 1966) was used to estimate the liquid water spectrum from the leaf diffuse spectral reflectance itself. In a first approximation single leaves are assumed to consist of distinct but well-mixed liquid water and dry components each characterized by intrinsic absorption (k_w, k_d) and scattering (s_w, s_d) functions (hereafter simply intrinsic functions). The dry components are in turn assumed to consist of well-mixed lignin, cellulose, starch, protein, and other organic compounds (see Elvidge, 1990, for representative visible and near-infrared spectra). In the KM theory, which was originally developed to calculate the reflectance of paint films, independent as well as purely backward scattering (van de Hulst, 1980) are assumed by all constituents. These assumptions are almost certainly violated to one extent or another in leaves. Comparing the k- and s-functions of KM theory with parameters of two-stream atmospheric models (see, for example, Coakley and Chylek, 1975), shows k is identified with particle absorption, given by $1 - \varpi_0$, where ϖ_0 is the single scattering albedo, and s with the scattered fraction $\varpi_0\beta$, where β is the average forward scatter for isotopically incident radiation (Wiscombe and Grams, 1976).

3. **Calculation of k- and s-functions.** We develop mixing laws that comprise relationships between bulk leaf scattering (S) and absorption (K) functions

and the intrinsic functions of assumed individual components; the bulk functions are simple linear sums of the intrinsic functions weighted by constituent concentrations (c_w, c_d). For a simple two-component system, the intrinsic functions are isolated individually by use of reflectance (R) and transmittance (T) measurements on single leaves, both wet and desiccated, together with theoretical relationships for R and T for single uniform layers from KM theory (Wendlandt and Hecht, 1966, p. 60). Allen and Richardson (1968) first used single leaf R and T data to calculate k- and s-coefficients for cotton leaves. The intrinsic functions derived in this way for *Liquidambar styraciflua* (sweetgum) are given in Figure 1.

4. **Leaf water reflectance.** Given k_w and s_w of Figure 1, the reflectance $R_{w\infty}$ of a semi-infinite body of "pure" liquid leaf water was calculated from the so-called KM remission function (Kortum, 1969, p.180, discusses the remission function). A light path through a stack of 5 or 6 leaves approximates an infinite thickness condition at all wavelengths between 400-2500 nm, since no change in reflectance occurs with addition of further layers. The resulting $R_{w\infty}$ is shown in Figure 2. The function represented has been smoothed once by a three-point "hanning" filter (Blackman and Tukey, 1958) to suppress fluctuations in the calculated k- and s-functions from noise in the reflectance data themselves. The curve of Figure 2 has been taken arbitrarily to represent a generic background water reflectance for derivation of dry constituent spectral residuals from the optically infinite thickness green leaf diffuse reflectance. An example comparing $R_{w\infty}$ with the equivalent semi-infinite reflectance for sweetgum, calculated from K and S via the remission function, is shown in Figure 3. Both curves have been translated to zero reflectance at 1452 nm, and the water reflectance was adjusted by a single scale factor to achieve the match shown. Similar adjustments of origin and scale in $R_{w\infty}$ were required in calculation of residuals for foliage of other species, as described next.

5. **Reflectance residuals.** We calculated fractional residual reflectances for sweetgum, sycamore (*Platanus racemosa)*, pinyon pine (*Pinus monophylla*) and bigberry manzanita (*Arctostaphylos glauca*) using the generic water reflectance curve. These results are given in Figure 4 for the spectral region 1400-1900 nm. The fractional residual reflectance is defined as $1 - (R_{w\infty} - R_{i\infty})/R_{w\infty}$ where $R_{i\infty}$ is the measured (or calculated) reflectance for infinite thickness of species i. The diffuse reflectance data for sycamore, pinyon pine, and manzanita were taken from Elvidge (1990). These examples are distinguished from one another by apparent systematic displacements of reflectance minima from one species to the next and by the presence of both major and minor structures in the pinyon and manzanita residuals that are not shared by the other examples. The noise-equivalent reflectance variation ($ne\Delta R$) in these data was estimated numerically by calculating residuals from a second-degree polynomial fit to a smooth piece of the raw sweetgum reflectance (1500-1600 nm, 24 points) with a resulting rss error of 0.0000016 in reflectance units and an average fractional uncertainty of 0.000001.

6. **Comparison of desiccated leaf and residual spectra.** From the derived k_d and s_d values given in Figure 1 we also calculated the expected reflectance $R_{d\infty}$ for desiccated sweetgum via the remission function, and compared structures in that reflectance with structures present in the (presumed liquid water-free) residual spectrum for sweetgum in Figure 3. This comparison is made in Figure 5. Apart from positions of minor features these curves do not resemble one another; the presence of important (lignin + cellulose + other) absorptions remains masked in the extracted residual spectrum. Features in the calculated sweetgum spectrum $R_{d\infty}$ are, on the other hand, present in the pinyon and manzanita residuals in Figure 4.

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8. **References.**

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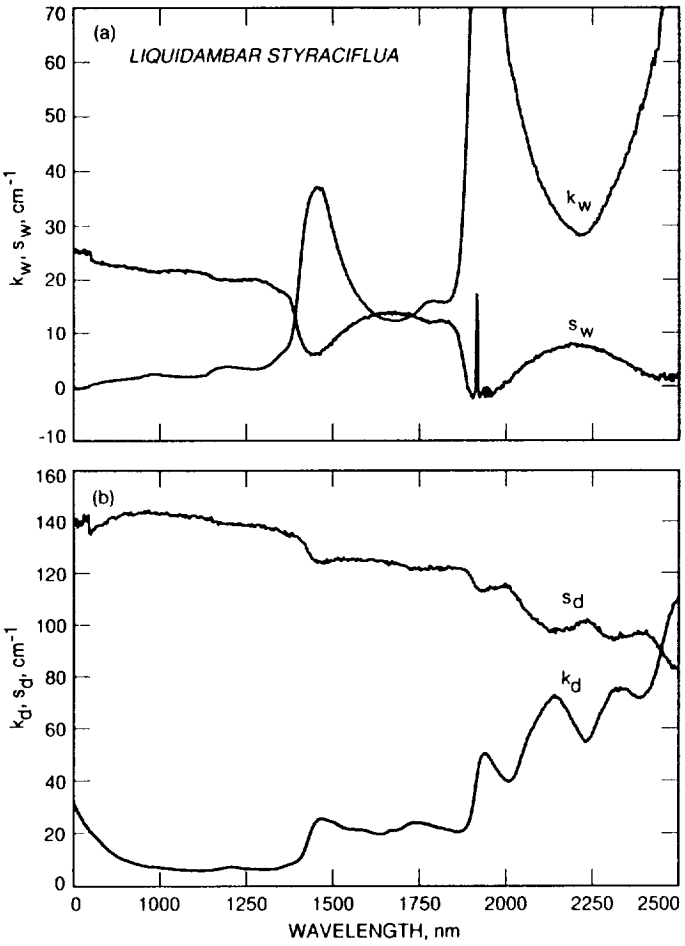

Figure 1. *L. styraciflua.* (a) intrinsic functions for leaf liquid water component. (b) intrinsic functions for bulk desiccated leaf components.

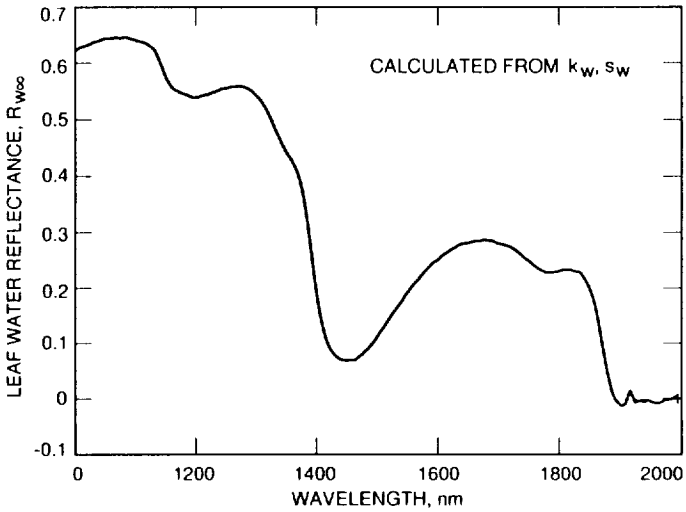

Figure 2. *L. styraciflua* leaf liquid water reflectance calculated from k_w and s_w.

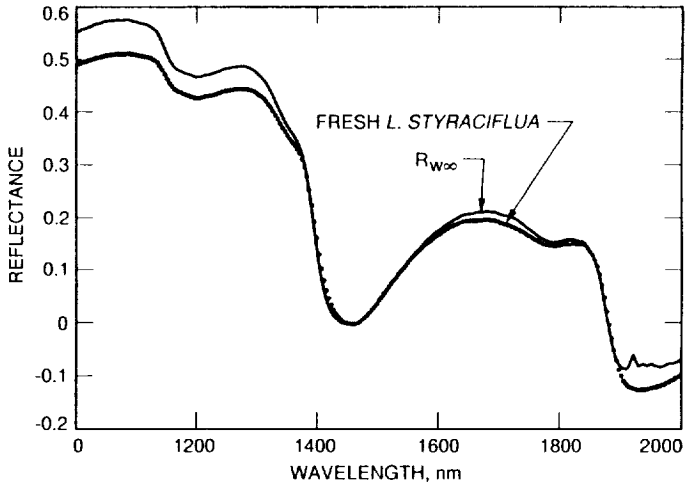

Figure 3. Liquid water reflectance $R_{w\infty}$ compared to the infinite thickness reflectance of *L. Styraciflua.*

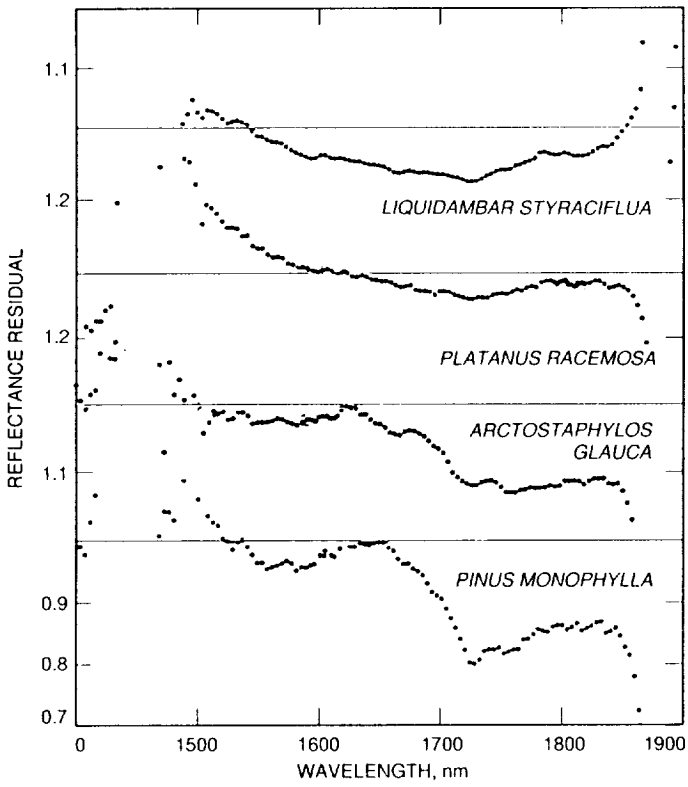

Figure 4. Reflectance residuals for fresh leaves and needles of four plant species.

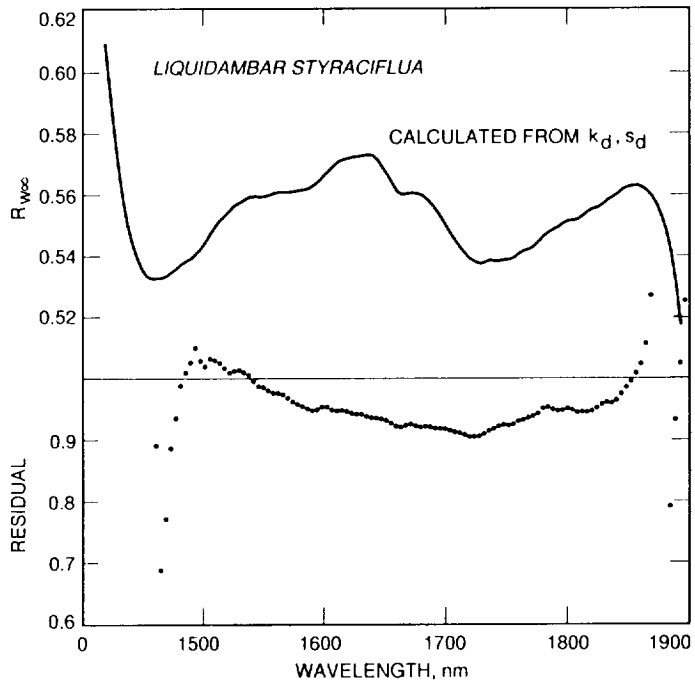

Figure 5. Comparison of the calculated desiccated leaf reflectance for *L. styraciflua* with its fresh leaf reflectance residual.