

LEAF REFLECTANCE A STOCHASTIC MODEL FOR ANALYSING THE BLUE SHIFT

W. Lüdeker, K.P. Günther

DLR - Oberpfaffenhofen, Institute of Optoelectronics, D- 8031 Wessling, West-Germany

ABSTRACT

In order to investigate the blue shift of the red edge in the reflectance spectra theoretically, the stochastic leaf model of Tucker and Garratt (1977) was used. This approach treats the radiative transfer of diffuse light as transitions of light with weighted probabilities according to the theory of homogeneous Markov processes with a finite number of states. The transition probabilities are determined by the optical parameters (e.g. specific absorption coefficients of different pigments, scattering coefficients and refractive index of cell membranes), the pigment concentrations and the geometrical dimensions of the leaf (e.g. total leaf thickness, thickness of palisade and spongy parenchyma and the geometrical cross section of chloroplasts and cells).

Assuming realistic leaf parameters our results showed that the modeled reflectance spectra were not in agreement with measured data and the spectra presented by Tucker and Garratt (1977).

Based on these findings the model was reinvestigated. By introducing a new radiation state and by revising the transition probabilities of Tucker and Garratt a successful modeling of reflectance spectra is possible assuming realistic leaf parameters.

In order to investigate the blue shift of the red edge the model parameters were varied systematically. It was shown that

- a reduced light absorption and / or
 - a shift in the absorption spectra of chlorophyll *a* and *b*
- are responsible for the observed blue shift of the red edge.

A reduced light absorption is not only caused by a reduced pigment concentration but also by a reduced light path. In turn the light path may be reduced by a decrease of the thickness of the palisade and / or spongy parenchyma or may be reduced by a decrease of the scattering coefficients.

The shift of the absorption bands of chlorophyll *a* or *b* may occur to a minor extent when the chlorophyll-protein aggregates make a phase transition from polymers to dimers or monomers due to environmental stress. By treating leaves with the herbicide DCMU in the laboratory the observed blue shift may be attributed to a shift of the absorption bands by partially extracting the chlorophyll pigments from the proteins.

Key Words: Leaf reflectance, stochastic model, Markov chain, blue shift, red edge

1 INTRODUCTION

Observing the reflectance spectra of vegetation in the visible domain a variation of the steep rise of the near-infrared reflection edge at about 690 nm can be seen. In the last few years the application of high resolution imaging spectroscopy stimulated the remote detection of this phenomenon, called the blue shift of the red edge, in order to monitor vegetative chlorophyll status and leaf area index independently (Horler et al. 1983) and plant stress induced e.g. by geochemical metal deposition (Collins et al. 1983). The trace metal-induced stress retards the pigment synthesis and in turn decreases the pigment

absorption leading to higher reflectance. Since the spectral shift is related not only to soil geochemistry but also to tree species (Singhroy et al. 1985) a uniform forest stand is best suited for studying the blue shift. A comparison of in situ and airborne spectral measurements of the blue shift in Vermont and West-Germany over homogeneous forest stands (Rock et al. 1988) showed that the blue shift is associated with damage in spruce needles. The authors suggested that the shift of the red edge to shorter wavelengths may be due to an absorption line narrowing when the chlorophyll *a* concentration decreases in contrast to the explanation of a shift in the position of the maximum of the chlorophyll absorption. Also Buschmann and Lichtenthaler (1988) correlated the observed blue shift of the red edge

for cherry-laurel leaves with the chlorophyll *a* and *b* concentration in agreement with Horler et al. (1980).

Recently, Lichtenthaler and Buschmann (1987) proposed an alternative explanation of the blue shift. They suggested that the fluorescence of chlorophyll *a* may account for the observed phenomenon because the chlorophyll *a* fluorescence spectrum coincides with reflectance spectrum at the red edge and because the fluorescence increases with decreasing pigment concentration.

A quite different explanation for the shift of the red edge observed during the growth of wheat is given by Schutt et al. (1984). These authors found that the leaf surface exposed to the incident light during heading and after emergence of the head determined the wavelength position of the red edge due to the amorphous nature of the cuticle layer of the lower leaf surface. Thus the increased reflectance of the lower leaf surface gave an indication of lower pigment absorption than the upper leaf surface.

Model simulations of Baret et al. (1988) demonstrated that the inflection point of the red edge shifts toward shorter wavelengths when the chlorophyll *a* concentration decreases. The authors derived a simple semi-empirical model for the reflectance of wheat introducing an equation for the reflectance depending on the chlorophyll concentration and the measured reflectance at 760 nm. Additionally, three constants are required for the model, while one parameter is used for adjusting the results to the experimental data.

Comparable with these theoretical findings are the calculated results of Guyot et al. (1988). In addition they found that the blue shift of the red edge is correlated with the decrease of the leaf area index (LAI).

The aim of our work is to model the reflectance spectra of leaves based on the stochastic description of radiative transfer. This technique needs the optical and geometrical parameters as well as the pigment concentrations as input parameters in contrast to semi-empirical models where the a priori knowledge of the reflectance spectrum is necessary.

2 THEORY

The time evolution of dynamic systems, which are not formalized in a classical and deterministical way, can be handled by a succession of stochastic states of the system. In the stochastic leaf model the states of the system are represented by different radiation states (diffuse solar input, reflectance at the upper cuticle, diffuse reflectance, absorption, scattering, diffuse transmittance) in different structures of the leaf (cuticle, palisade parenchyma, spongy

mesophyll).

The stochastic process is called Markov chain, when the system can be separated in well distinguishable finite number of states and the probability for the appearance of every state can be described by a chain of random numbers.

If the development of the system in time is independent from the history of the process the Markov chain is named "homogeneous". In consequence, homogeneous Markov chains are without memory.

The realisation of the leaf model in a Markov chain by defining the states of the system is shown in figure 1.

Tucker and Garratt (1977) proposed in their model to divide the leaf in three compartments:

- the epidermal layer, which is regarded as a totally homogeneous and transparent medium. It is responsible for a partial reflectance at the cuticle.
- the palisade parenchyma, where light scattering at the parenchyma cells and absorption in the pigmentation occurs.
- the spongy mesophyll, where light scattering and absorption occurs as in the palisade parenchyma. But the scattering coefficient will be much greater, because the cell density is very high and there are many intracellular airspaces localized. The absorption will be very low, because the pigment concentration in this cell layer is very low.

In contrast to the model of Tucker and Garratt (1977) a new compartment was introduced. This radiation state allows partially direct transmittance of the scattered light of the spongy mesophyll through the palisade parenchyma.

After the definition of the states of the system the radiative transfer from one state to another state is treated as transitions of light with weighted probability. The basis for the probabilities are the optical, the geometrical and the physiological parameters of the leaf.

At least one has to arrange the transition probabilities in a square transition-matrix $R[i][j]$, which has as much columns as states are included in the model. Running the model leads to iterative multiplication of an input vector at time 0, $v[j](t=0)$, with the transition-matrix $R[i][j]$. In general $v[j](t)$ represents the probability distribution at a given time of the process. Every iteration step modifies the vector to an vector $v[j](t+dt)$. This new vector is taken as input for the next step. After a finite number of iterations the vector comes to a steady state if the process is a "finite" Markov process.

Irradiance-Flow-Model

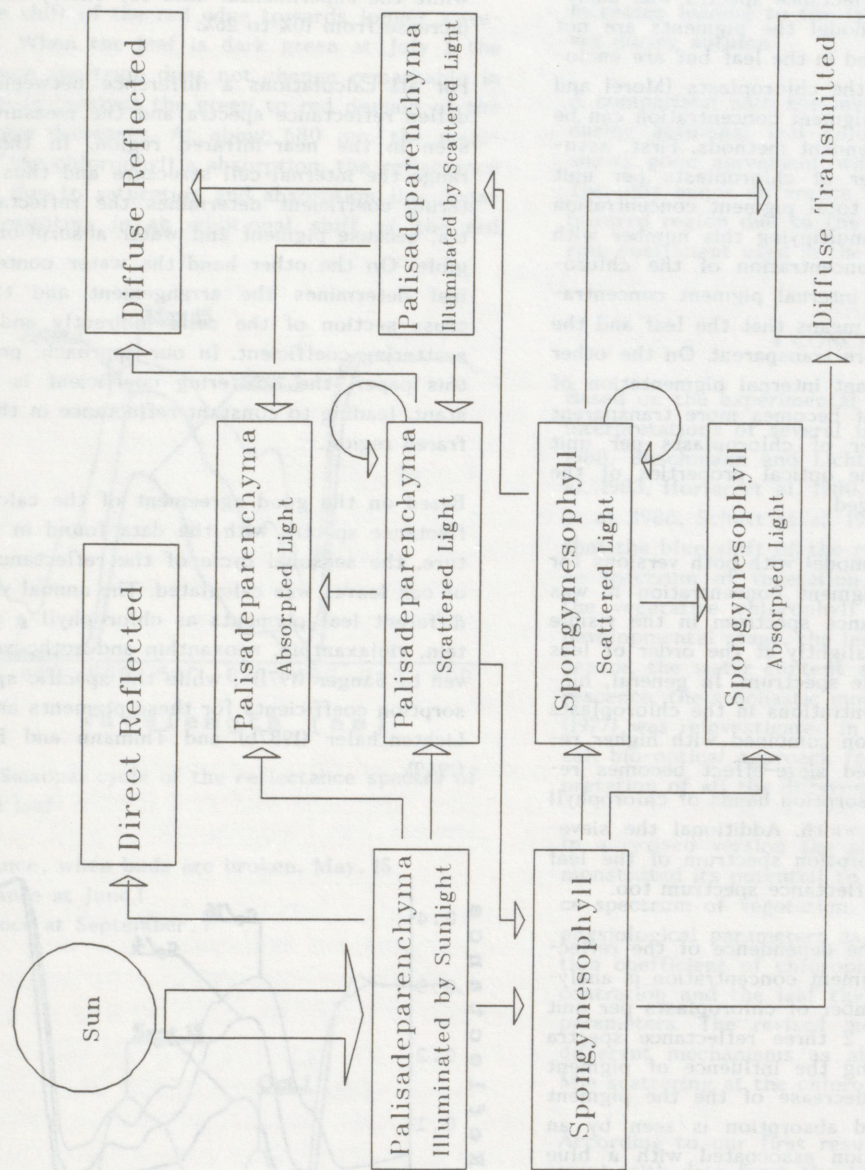


Figure 1: Schematic diagram of the structural entities of the revised model leaf including the physical mechanisms as absorption, reflection, scattering and transmission. All compartments are forming the state of the system.

3 RESULTS

Some results of the model simulations are presented in figure 2 to 4. All parameters needed for the calculations are taken from the literature, but in some cases not all optical, geometrical or physiological parameters were found so that some estimates had to be made.

In our first approach the influence of the pigment concentration on the reflectance spectra was analyzed. According to our model the pigments are not homogeneously distributed in the leaf but are enclosed in small particles, the chloroplasts (Morel and Bricaud 1981). Thus the pigment concentration can be calculated by two independent methods. First, assuming a constant number of chloroplasts per unit volume in the leaf, the total pigment concentration of the leaf is given by multiplying this number with the internal pigment concentration of the chloroplasts. By reducing the internal pigment concentration of the chloroplasts means that the leaf and the chloroplasts become more transparent. On the other hand, assuming a constant internal pigmentation of the chloroplasts the leaf becomes more transparent by reducing the number of chloroplasts per unit volume. In this case the optical properties of the chloroplasts are unchanged.

Running the stochastic model with both versions for calculating the total pigment concentration it was shown that the reflectance spectrum in the visible part is influenced only slightly at the order of less than 0.5% over the whole spectrum. In general, higher local pigment concentrations in the chloroplasts induce reduced absorption combined with higher reflectance. This so called sieve-effect becomes remarkable only in the absorption bands of chlorophyll *a* by increasing the linewidth. Additional the sieve-effect flattens the absorption spectrum of the leaf and thus flattens the reflectance spectrum too.

Based on this result, the dependence of the reflectance spectra on the pigment concentration is analyzed by reducing the number of chloroplasts per unit volume only. In figure 2 three reflectance spectra are shown demonstrating the influence of pigment reduction. Due to the decrease of the the pigment concentration a reduced absorption is seen by an increase of the reflection associated with a blue shift of the red edge. The increase of the calculated reflectance at e.g. 680 nm is about 6%, when the pigment concentration decreases to about 1/16 of the initial concentration which was about 3 mg/cm³ of chlorophyll *a* and *b*. The shift of the red edge is typical nm, when the leaf color changes from fully green leaves (3 mg/cm³) to light-green leaves (about 0.2 mg/cm³). This result is in very good agreement with the experimental results of Buschmann and Lichtenthaler (1988) for cherry-laurel leaves, having

comparable pigmentation.

Also in the green spectral range at about 560 nm a quite good agreement between the modeled reflectance spectra and the experimental data of Buschmann and Lichtenthaler (1988) is seen. The increase of the reflectance at 560 nm by decreasing the pigment concentration at an equal amount is nearly identical for the measured and modeled data. The model shows an increase of the reflectance from 9% for fully green leaves to 25% for light green leaves while the experimental data for cherry-laurel leaves increase from 10% to 26%.

For all calculations a difference between the modeled reflectance spectra and the measured data is seen in the near-infrared region. In this spectral range the internal cell structure and thus the scattering coefficient determines the reflectance spectra, because pigment and water absorption is negligible. On the other hand the water content of the leaf determines the arrangement and the optical cross section of the cells indirectly and thus the scattering coefficient. In our approach, presented in this paper, the scattering coefficient is held constant, leading to constant reflectance in the near-infrared region.

Based on the good agreement of the calculated reflectance spectra with the data found in the literature, the seasonal cycle of the reflectance features of oak leaves was calculated. The annual variation of different leaf pigments as chlorophyll *a* and *b*, lutein, violaxanthin, neoxanthin and anthocyanin is given by Sanger (1971), while the specific spectral absorption coefficients for these pigments are found in Lichtenthaler (1987b) and Thimann and Edmondson (1949).

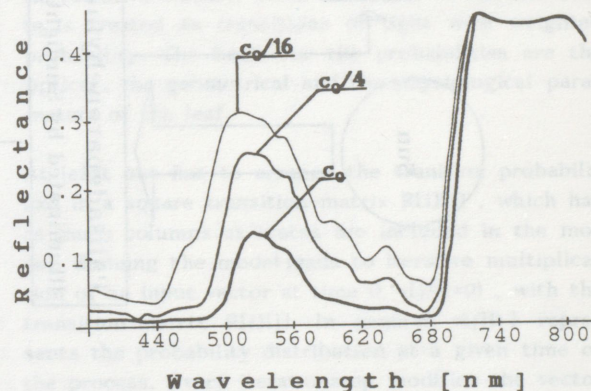


Figure 2: Reflectance spectra of the model leaf depending on the pigment concentration. All other leaf parameter are held constant.

- | | | |
|----|-----------------------|------------|
| 1: | maximum concentration | c_0 |
| 2: | reduced concentration | $c_0 / 4$ |
| 3: | reduced concentration | $c_0 / 16$ |

Figures 3 and 4 show the development of leaf reflectance from the early beginning in May when the buds are broken and the leaves are light-green. With the increasing pigment concentrations from May 15 to June 1 the reflectance spectrum changes dramatically. In the blue region of the spectrum the flattening of the reflectance spectrum is observed due to the saturation of the absorption. The chloroplasts are no more transparent in the blue absorbing all incoming light. In the red part of the spectrum a linear decrease of the reflectance is seen associated with the shift of the red edge towards longer wavelengths. When the leaf is dark green at July 1 the reflectance spectrum does not change remarkable in the blue. In contrast the green to red domain of the reflectance decreases. At about 680 nm, the maximum of the chlorophyll *a* absorption, the reflectance flattens due to saturation and absorption line broadening resulting in an additional shift of the red edge.

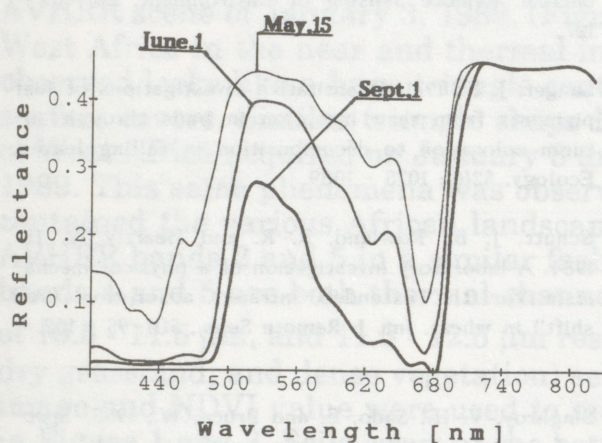


Figure 3: Seasonal cycle of the reflectance spectra of the model leaf

- 1: reflectance, when buds are broken, May, 15
- 2: reflectance at June, 1
- 3: reflectance at September, 1

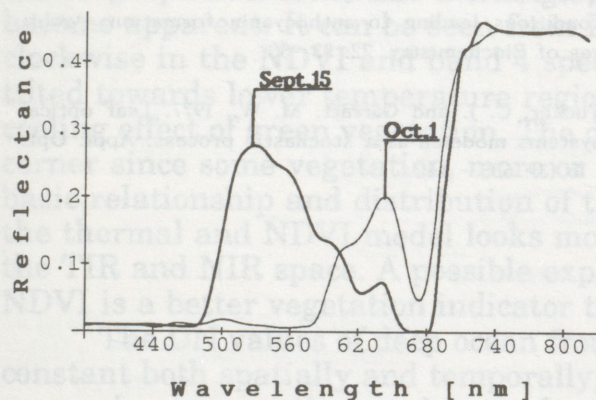


Figure 4: Seasonal cycle of the reflectance spectra of the model leaf

- 4: reflectance at September, 15
- 5: reflectance at October, 1

During summer, the pigment concentration remains relatively constant. As seen in figure 4, the reflectance spectrum for September 15 is comparable with the spectrum from July 1. During the next two weeks, the chlorophyll concentration breaks down accompanied by an increase of a new pigment, the anthocyanin. This pigment occurs during the autumn and is localized in the vacuoles of the epidermis. Due to the strong absorption of anthocyanin in the 500nm to 600nm region the green reflectance decreases while the reflectance in the domain of the red edge increases leading to the typical red coloring of leaves during autumn.

A comparison with the measured reflectance spectra during autumnal leaf coloring (Boyer et al. 1988) shows good agreement with our calculated spectra. The only major difference is seen again in the near-infrared region due to the constancy of the scattering coefficient used in the model.

4 CONCLUSION

Based on the experimental findings and the different interpretations of several investigators (Boyer et al. 1988, Buschmann and Lichtenthaler 1988, Collins et al. 1983, Horler et al. 1980, Horler et al. 1983, Rock et al. 1988, Schutt et al. 1984, Singhroy et al. 1985), that the blue shift of the red edge of the reflectance spectrum of vegetation may be correlated with the vegetative chlorophyll status, the species, the developmental stage, the leaf surface exposed to the sensor, the water content and the chlorophyll fluorescence, the stochastic model of Tucker and Garratt (1977) was reinvestigated in order to find a theoretical, bio-optical approach for a comprehensive interpretation of all the different explanations.

In a revised version the stochastic leaf model demonstrated its potential to calculate the reflectance spectrum of vegetation. Optical, geometrical and physiological parameters as e.g. the specific absorption coefficient of chlorophyll *a*, the pigment concentration and the leaf thickness are used as input parameters. The revised model takes into account different mechanisms as absorption, reflection and Mie scattering at the chloroplasts and the leaf cells.

According to our first results showing good agreement with data from the literature, the model presents two ways for interpreting the blue shift. First, by reducing the light absorption in the leaf, a blue shift of the red edge can be produced because the absorption line in the red part of the spectrum narrows. In turn a reduced light absorption can be modeled twofold by reducing the pigment concentration of the leaf or by reducing the thickness of the leaf assuming constancy of the pigment concentration. Thinner leaves have in general a shorter light path resulting in an overall less absorption.

From a physiological point of view thin leaves can be found in spring when young leaves are developing or under stress conditions as e.g. water stress. In this paper we presented only the effect of different pigmentations.

As mentioned before a second effect may influence the blue shift of the red edge, the shift of the absorption line to shorter wavelengths. This phenomenon can be observed in the laboratory when leaves are treated with the herbicide DCMU, solved in alcoholic solution, in order to investigate e.g. the Kautsky effect to obtain physiological data of the plant. Under these special conditions, the pigment concentration remains constant as well as the leaf thickness so that the observed shift of the red edge may be attributed to a shift of the absorption line due to the influence of the solvent and the herbicide. It is well known that the type of solvents can change the position of absorption lines.

The revised version of the stochastic leaf model has demonstrated its usefulness in calculating reflectance spectra.

5 REFERENCES

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. Kluwer Academic Publisher, Dordrecht, pp. 345 - 351.

Boyer M., Miller, J., Belanger M. and Hare, E., 1988. Senescence and spectral reflectance in leaves of northern pin oak (*Quercus palustris* Muenchh.). Remote Sens. Environment, 25: 71 - 87.

Buschmann, C. and Lichtenthaler H. K., 1988. Reflectance and fluorescence signature of leaves. In: Applications of chlorophyll fluorescence. Kluwer Academic Publisher, Dordrecht, pp. 325 - 332.

Collins, W., Chang, S.-H., Raines, G., Canney, F. and Ashley, R., 1983. Airborne biogeophysical mapping of hidden mineral deposits. Economic Geology, 78: 737 - 749.

Guyot, G., Baret, F. and Major, D., 1988. La haute résolution spectrale. détermination des déformations spectrales entre le rouge et proche infrarouge. In: Proc. 6eme Congres de l'Association Quebecoise de Teledetection. Sherbrooke, May 3-6, 1988.

Horler, D. N. H., Barber, J. and Barringer A. R., 1980. Effects of heavy metal on the absorbance and reflectance spectra of plants. Int. J. Remote Sensing, 1 (1): 121 - 136.

Horler, D. N. H., Dockray, M. and Barber, J., 1983. The red edge of plant reflectance. Int. J. Remote

Sensing, 4 (2): 273 -288.

Lichtenthaler, H. K., 1987. Chlorophylls and carotenoids: pigments of photosynthetic biomembranes. In: Methods in Enzymology, Vol. 148, Academic Press Inc., pp. 350 - 382.

Lichtenthaler, H. K. and Buschmann, C., 1987. Reflectance and fluorescence signature of leaves, Proc. IGARSS '87, May 18-21, 1987, pp. 1201 - 1207.

Morel, A. and Bricaud, A., 1981. Theoretical results concerning light absorption in a discrete medium, and application to specific absorption by phytoplankton. Deep Sea Res., 28A (11), 1375 - 1393.

Rock, B. N., Hoshizaki, T. and Miller, J. R., 1988. Comparison of in situ and airborne spectral measurements of the blue shift associated with forest decline. Remote Sensing of Environment, 24: 109 - 127.

Sanger, J. E., 1971. Quantitative investigations of leaf pigments from their inception in buds through autumn coloration to decomposition in falling leaves. Ecology, 52(6): 1075 - 1089.

Schutt, J. B., Rowland, R. R. and Heartly W. H., 1984. A laboratory investigation of a physical mechanism for the extended infrared absorption ('red shift') in wheat. Int. J. Remote Sens., 5(1): 95 - 102.

Singhroy, V. H., Sado, E. and Bruce, W., 1985. Spectral geobotany in glaciated environments: test over a mineralized till site in northern Ontario. Proc. Fourth Them. Conf. on Remote Sensing for Exploration Geology, San Francisco, April 1-4, 1985, pp. 701 - 720.

Thimman, K. V. and Edmondson, Y. H., 1949. The biogenesis of the anthocyanins. I. General nutritional conditions leading to anthocyanin formation. Archives of Biochemistry, 22: 33 -53.

Tucker, C. J. and Garratt, M. W., 1977. Leaf optical systems modeled as a stochastic process. Appl. Opt., 16 (3): 635 - 642.