A New Leaf Fluorescence Model

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ABSTRACT

Passive remote sensing of plant fluorescence emerged as a possible approach for monitoring vegetation health from an airplane or even from space. However, the fluorescence signal is a complex response of both light interception and physiological parameters, which necessitates developing models to interpret the data. In the frame of the FluorMOD project − Development of a Vegetation Fluorescence Canopy Model − funded by ESA, a leaf fluorescence model has been designed which predicts the reflectance and transmittance of a fresh leaf including the emission of chlorophyll fluorescence.

The model is based on the PROSPECT leaf optical properties model which is widely used in the scientific community. It is one of the first radiative transfer codes to accurately simulate the hemispherical reflectance and transmittance of various plant leaves (monocots, dicots or senescent leaves) over the solar spectrum, with only four input parameters: the leaf structure parameter (number of compact layers specifying the average number of air/cell walls interfaces within the mesophyll), the chlorophyll a+b concentration, the equivalent water thickness, and the dry matter content. We introduced the fluorescence emission into PROSPECT, viewing fluxes within the leaf as a network. The core of the model is the fluorescence emission elementary spectrum, a combination of Photosystem I (PSI) and Photosystem II (PSII) fluorescence spectra. The additional input parameters are the fluorescence quantum efficiency, the relative contribution of the two photosystems (stoichiometry of the PSII to PSI reaction centers), the leaf temperature, and the light level. The influence of these parameters on the fluorescence emission changes from one species to the other. Using the flux network diagram, the elementary spectrum is re-absorbed within the leaf so we can describe the leaf fluorescence spectrum upward and downward, for different wavelengths of excitation. Outputs of the model have been compared with experimental measurements.

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1. Introduction

As only passive techniques to measure vegetation fluorescence from space are technically conceivable (Ounis, 2001), the FLEX (Fluorescence Explorer) mission was put forward in 1998 by the European Space Agency (ESA) to explore the possibility of using the Fraunhofer lines of the solar spectrum for passive measurements of natural sunlight-induced fluorescence. In October 2002, ESA initiated a study to speed up the underlying science of a possible vegetation fluorescence space mission by addressing the need for an integrated canopy fluorescence model. The objective of this study is to review and advance existing fluorescence models at the leaf level and to integrate these into canopy reflectance models. In this paper, we describe a new leaf fluorescence model developed in the frame of the FluorMod project (Development of a Vegetation Fluorescence Canopy Model). We propose a new approach since none of the existing models fullfiled all the requierements for an application in fluorescence detection from space, *i.e.* a simple and fast code, with a limited number of input variables, easily invertible and including meaningful variables connected to plant physiology. The model outputs have been compared with experimental measurements by way of validation.

2. Model description

The new leaf fluorescence model is based on the PROSPECT model in widespread use in the remote sensing community. We selected it because of its small number of variables, which can be measured experimentally and estimated by inversion.

2.1 The PROSPECT model

PROSPECT (Jacquemoud and Baret, 1990) was one of the first radiative transfer codes to accurately simulate the hemispherical reflectance and transmittance of various plant leaves (monocots, dicots or senescent leaves) over the solar spectrum (from 400 nm to 2500 nm). It represents the leaf as one or several absorbing plates with rough surfaces giving rise to diffuse scattering (Fig. 1).

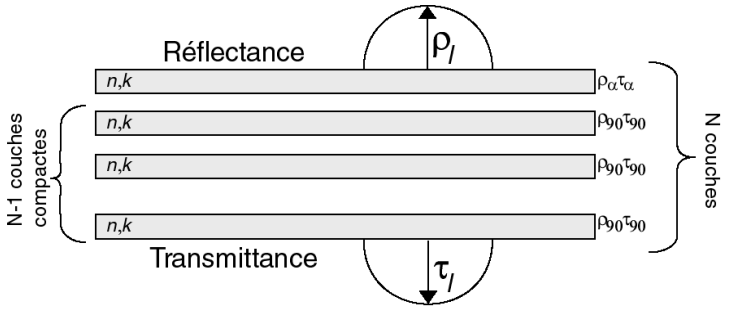

Figure 1. Schematic representation of PROSPECT.

It accepts four input parameters: the structure parameter (N) (number of compact layers specifying the average number of air/cell walls interfaces within the mesophyll), the chlorophyll (hereafter Chl) a+b concentration (Cab), the equivalent water thickness (Cw), and the dry matter content (Cm).

2.2 Fluorescence excitation

We propose an algebraic method to calculate the fluorescence, first of an elementary layer, and then of a pile of N layers by considering fluxes as a network (Fig. 2). We can set down a system of linear equations:

$$\begin{aligned} &i_0 = 1,\ i_1 = i_0,\ i_2 = i_1 t_{12}\,\tau(1) + i_4 r_{21}\,\tau(1),\ i_3 = i_2 t_{21},\ i_4 = i_2 r_{21}\,\tau(1),\ i_5 = i_1 r_{12} + i_4 t_{21} \\ &i_{12} = i_1 t_{12}\,\tau(x),\ i_{24} = i_2 r_{21}\,\tau(1-x),\ i_{42} = i_4 r_{21}\,\tau(x) \end{aligned} \quad (1)$$

whose solution provides the same expressions for reflectance (i_5) and transmittance (i_3) as in PROSPECT, and the following values for i_{12}, i_{24} and i_{42} at position x:

$$i_{12}(x) = t_{12}\,\tau(x) \text{ and } i_{24}(x) = \frac{t_{12}\,r_{21}\,\tau(1)\tau(1-x)}{1-r_{21}^2\,\tau^2(1)} \text{ and } i_{42}(x) = \frac{t_{12}\,r_{21}^2\,\tau^2(1)\tau(x)}{1-r_{21}^2\,\tau^2(1)} \tag{2}$$

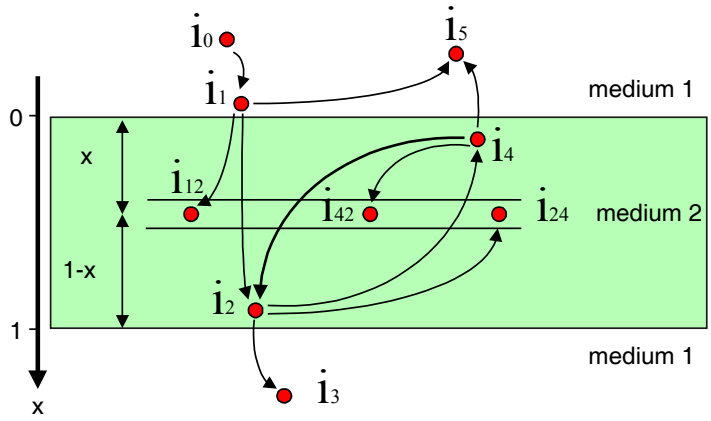

Figure 2. Flux network showing the excitation fluxes at position x.

The total flux at position x is given by the algebraic sum $i_{12}(x) + i_{24}(x) + i_{42}(x)$. $i_{12}(x)$ and $i_{42}(x)$ are propagating towards positive values of x, while $i_{24}(x)$ is propagating towards negative value of x. The absorbed flux in the medium between the x and x+dx levels is calculated by considering the difference of a given flux along the direction of propagation between these two levels. Thus, we have for $i_{12}(x)$ and $i_{42}(x)$:

$$\begin{cases} i_{12}(x+dx) = i_{12}(x) - a_{12}(x)dx \\ i_{42}(x+dx) = i_{42}(x) - a_{42}(x)dx \end{cases} \tag{3}$$

And for $i_{24}(x)$:

$$i_{24}(x+dx) = i_{24}(x) + a_{24}(x)dx \tag{4}$$

Then, by returning to the definition of the derivative of a function, we can link the absorbed flux with the derivative of the fluxes:

$$a(x) = \pm\frac{i(x+dx)-i(x)}{dx} = \pm i'(x) \tag{5}$$

So the amount of flux absorbed along dx is:

$$\begin{aligned} a(x)dx &= \left(a_{12}(x) + a_{24}(x) + a_{42}(x)\right)dx = -\left(i'_{12}(x) - i'_{24}(x) + i'_{42}(x)\right)dx \\ &= -t_{12}\,\tau'(x) + \frac{t_{12}\,r_{21}\,\tau(1)\tau'(1-x)}{1-r_{21}^2\,\tau^2(1)} - \frac{t_{12}\,r_{21}^2\,\tau^2(1)\tau'(x)}{1-r_{21}^2\,\tau^2(1)} \end{aligned} \tag{6}$$

2.3 Fluorescence emission

At a given wavelength λ, one can now define ϕ(λ) (noted ϕ in the following for convenience) as the product of the fluorescence quantum yield, i.e. the fraction of absorbed flux that contributes to fluorescence excitation, by the fluorescence emission spectral distribution function. The network in Figure 3 corresponds to the following set of linear equations:

$$\begin{cases} dy_1 = a(x).\phi.dx \\ dy_2 = \dfrac{1}{2} dy_1\, \tau f(x) + dy_4\, rf_{21}\, \tau f(1) \\ dy_3 = dy_2\, tf_{21} \\ dy_4 = \dfrac{1}{2} dy_1\, \tau f(1-x) + dy_2\, rf_{21}\, \tau f(1) \\ dy_5 = dy_4\, tf_{21} \end{cases} \tag{7}$$

Where the subscript f indicates the wavelength of fluorescence. The emitted photons are equally distributed between the upward and downward directions in the infinitesimal layer because light emission occurs isotropically. The system of equations (7) can be easily solved in dy_3 and dy_5:

$$\begin{cases} dy_3 = -\dfrac{t_{12}\, tf_{21}\, \phi}{2} \dfrac{\left(rf_{21}\, \tau f(1) \tau f(1-x) + \tau f(x)\right)\left(r_{21}\, \tau(1) \tau'(1-x) + \tau'(x)\right)}{\left(1 - r_{21}^2\, \tau^2(1)\right)\left(1 - rf_{21}^2\, \tau f^2(1)\right)} \\ dy_5 = -\dfrac{t_{12}\, tf_{21}\, \phi}{2} \dfrac{\left(rf_{21}\, \tau f(1) \tau f(x) + \tau f(1-x)\right)\left(r_{21}\, \tau(1) \tau'(1-x) + \tau'(x)\right)}{\left(1 - r_{21}^2\, \tau^2(1)\right)\left(1 - rf_{21}^2\, \tau f^2(1)\right)} \end{cases} \tag{8}$$

The upward and downward fluorescence signals of the plate (N = 1) are then equal to the integral of dy_3 and dy_5, respectively, between x = 0 and x = 1:

$$Fu(1) = \int_0^1 dy_3\, dx \quad \text{and} \quad Fd(1) = \int_0^1 dy_5\, dx \tag{9}$$

For N layers we can use a similar approach to Jacquemoud and Baret (1990) in the PROSPECT model except that there is no analytical solution for a real number of layers. We consequently calculate fluorescence for N = 1, 2, 3,… layers, recursively. At N = 5, both the upward and downward fluorescence reache a plateau so that no significant variation is observed when this value is exceeded. The upward Fu(N) and downward Fd(N) Chl fluorescence is stored in a cube of dimension A×B×5: A is the number of wavelengths of excitation, B is the number of wavelengths of emission, and we have considered 5 layers. The determination of the fluorescence for any real value of N amounts to « cut a slice » in the cube, i.e. to make a three-dimensional data interpolation (lookup table).

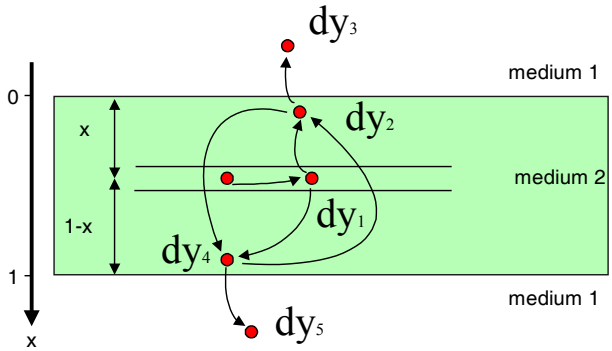

Figure 3. Flux network showing the emission flux at position x.

2.4 Fluorescence emission spectrum

Once the equations describing the fluorescence excitation and fluorescence emission have been solved, we need to know the fluorescence emission distribution spectrum, hereafter the elementary spectrum $\eta(\lambda)$. The latter represents the emission of the differential width of the leaf dx where the fluorescence is produced. The fluorescence source $\phi(\lambda)$ is the product of the quantum yield of fluorescence (or fluorescence quantum efficiency) φ by the fluorescence elementary spectrum $\eta(\lambda)$. This fluorescence source will provide the fluorescence with the right units (number of photons), instead of the widespread used arbitrary units.

The quantum yield of fluorescence usually ranges over a few percents (3-5%), between 0% (no fluorescence) and a maximum of 10%, depending on the state of the leaf photosynthetic apparatus.

Although some elementary spectra are available in the literature (Meier, 2000; Gitelson et al., 1998; Subhash and Mohanan, 1997), we decided to propose a new fluorescence emission spectrum for two reasons. First, the Gaussian decomposition suggested by Subhash and Mohanan (1997) does not rely on physical basis. We consequently decided to separate the contribution of the two photosystems that, in photosynthesis, act in the emission spectrum. Second, by introducing the two photosystems, we will be able to describe the dynamics of the transition between fluorescence spectra at F_0 (minimum of fluorescence) and F_M (maximum of fluorescence) as this difference reflects different relative contributions of PSI and PSII fluorescence (Franck et al., 2002).

The elementary spectrum is a combination of the PSI spectrum measured by Croce et al. (1996, 2000) and the PSII spectrum measured by Franck et al. (2002). For the contribution of each photosystem we used the stoichiometry of PSII to PSI reaction centers. The advantage of this approach is that plants adjust their PSI and PSII stoichiometry as a long-term regulatory response to environmental conditions (Murakami, 1997). Taiz and Zeiger (1998) suggest that the ratio of PSII to PSI is about 1.5:1 under many conditions, but it may change according to growth conditions. Nevertheless the two photosystems do not have the same fluorescence lifetimes, and consequently the Chl fluorescence quantum yield is different. The quantum yield at Fs can be deduced from lifetime measurements data (Schmuck and Moya, 1994), according to $\Phi = \tau/\tau 0$ ($\tau 0$ is about 15-18 ns). Measured mean values at Fs are $\Phi^{PSII} = 0.5/15 = 3.3\%$ for PSII and $\Phi^{PSI} = 0.1/15 = 0.66\%$ for PSI. Therefore we will consider that the PSII is five times more efficient than the PSI by multiplying the values of the stoichiometry for a weight factor of 5. Figure 4 shows the elementary spectrum for several values of the stoichiometry of PSI and PSII, that modify the shape of the spectrum.

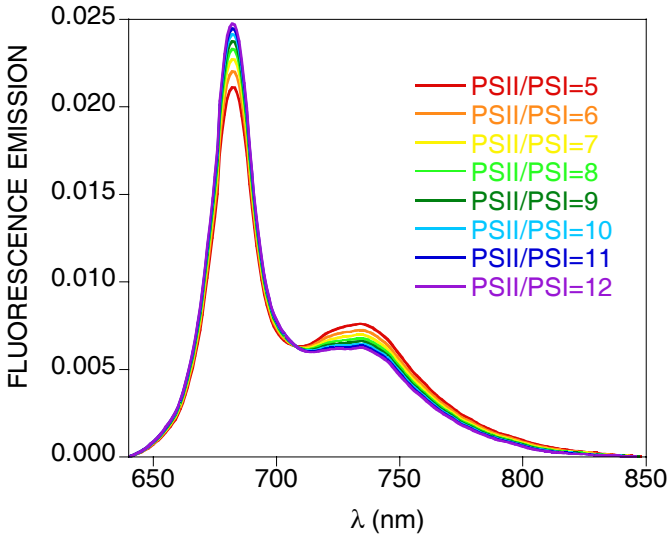

Figure 4. Elementary spectrum for several values of the contribution of PSII. PSI spectrum after Croce et al. (1996, 2000); PSII spectrum after Franck et al. (2002).

2.5 Physiological parameters

A set of variables has been included to connect the fluorescence emission to the plant physiology. These variables have been chosen because they describe the fluorescence emission and because they are accessible to measurement. We introduced the stoichiometry of PSI and PSII (sto), the fluorescence quantum efficiency (Qeff), the temperature (t), and the light level. Fluorescence increases when temperature decreases. An empirical dependence with temperature has been taken from Agati (1998). Fluorescence increases with PAR (Photosynthetic Active Radiation) until a saturation point and then decreases slowly. The functional dependence with light level has been taken from Rosema et al. (1998). The stoichiometry of the two photosystems has been included as refered in section 1.4. Fluorescence quantum efficiency has been included in the model as a multiplier factor in the elementary spectrum, as described in section 1.4.

3. Materials and methods

We measured the fluorescence emission spectra of fresh green bean (*Phaseolus vulgaris* var. Contender) leaves with the Cary Eclipse fluorimeter which is equipped with two monochromators, one for fluorescence excitation and another one for fluorescence detection, allowing a measurement at 1 nm step. The plants were grown in pots and maintained outdoors. Some leaves with different Chl content were cut off and kept in a moistured cloth until the measurement time, in a span of an hour. The Chl content was estimated with the Minolta SPAD-502 chlorophyll meter.

4. Results and discussion

The modeled fluorescence has been compared with measurements carried out on leaves with different Chl contents, for an excitation at 440 nm. The results shown in figures 5 and 6 correspond to Cab = 17 and 33 μg cm^{-2}, respectively. The measurements are in arbitrary units. The model reproduces well the variation in the spectrum shape while Chl changes. When Chl increases the ratio of the fluorescence at 685 nm and 730 nm, namely F685/F730, decreases because F685 is more reabsorbed. We considered a white light excitation using a typical global solar irradiance file simulated with the MODTRAN 4.0 radiative transfer code. The contribution of the fluorescence to the reflectance and the transmitance is shown in figure 7. The values are 10.2% at 685 nm and 1.0% at 730 nm which is in agreement with the results published by Kim et al. (1993).

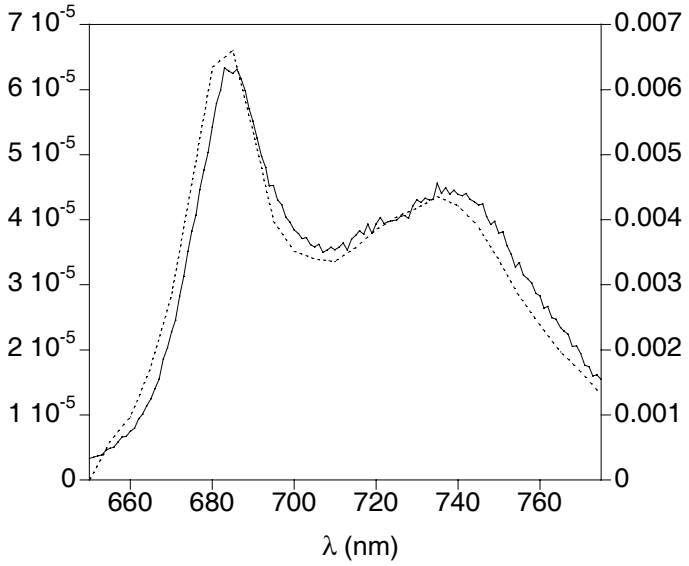

Figure 5. Fluorescence upward emission spectrum for a green bean leaf with Cab = 17 μg cm^{-2} (solid line). Modeled emission spectrum using a ratio of PSII/PSI=10/1 (dotted line). The excitation wavelength is 440 nm. N=1.5; Cab=33; Cw=0.025; Cm=0.01; Qeff=0.04; t=20; sto=2.0.

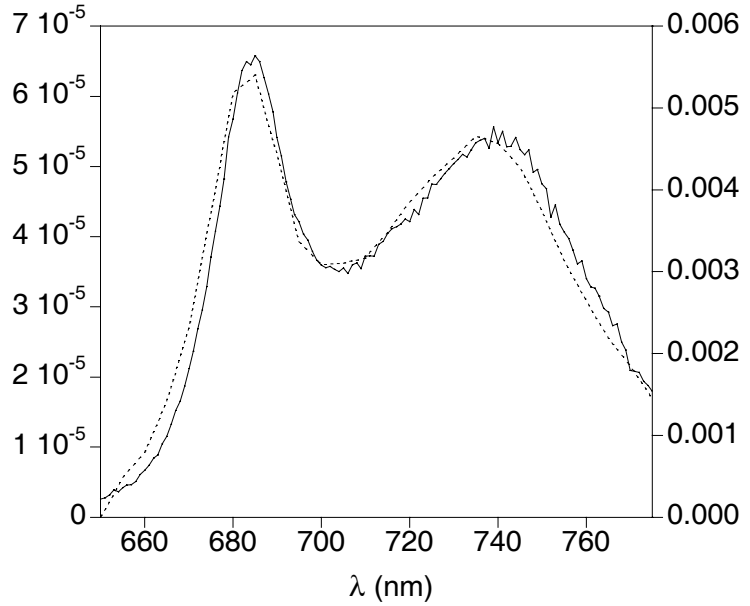

Figure 6. Fluorescence upward emission spectrum for a green bean leaf with Cab = 33 µg cm^{-2} (solid line). Modeled emission spectrum using a ratio of PSII/PSI=10/1 (dotted line). The excitation wavelength is 440 nm. N=1.5; Cab=33; Cw=0.025; Cm=0.01; Qeff=0.04; t=20; sto=2.0.

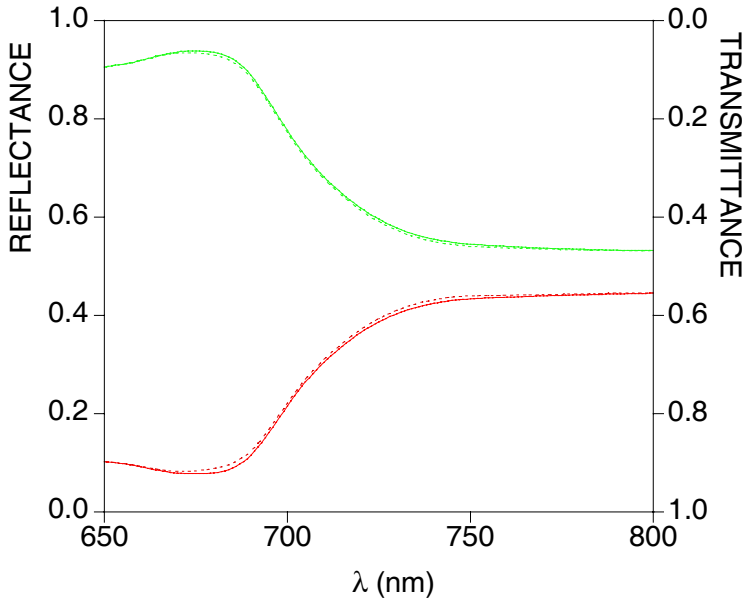

Figure 7. Reflectance (green) and transmittance (red) with (dotted line) and without (solid line) fluorescence for green bean. N=1.5; Cab=33; Cw=0.025; Cm=0.01; Qeff=0.04; t=20; sto=2.0.

5. Conclusion

We have designed a new reflectance and transmittance model of a fresh-green leaf, including Chl fluorescence emission. The model is based on the PROSPECT model, adding several variables to connect plant physiology and fluorescence emission. The variables are fluorescence quantum efficiency, light level, temperature and stoichiometry of the photosystems. The influence of these parameters on the fluorescence emission changes from one species to another. The core of the model is the spectral distribution of the fluorescence emission, the elementary spectrum, a combination of the PSI and PSII emission spectra. The model outputs have been compared to actual measurements, for one wavelength of excitation. The model reproduces the variation in shape associated with Chl variation caused by a modification in the reabsorption. In addition, the model predicts well the contribution of the fluorescence to reflectance and transmittance.

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