Remote Sensing of Environment 211 (2018) 345–356

Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

Extending Fluspect to simulate xanthophyll driven leaf reflectance dynamics

Nastassia Vilfan[a,*], Christiaan Van der Tol[a], Peiqi Yang[a], Rhys Wyber[b], Zbyněk Malenovský[b,c,d], Sharon A. Robinson[b], Wouter Verhoef[a]

[a] *University of Twente, Faculty of Geo-Information Science and Earth Observation (ITC), P.O. Box 217, Enschede 7500 AE, The Netherlands*
[b] *Centre for Sustainable Ecosystem Solutions, School of Biological Sciences, University of Wollongong, NSW 2522, Australia*
[c] *Surveying and Spatial Sciences Group, School of Land and Food, University of Tasmania, Private Bag 76, TAS, Hobart 7001, Australia*
[d] *Department of Remote Sensing, Global Change Research Institute CAS, Bělidla 986/4a, Brno CZ-60300, Czech Republic*

ARTICLE INFO

Keywords:
PRI
Fluspect
Reflectance
Xanthophyll cycle
Leaf chlorophyll fluorescence
SCOPE

MSC:
00-01
99-00

ABSTRACT

The xanthophyll cycle regulates the energy flow to photosynthetic reaction centres of plant leaves. Changes in the de-epoxidation state (*DEPS*) of xanthophyll cycle pigments can be observed as changes in the leaf absorption of light with wavelengths between 500 to 570 nm. These spectral changes can be a good remote sensing indicator of the photosynthetic efficiency, and are traditionally quantified with a two-band physiologically based optical index, the Photochemical Reflectance Index (PRI). In this paper, we present an extension of the plant leaf radiative transfer model Fluspect (Fluspect-CX) that reproduces the spectral changes in a wide band of green reflectance: a radiative transfer analogy to the PRI. The idea of Fluspect-CX is to use *in vivo* specific absorption coefficients for two extreme states of carotenoids, representing the two extremes of the xanthophyll de-epoxidation, and to describe the intermediate states as a linear mixture of these two states. The 'photochemical reflectance parameter' (C_x) quantifies the relative proportion of the two states. Fluspect-CX simulates leaf chlorophyll fluorescence (*ChlF*) excitation-emission matrices, as well as reflectance (R) and transmittance (T) spectra as a function of leaf structure, pigment contents and C_x. We describe the calibration of the model and test its performance using various experimental datasets. Furthermore, we retrieved C_x from optical measurements of various datasets. The retrieved C_x correlates well with xanthophyll *DEPS* ($R^2 = 0.57$), as well with non-photochemical quenching (NPQ) of fluorescence ($R^2 = 0.78$). The correlation with NPQ enabled us to incorporate Fluspect-CX in the model SCOPE to scale the processes to the canopy level. Introducing the dynamic green reflectance into a radiative transfer model provides new means to study chlorophyll fluorescence and PRI dynamics on leaf and canopy scales, which is crucial for the remote sensing.

1. Introduction

Under excess irradiance the amount of absorbed photosynthetically active radiation (PAR) exceeds the capacity of photosynthetic reactions, which can cause irreversible damage to the photosystem II reaction centre resulting in photoinhibition. In order to regulate the energy dissipation, photosynthetic eukaryotes have developed many protective mechanisms, in one of which, the excess energy is diverted from the photosystem reaction centres to the pigments of the xanthophyll cycle (Niyogi et al., 1998).

The xanthophyll cycle is an interconversion of three xanthophylls belonging to a carotenoid pigment group: zeaxanthin, antheraxanthin and violaxanthin. Under high PAR levels an increase in the proton gradient across the thylakoid membrane activates the enzymatic conversion of violaxanthin to antheraxanthin and then to zeaxanthin. This interconversion provides a sink for the excess absorbed energy in a process called non-photochemical quenching (NPQ) of chlorophyll fluorescence: the energy is dissipated as heat in the light harvesting complexes associated with photosystem II (Björkman and Demmig-Adams, 1995; Horton et al., 1994; Jahns and Holzwarth, 2012; Niyogi et al., 1998; Ruban, 2016). Under low light conditions or in darkness, the process is readily reversed and zeaxanthin is converted back to violaxanthin.

Numerous studies have shown that NPQ is positively correlated with zeaxanthin formed by the xanthophyll cycle (for reviews, see Demmig-Adams, 1990; Jahns and Holzwarth, 2012).

In practice, the xanthophyll cycle can be observed as dynamic changes in green reflectance between approximately 500 to 570 nm. In order to express these changes with a simple physiologically based optical index, the narrow band photochemical reflectance index (PRI) was defined by Gamon et al. (1992) (for a review, see Garbulsky et al., 2011). PRI is usually calculated as $(R531 - R570)/(R531 + R570)$,

---

[*] Corresponding author.
E-mail address: n.rajhvilfan@utwente.nl (N. Vilfan).

https://doi.org/10.1016/j.rse.2018.04.012
Received 19 May 2017; Received in revised form 28 March 2018; Accepted 5 April 2018

comparing the xanthophyll induced reflectance (*R*) change at 531 nm to a xanthophyll independent reference band at 570 nm. PRI has been shown to vary significantly over different time scales, in response to different levels of sunlight and to various stresses, from the leaf to the satellite levels. Its empirical relationship to light use efficiency (LUE) has been confirmed over a wide range of species, providing means for global tracking of primary productivity (Garbulsky et al., 2011; Magney et al., 2016; Sims and Gamon, 2002). Moreover, a functional link has been documented between PRI, DEPS of the xanthophyll cycle and NPQ (Evain et al., 2004; Gamon et al., 1992; Peñuelas et al., 1997).

However, the applicability of PRI is limited. In general, correlations are most convincing at the leaf scale, but become far less reliable when we move to the higher levels, due to the influences of canopy structure, viewing and illumination angles on the *R* signal (Barton and North, 2001; Garbulsky et al., 2011; Zhang et al., 2017).

On the leaf level, the shape of the *R* signal in the visible range depends primarily on leaf biochemistry. In particular, in the spectral range of 500–570 nm, at least three types of pigments contribute to the shape of the *R* spectrum, namely chlorophylls, anthocyanins and carotenoids, the later include carotenes and xanthophylls. The absorption spectra of these pigments not only strongly overlap, but also vary with their local chemical environment and scattering conditions (Lichtenthaler and Buschmann, 2001; Ustin et al., 2009). In order to decouple the individual pigments contributions to the *R* signal, an index with only 2 bands, such as PRI, is not sufficient.

PRI has been shown to correlate with the ratio of carotenoid to chlorophyll pool sizes. On the diurnal scale it is mostly affected by changes in the xanthophyll cycle, whereas on the longer time scales it primarily depends on the carotenoid and chlorophyll concentration changes (Fréchette et al., 2016; Porcar-Castell et al., 2014; Wong and Gamon, 2015). The use of the index is further complicated by a lack of clear consensus on both the wavelengths used and the normalization methods (Magney et al., 2016; Panigada et al., 2014). A common normalization method is the use of delta PRI (ΔPRI), calculated by subtracting the dark adapted reference value from the light adapted values. The method is used to measure absolute diurnal as well as seasonal changes in xanthophyll de-epoxidation (Hmimina et al., 2014; Magney et al., 2016).

Besides PRI, few other attempts have been made to model dynamic changes in green *R* by using the continuous spectral information rather than just two bands (Kováč et al., 2013, 2012), but to our knowledge, a model that can reproduce changes over a broad band of green *R* in a radiative transfer (RT) manner has never been published.

In this paper, we present an extension to the leaf RT model Fluspect-B (Vilfan et al., 2016), called Fluspect-CX, which is able to reproduce dynamic spectral changes in a broad band of green *R*, from 500 to 570 nm. Fluspect-CX now provides a dynamic green *R* together with chlorophyll fluorescence (ChlF) spectrum, using the incoming light and ten parameters as input.

First, we describe a way of calibrating Fluspect-CX specific spectral absorption coefficients (SAC). Next, we present the model routine for retrieving dynamic changes in green *R*, represented by a parameter C_x. We retrieve C_x for various datasets and link it empirically to leaf chlorophyll fluorescence dynamics.

Moreover, Fluspect-CX was implemented as a routine within the Soil Canopy Observation of Photosynthesis and Energy (SCOPE) balance model (Van der Tol et al., 2009), and lately also in the three-dimensional Discrete Anisotropic Radiative Transfer (DART) model (Gastellu-Etchegorry et al., 2017). By including the spectral coefficient for dynamic green *R*, the leaf model can be up-scaled to the canopy scale, giving the potential to study PRI dynamics in real time at the canopy level.

2. Model description

Fluspect is a radiative transfer model that simulates *R* and *T* from 400 nm to 2500 nm and ChlF spectra from 640 nm to 850 nm. It is implemented in Matlab and published under GNU General Public License at https://github.com/christiaanvandertol.

Fluspect is based on the model PROSPECT (Jacquemoud and Baret, 1990). Recently, a new version was published, called PROSPECT-D (Féret et al., 2017), which has made a leap further towards modelling leaf optical properties through a complete plant life cycle by introducing anthocyanins as a new model input and re-calibrating the existing SACs of carotenoids and chlorophylls.

Here, we present an extension of Fluspect-B (Vilfan et al., 2016), called Fluspect-CX, in which we: 1) incorporate the absorption of anthocyanins and replace the SACs of carotenoids and chlorophylls, as defined in PROSPECT-D and 2) include the SACs for the two extreme states of the violaxanthin de-epoxidation.

The spectral absorption (*k*) by leaf constituents is simulated in Fluspect by:

$$k(\lambda) = \sum_{i=0}^{n} K_i(\lambda)\cdot C_i \tag{1}$$

where *C* is the pigment concentration and *K* the specific spectral absorption coefficient. Fluspect-B uses five SACs (chlorophylls (C_{ab}), carotenoids (C_{car}), leaf water (C_w), dry matter (C_{dm}) and senescent material (C_s)). In Fluspect-CX, we incorporate a sixth, representing anthocyanins (C_{ant}), and we add a seventh (C_x), which is a radiative transfer analogue to the PRI: it represents the spectral effect of the leaf xanthophyll de-epoxidation, described in the model as change in the absorption of the total carotenoids. The model input parameters, together with their range and standard values, are defined in Table 1.

Because of the strong overlap of viola- and zeaxanthin absorption spectra with the absorption spectrum of total carotenoids, we could not include them as separate SACs. Instead, we describe the carotenoid absorption spectrum as a linear combination of two coefficients representing the two extreme situations: one for an unstressed leaf, where *NPQ* and the associated xanthophyll *DEPS* are 0 (K_{car0}), and one for the state where maximum *NPQ* activity occurs and *DEPS* is 1 (K_{car1}):

$$K_{car} = (1 - C_x)\cdot K_{car0} + C_x\cdot K_{car1} \tag{2}$$

where C_x is the parameter representing the xanthophyll *DEPS*.

Table 1
Fluspect-CX input parameters.

Parameter	Symbol	Range	Standard value	Unit	Reference	Origin
Chlorophyll a + b content	C_{ab}	0–100	40	$\mu g\,cm^{-2}$	Féret et al. (2017)	PROSPECT-D
Total carotenoid content	C_{car}	0–30	10	$\mu g\,cm^{-2}$	Féret et al. (2017)	PROSPECT-D
Anthocyanin content	C_{ant}	0–10	0	$\mu g\,cm^{-2}$	Féret et al. (2017)	PROSPECT-D
Water content	C_w	0–0.4	0.009	cm	Jacquemoud and Baret (1990)	PROSPECT
Dry matter content	C_{dm}	0–0.5	0.012	$g\,cm^{-2}$	Jacquemoud and Baret (1990)	PROSPECT
Leaf mesophyll structure parameter	N	1–4	1.4	–	Jacquemoud and Baret (1990)	PROSPECT
Senescence material (brown pigments)	C_s	0–0.6	0	In arbitrary units	Jacquemoud and Baret (1990)	PROSPECT
Fluorescence quantum efficiency	η	0–0.2	0.002	–	Miller et al. (2005)	Fluspect
Photochemical reflectance parameter	C_x	0–1.5	0	–	/	Fluspect