PHOTOSYNTHESIS-SUN INDUCED FLUORESCENCE RELATIONSHIP IN A MEDITERRANEAN GRASSLAND

David Martini (1), Javier Pacheco-Labrador (1), Oscar Perez-Priego (1), Christiaan van der Tol (3), Tarek El Madany (1), Tommaso Julitta (5), Micol Rossini (2), Anatoly Gitelson (4), Markus Reichstein (1) and Mirco Migliavacca (1)

(1) Max Planck Institute for Biogeochemistry, Jena, Germany. (2) University of Milano Bicocca, Milan, Italy. (3) University of Twente, Enschede, The Netherlands. (4) University of Nebraska, Lincoln, USA. (5) JB Hyperspectral devices.

ABSTRACT

Sun induced fluorescence at 760 nm (F_{760}) has shown to provide a valid approach to quantify gross primary production (GPP) at various scales, however the relationship between GPP and F_{760} is influenced by the escape probability of fluorescence (Fesc), a variable which is not still fully understood. Combining radiative transfer modelling approaches, by means of the SCOPE model, and a data driven methodology based on variable selection methods we identify the predictors of Fesc, focusing on the effect of functional and structural traits. We show that Fesc is mainly predicted by structural variables such as fraction of grasses and near infrared reflectance. Building on the analysis of the predictor of Fesc, LUE_p and LUE_f we present a semi-empirical model formulation based only on optical data that significantly improves the GPP prediction.

Index Terms— sun induced fluorescence, Fesc, functional traits, canopy structure, GPP, SCOPE model

1. INTRODUCTION

Gross primary production (GPP) by terrestrial plants drives the terrestrial carbon cycle and strongly influences the water and energy exchanges between atmosphere and the biosphere, ultimately sustaining all terrestrial life. Sun induced chlorophyll fluorescence (SIF) has increasingly been used as a tool to quantify GPP, and its application has been tested and validated at various scales, ranging from an individual leaf to the global scale [1] [2].

The reason why GPP and SIF correlate is that both photosynthesis and chlorophyll fluorescence originate from the same excitation energy; the excited state of chlorophyll. Once a photon reaches a chlorophyll molecule of the photosystem 2 (PSII), the excited state of chlorophyll can be quenched by three main pathways; it can follow the linear electron transport producing ATP and NADPH through photochemistry or photochemical quenching (PQ), it can be re-emitted as a photon of fluorescence or can be dissipated through non-photochemical quenching (NPQ) [3].

The SIF yield is influenced by the other competing process that unlike SIF can be physiologically regulated; the PQ and NPQ. NPQ represents the thermal dissipation of the excitation energy through the xanthophyll cycle. The NPQ is triggered when the electron transport chain saturates, as the light reactions are bottlenecked by the CalvinBenson cycle under high light conditions. The changes in xanthophyll pigments and therefore the NPQ can be observed with the photochemical reflectance index (PRI) [4]. SIF and PRI are both optical signals that are generated within the leaf; after the signals are produced, a radiative transfer process takes place, resulting in a structural effect on both signals. The relationship between SIF at 760 nm (F_{760}) and GPP has been described with the Monteith's light use efficiency equation (equation 1) [2], where LUE_p is GPP / APAR and LUE_f is F_{760} / APAR.

$$GPP \approx F_{760} \times \frac{LUE_p}{LUE_f \times Fesc} \tag{1}$$

Although SIF has been successfully used to predict GPP in various ecosystems, the mechanistic link between GPP and SIF remains not fully understood, and especially the effect of function and structure on SIF at the canopy scale remains an active area of research [5]. SIF is emitted by the whole canopy, but only a fraction of the total emission is observed with remote sensing techniques. The escape probability of SIF (Fesc) is defined as the probability of a photon of fluorescence of reaching the sensor and it can be conceptualized as the ratio between F_{760} observed and the F_{760} emitted, as showed in equation 2, where Fesc is the escape probability of

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F_{760} emitted at leaf level.

$$Fesc = \frac{F_{760}}{F_{760\ emitted}/\pi} \quad (2)$$

As the escape probability of fluorescence strongly affects the fluorescence observation, and the LUE_p and LUE_f influence the fluorescence emission [6], it is pivotal to understand the factors controlling Fesc, LUE_p and LUE_f in order to improve the accuracy of the prediction of GPP from SIF.

The objectives of this work are twofold: i) to assess the factors controlling Fesc, LUE_p and LUE_f in a Mediterranean grassland with different levels of nitrogen and phosphorous fertilization; ii) to obtain more accurate prediction of GPP from SIF using only remote sensing information. We therefore i) explore the predictors of Fesc, LUE_p and LUE_f (functional traits and canopy structural parameters) combining radiative transfer modelling approaches, by means of the SCOPE model, and a data driven methodology based on variable selection methods, and ii) on the basis of the results obtained in the first step we developed an empirical model to predict GPP from SIF using only optical data.

2. MATERIALS AND METHODS

The study was conducted in a Mediterranean savannah located in Spain (39°56′24.68″N , 5°45′.40.27″W; Majadas de Tietar, Cáceres), characterized by a continental Mediterranean climate. The site is managed as a typical wood pasture (Iberian Dehesa). The herbaceous stratum is dominated by species of the three main functional plant forms: grasses, forbs and legumes.

A small-scale manipulation experiment focused on the herbaceous layer was set-up with Nitrogen, Phosphorus and Nitrogen and Phosphorus addition with a randomized block design. Measurements taken that are used in the study are: CO_2 flux measurements with transparent and opaque chambers [4], leaf area index (LAI), leaf mass per area (LMA) and plant type composition identification. Leaf angle distribution parameters (LIDFa, LIDFb) were estimated from plant type composition, assuming erectophile distribution for grasses, spherical distribution for forbs and planophile distribution for legumes. Top of canopy spectral radiance were collected at midday under clear sky conditions with two portable spectrometers (HR4000; OceanOptics, Dunedin, FL, USA). Sun induced fluorescence was retrieved exploiting the spectra fitting method [7]. The four phenological phases referred in the study are Tillering, Flowering and Ripening that correspond to the growing season and Senescence that corresponds to the dry season.

The coupled fluorescence photosynthesis model SCOPE 1.7 [8] modified to provide dynamic LAD in time [5], was used to simulate photosynthesis, radiative transfer in the leaf and canopy, SIF for both emission peaks, and the surface energy balance for each campaign of the two years. Input variables provided for the model are: incoming and outgoing radiation, wind speed, air humidity, air temperature, air pressure, LAI, chlorophyll concentration, the maximum carboxylation rate (V_{cmax}) and soil moisture content. Data were analyzed by means of k-fold cross-validation to select the best GPP model, using R^2 and Akaike information criterion (AIC) for model selection. Several different PRI formulations and NIR integration intervals were tested. Principal component analysis for the multivariate analysis and relative importance analysis with "lmg" method was used to determine the importance of the predictors.

From equation 1 we express the relationship between GPP and F_{760} as shown in equation 3, where ϵ represents the unexplained variation.

$$GPP = \frac{F_{760}}{\frac{LUE_f\ Fesc}{LUE_p}} + \epsilon \quad (3)$$

3. RESULTS

A good relationship between GPP and SIF in both years is observed as reported in the first row of Table 1.

predictors	r.squared	p.value	df	AIC
F760	0.70	<0.01	2	738.76
F760 /NIR + PRI	0.86	<0.01	3	636.52

Table 1. $GPP \sim F_{760}$ and $GPP \sim F_{760}/NIR_{680-770} + PRI_{667-531}$ for grasses in a Dehesa in Majadas, Spain in 2014 and 2015.

The 7 variables measured and Fesc are represented in a principal component analysis in Figure 1. The first main axis of variation is mainly influenced by PRI, LAI and leaf nitrogen content (N%), and the second main axis of variation, independent from the first, is driven mainly by "% of grasses". The first three phenological phases, called Tillering, Flowering and Ripening overlap and the only phase that clearly clusters is the Senescence. Together, the first two axis explain 70% of the total variation.

Figure 2 shows that by means of a relative importance analysis, the main predictor of Fesc is "% of grasses", with R^2 of 0.34, with NIR $_{680\text{-}770}$ as secondary predictor. The main predictors of the residuals of the linear model between GPP and F_{760} are $PRI_{667\text{-}531}$ with R^2 of 0.16 and $NIR_{680\text{-}770}$ as secondary predictor. Finally the main predictor of the lumped term (LUE_f * Fesc) / LUE_p is $NIR_{680\text{-}770}$ with R^2 of 0.1.

$NIR_{680\text{-}770}$ and $PRI_{667\text{-}531}$ are therefore potential candidates to empirically approximate components of the LUE equation that usually difficult to obtain, such as LUE_f, LUE_p and Fesc.

Different empirical model formulations, were tested and the one selected as the best according to model performance and AIC is described in equation 4 where (LUE_f x Fesc) /

$LUE_p = NIR_{680\text{-}770}$ and $\epsilon = PRI_{667\text{-}531}$. In doing so, we obtain a new formulation that describes GPP using only optical data.

$$GPP \approx \frac{F_{760}}{NIR_{680-770}} + PRI_{667-531} \quad (4)$$

This new formulation significantly improves the prediction of GPP, as shown in the second row of Table 1, opening new exciting pathways for GPP quantification.

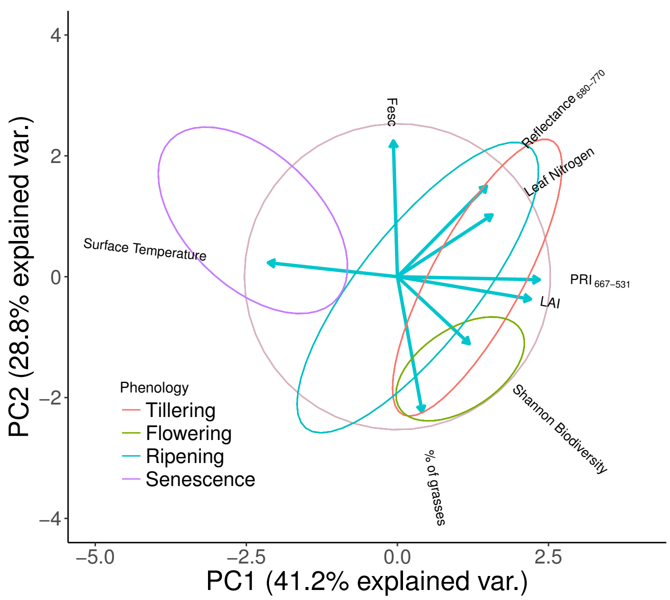

Fig. 1. Principal Component Analysis for 9 variables in 2014 and 2015. All varialbes are centered and scaled before inclusion in the PCA. Ellipses represent 95 % confidence intervals of the phenology factor

4. DISCUSSION

The predictors of Fesc, the lumped term (LUE_f * Fesc) / LUE_p and the residuals of GPP - F_{760} were analyzed with a relative importance analysis with various degrees of success, being Fesc easier to predict, while the lumped term and the residuals GPP - F_{760} remain elusive and harder to fully understand. "% of grasses", the main predictor of Fesc, is in itself a biodiversity proxy, but it also a variables that strongly influences LAD and canopy structure as grasses are mainly erectophiles [5]. LAD has not been included as a predictor in the relative importance analysis, as it was one input of the SCOPE simulation but, LAD parameters such as LIDFa strongly correlate with "% of grasses" (R^2= 0.64, p <0.01); for this reason "% of grasses" is considered a structural variable. Both F_{760} and Fesc are affected by functional and structural traits. Functional traits such as V_{cmax}, nitrogen content and chlorophyll content influence F_{760}, as they directly affect the PQ, through RuBisCO availability, and NPQ, by setting the ceiling of photosynthetic active radiation (PAR) at which the photosynthesis becomes saturated and the excessive energy needs to be dissipated through the xanthophyll cycle [6].

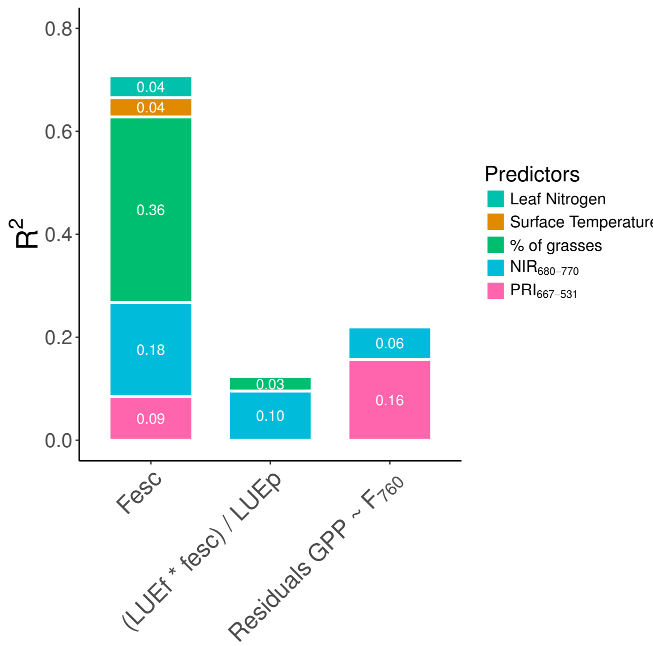

Fig. 2. Relative importance of 5 independent variables with "lmg" method for Fesc, the lumped term (LUE_f * Fesc) / LUE_p and the residuals of the linear model between GPP and F_{760}. The phenological period Senescence is filtered.

Structural traits such as leaf area index (LAI) and leaf angle distribution (LAD) have a strong influence on the F_{760} reabsorption and scattering, but structure has also a physiological influence on F_{760} through the sun-shade ratio. Sunlit leaves are more likely to have photosynthesis limited by radiation and have therefore lower LUE_p than shaded leaves; sunlit leaves therefore dissipate the excess of energy mainly through the NPQ pathway.

The lumped term (LUE_f * Fesc) / LUE_p was predicted with R^2 of only 0.13, highlighting the difficulty of predicting a term that carries both functional and structural information. The main predictor was $NIR_{680\text{-}770}$, a variable that is mostly influenced by canopy structure, suggesting that most of the variation of this lumped term is due to the structure. Even though it is challenging to describe (LUE_f * Fesc) / LUE_p, the inclusion of $NIR_{680\text{-}770}$ in the model improves GPP estimates.

One explanation could be related to the fact that as $NIR_{680-770}$ penetrates deeper into the canopy than visible light, it provides information on canopy structure. Moreover $NIR_{680-770}$ correlates well also with scattered F_{760} (R^2= 0.29, $p < 0.01$) indirectly revealing the degree of shade within the canopy and therefore explaining the structural component of Fesc. Furthermore $NIR_{680-770}$ correlates well with Nitrogen content as shown in the principal component analysis in Figure 1, which is bound to affect the LUE_p.

$PRI_{667-531}$ is the main predictor of the residuals of the linear model between GPP and F_{760} and its inclusion in the model improves GPP estimates; the reason for this is twofold. From the PCA in Figure 1 we can clearly see that $PRI_{667-531}$ correlates positively with LAI and negatively with surface temperature. $PRI_{667-531}$ is therefore a good indicator of the phenological variability and might help to explain part of the photosynthetic information that is not accounted by F_{760}. On the other hand, $PRI_{667-531}$ is also a proxy for NPQ. As it has been shown that the correlation between F_{760} and GPP is driven by the NPQ activity [3], it follows that $PRI_{667-531}$ should be able to explain the degree of coupling and uncoupling between photochemistry and fluorescence, hence providing a second explanation why its inclusion in the model also improves GPP estimates.

It is important to stress that the approach proposed in this study is based on an empirical analysis and therefore cannot be easily extrapolated to other sites.

In conclusion, we demonstrate that Fesc, a critical factor to predict GPP from F_{760} in light use efficiency modeling approach, it is mainly influenced by structural variables. Morever, based on the analysis of the predictor of Fesc, LUE_f and LUE_p we present a semi-empirical model formulation based only on optical data that significantly improves the GPP prediction. Additional research is needed to test this new approach across different ecosystems, and to further comprehend what are the processes responsible for the increased GPP predictions with the model proposed.

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