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# Multiple-constraint inversion of SCOPE. Evaluating the potential of GPP and SIF for the retrieval of plant functional traits



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#### ABSTRACT

The most recent efforts to provide remote sensing (RS) estimates of plant function rely on the combination of Radiative Transfer Models (RTM) and Soil-Vegetation-Atmosphere Transfer (SVAT) models, such as the Soil-Canopy Observation Photosynthesis and Energy fluxes (SCOPE) model. In this work we used ground spectroradiometric and chamber-based  $CO_2$  flux measurements in a nutrient manipulated Mediterranean grassland in order to: 1) develop a multiple-constraint inversion approach of SCOPE able to retrieve vegetation biochemical, structural as well as key functional traits, such as chlorophyll concentration ( $C_{ab}$ ), leaf area index (*LAI*), maximum carboxylation rate ( $V_{cmax}$ ) and the Ball-Berry sensitivity parameter (*m*); and 2) compare the potential of the of gross primary production (*GPP*) and sun-induced fluorescence (SIF), together with up-welling Thermal Infrared (TIR) radiance and optical reflectance factors (RF), to estimate such parameters. The performance of the proposed inversion method as well as of the different sets of constraints was assessed with contemporary measurements of water and heat fluxes and leaf nitrogen content, using pattern-oriented model evaluation.

The multiple-constraint inversion approach proposed together with the combination of optical RF and diel *GPP* and TIR data provided reliable estimates of parameters, and improved predicted water and heat fluxes. The addition of SIF to this scheme slightly improved the estimation of *m*. Parameter estimates were coherent with the variability imposed by the fertilization and the seasonality of the grassland. Results revealed that fertilization had an impact on  $V_{\rm cmax}$ , while no significant differences were found for *m*. The combination of RF, SIF and diel TIR data weakly constrained functional traits. Approaches not including *GPP* failed to estimate *LAI*; however *GPP* overestimated  $C_{\rm ab}$  in the dry period. These problems might be related to the presence of high fractions of senescent leaves in the grassland. The proposed inversion approach together with pattern-oriented model evaluation open new perspectives for the retrieval of plant functional traits relevant for land surface models, and can be utilized at various research sites where hyperspectral remote sensing imagery and eddy covariance flux measurements are simultaneously taken.

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#### 1. Introduction

Modeling and prediction of photosynthetic CO<sub>2</sub> uptake fluxes from regional to global scales is relevant for several areas involving policy, management and science; as it is the major flux in the global carbon cycle (Beer et al., 2010; Pfeifer et al., 2012). Land Surface Models (LSM) combine climatic and surface variables to predict biosphere-atmosphere exchanges in space and time. Accurate simulation of these fluxes requires certain knowledge on Earth surface properties at sufficient spatial and temporal resolutions. Currently, LSM predictions include large uncertainties originated in terrestrial carbon cycle modeling due to inadequate process understanding and/or parameterization (Friedlingstein et al., 2014: Knutti and Sedláček, 2012); but also due to unrealistic spatial and temporal representation of key plant functional traits controlling CO<sub>2</sub> uptake (Rogers, 2014; Rogers et al., 2016; Schaefer et al., 2012). Many of these parameters, - in particular maximum carboxylation rate  $(V_{cmax})$  and the Ball-Berry sensitivity parameter (m)-, are known to have a certain dynamic in space and time; however LSM typically use fixed values assigned to different plant functional types (PFT) (Bonan et al., 2011; Rogers, 2014; Walker et al., 2017; Wullschleger et al., 2014).

Other parameters also relevant for LSM describe vegetation structure and foliar constituents such as leaf area index (*LAI*), chlorophyll concentration ( $C_{ab}$ ) and other pigments. These parameters are relevant to describe both light absorption and the photosynthetic active biomass, and therefore control photosynthesis (Croft et al., 2015; Liu et al., 2017; Zhang et al., 2014a). The remote estimation of these parameters is possible because they directly influence radiation-canopy interaction; and therefore Radiative Transfer Models (RTM) can be inverted against spectrodirectional observations to characterize vegetation state (Jacquemoud et al., 2009). Nonetheless, the inversion or RTM is illposed and can be quite uncertain as extensively discussed in the literature (Combal et al., 2003; Homolová et al., 2013; Kimes et al., 2000; Pfeifer et al., 2012; Ustin et al., 2009; Zurita-Milla et al., 2015).

Contrarily, functional traits related to photosynthetic processes and stomatal conductance (e.g.,  $V_{cmax}$ , m, as well as fluorescence quantum efficiency ( $f_{qe}$ ), maximum rate of electron transport ( $J_{max}$ ), etc.) only have an indirect and reduced effect on the radiation leaving the top of the canopy (TOC). They modify optical signals mainly via sun-induced chlorophyll fluorescence (SIF) emission (Verrelst et al., 2015) and/or reflectance variations related to non-photochemical quenching reactions involving xanthophyll cycle (Gamon et al., 1992). In addition, photosynthesis and stomatal conductance are intimately related (Farquhar and Sharkey, 1982) and therefore a relationship between photosynthesis and the Thermal Infrared (TIR) domain is expected, in particular under stress conditions (Sellers et al., 1997). Variations in the optical up-welling radiance induced by these processes can be only sensed from narrow or very narrow spectral bands, and ideally from hyperspectral sensors. This fact, combined with the weak and indirect connection between traits and TOC optical radiance explains the lack of RS-based spatiotemporal information on these photosynthetic variables. Recently,  $V_{\rm cmax}$  was retrieved from hyperspectral data at leaf and canopy scales using partial least squares regression techniques thanks to spectral bands related to protein absorption features (Dechant et al., 2017; Serbin et al., 2015; Silva-Perez et al., 2018). These works indirectly linked reflected radiation and V<sub>cmax</sub> via nitrogen (N) - V<sub>cmax</sub> covariation. More mechanistic approaches used the  $C_{\rm ab}$  -  $J_{\rm max}$  -  $V_{\rm cmax}$ relationship (Alton, 2017); or inverted the Boreal Ecosystem Productivity Simulator model (Xie et al., 2018) to retrieve  $V_{cmax}$  from RS data in combination with eddy covariance (EC) fluxes. Empirical models have related spectral indices and canopy temperature to stomatal conductance (Damm et al., 2018; Jarolmasjed et al., 2018; Vaz et al., 2016; Zarco-Tejada et al., 2012; Zarco-Tejada et al., 2013), but to the best to our knowledge, not to the underlying parameter m. Only recently, *m* has been retrieved from RS data thanks to the combination of RTM and Soil-Vegetation-Atmosphere Transfer (SVAT) models (Bayat et al., 2018). An alternative to obtain information about photosynthetic parameters is the retrieval and analysis of SIF, the reemission of the absorbed photosynthetically active radiation (*APAR*) at larger wavelengths. SIF is linked to the electron transport rate in photosystem II (Porcar-Castell et al., 2014), and mechanistically related with  $V_{\rm cmax}$ : The latter imposes the ceiling on the rate of *APAR* that can be used in photochemistry, thus affecting charge dissipation and SIF (Frankenberg and Berry, 2018; Vilfan et al., 2019).

As described, various signals in the optical and the thermal domains can be related to plant photosynthesis through different mechanisms, and therefore could jointly be used to estimate functional parameters of vegetation. Currently, the state-of-the-art model that describes all these processes and the related spectroradiometric signals is SCOPE (van der Tol et al., 2009). This model combines Visible, TIR and SIF radiative transfer with energy balance and photosynthesis models. Using SCOPE, Zhang et al. (2014b) used RS-based SIF and vegetation indices to retrieve  $V_{\rm cmax}$  in crops. Zhang et al. (2018) inverted SCOPE against optical RS data and EC fluxes to retrieve  $V_{cmax}$ ; then they fit models to predict GPP from SIF in crops at regional scale. Also recently, Bayat et al. (2018) inverted SCOPE combining Landsat optical and TIR imagery to retrieve  $V_{\rm cmax}$  and *m* parameters in a grassland. Dutta et al. (2019) used a modified version of SCOPE to constrain LAI,  $V_{\rm cmax}$  and m against carbon and energy fluxes together with multiband optical RS data. In addition, Hu et al. (2018) estimated  $V_{cmax}$  and  $f_{qe}$  by inverting SCOPE against a combination of proximal sensing data (i.e. SIF) and GPP. These works represent the state-of-the-art in the estimation of functional traits such as  $V_{\rm cmax}$  and/or m parameter from RS observations. Despite the fact that different works provided estimates of  $V_{\rm cmax}$ and other functional traits using GPP (Dutta et al., 2019; Xie et al., 2018; Zhang et al., 2018) as well as SIF (Zhang et al., 2014b), it is not clear whether both variables can provide comparable estimates; and therefore, whether they can be used indistinctly or not. A robust evaluation is needed to understand the potential of SIF and GPP to retrieve  $V_{\rm cmax}$  and other functional parameters, as well as and to identify the most suitable methodologies for this task.

One of the most critical aspects of the retrieval of functional traits is the validation or evaluation of the results. The evaluation of functional trait estimates at canopy/ecosystem scale requires leaf level measurements that are not feasible at large spatial scales, or in ecosystems featuring numerous species. So far, the inversion of SCOPE model has rarely been evaluated against either field observations or proxies of the functional parameters. Most commonly, SCOPE inversion has been indirectly assessed by comparing predicted and observed EC fluxes that were not included in the optimization process, as for example, water and heat fluxes (Bayat et al., 2018; Zhang et al., 2014b). However, this comparison can result largely uncertain due to the spatial mismatch existing between the spectral and the EC footprints under comparison (Cescatti et al., 2012; Chen et al., 2009; Gamon, 2015; Gelybó et al., 2013; Migliavacca et al., 2015). Nonetheless, pattern-oriented model evaluation (Carvalhais et al., 2014; Grimm and Railsback, 2012; Luo et al., 2012; Migliavacca et al., 2013; Reichstein et al., 2011) is a viable alternative strategy to diagnose model performances when traditional model evaluation is problematic for several reasons, including lack of robust ground data, as in the case of canopy scale plant functional traits. The pattern-oriented model evaluation - as intended here - is a strategy to evaluate the physical consistency of model inversion or of the estimated parameters. This is conducted in two ways:

1) By comparing the relationship between estimated parameters and proxies that are i) known to be related with the parameter under evaluation and ii) more easily measureable and scalable at plot level. For example, retrieved  $V_{\rm cmax}$  (and  $C_{\rm ab}$ ) are known to be related with nitrogen concentration ( $N_{\rm mass}$ ) (Quebbeman and Ramirez, 2016; Walker et al., 2014), and relationships for different plant types can be found in published meta-analyses (e.g., Feng and Dietze (2013) for grasslands) or in global databases such as TRY (Kattge

et al., 2011). Such information can be used to evaluate indirectly whether the inversion of the models produces patterns that are physically and biologically plausible, even in absence of direct observation of the target variable.

2) By comparing a combination of variables predicted by the model and not included in the cost function to verify whether the underlying processes represented by the model structure are coherent with the observations. For example, the comparison of predicted and observed evaporative fraction (*EF*, i.e. the ration between latent heat fluxes and available energy – the sum of latent and sensible heat fluxes) informs on the consistency of energy partition, and therefore of the plausibility of *m* estimates. This method is meant to be more robust to biases that might exist in the latent and sensible heat fluxes induced by footprint mismatch.

In this work, we test the inversion of SCOPE model in a two-steps multiple-constraint approach combining simultaneously observations of hyperspectral optical data and TIR radiation, together with *GPP* and/ or SIF. We aim to 1) develop the best scheme to retrieve biochemical and structural (e.g.  $C_{ab}$ , *LAI*) as well as functional traits ( $V_{cmax}$ , m) in a Mediterranean grassland manipulated with N and phosphorus (P) fertilization; 2) evaluate the performance *GPP* and SIF to constrain these traits in a multiple-constraint inversion approach; and 3) assess the performance and the sensitivity to uncertainties of the method proposed as well as of the different constraints using a pattern-oriented model evaluation approach by comparing  $V_{cmax}$  (and  $C_{ab}$ ) estimates from their relationship with measured leaf  $N_{mass}$ , and by assessing m estimates from the evaluation of energy partition with *EF*.

## 2. Methods

## 2.1. Study site and experimental design

The current study is located in a Mediterranean tree-grass ecosystem in the research facility of Majadas de Tiétar, Cáceres, Spain (39° 56′ 24.68″N, 5° 45′50.27″W). This is a managed savannah combining sparse trees and an annual grassland under low intensity grazing (< 0.3 cows/Ha). Trees (mainly *Quercus ilex* L. subsp. *ballota* [Desf.] Samp.) present a fractional cover ~20% and average tree distance ~18.8 m ( $\sigma$  = 5.0 m) (Pacheco-Labrador et al., 2016). The herbaceous layer is spatially and temporally diverse, comprehending species of the three main functional plant forms: grasses, forbs and legumes such as *Tolpis barbata, Anthoxanthum aristatum, Ornithopus compressus, Trifolum striatum, Lotus parviflorus* and *Plantago lagopus* (Migliavacca et al., 2017).

The climate is continental Mediterranean and therefore seasonality and inter-annual variability are strong. Mean annual temperature is 16.7 °C and mean annual precipitation ~650 mm. Rain concentrates between October and April, whereas summers are hot and dry. The herbaceous layer strongly responds to radiation and water availability: Biomass peaks in spring, completely dries in summer, re-greens in autumn and goes dormant in winter (Luo et al., 2018; Mendiguren et al., 2015). Senescent material accumulates within the canopy already during the growing period, and can represent up to 30% of *LAI* before the dry season starts.

The current work focuses on the herbaceous layer, in the context of the Small-scale MANIpulation Experiment (SMANIE). This is a full factorial fertilization experiment assessing the responses of the herbaceous layer N, P and N plus P fertilization (Migliavacca et al., 2017; Perez-Priego et al., 2015a). The experiment consists of four replicates of  $20 \times 20$  m blocks containing four  $9 \times 9$  m plots with a different treatment each: control -not fertilized- (C), fertilized with nitrogen (N), with phosphorous (P) or both (NP). Plots are separated by a 2 m buffer to prevent boundary effects and are located in an open area to minimize the influence of trees. Some of the ancillary data and meteorological measurements used in this work come from the nearby EC site, and are acquired both at ecosystem scale ( $EC_{eco}$ ) and over the herbaceous layer ( $EC_{sub}$ ) (El-Madany et al., 2018; Perez-Priego et al., 2017).

#### 2.2. Spectral, flux and ancillary measurements

Between spring 2014 and 2016, 9 field campaigns monitored the experimental blocks with the different treatments. In each campaign, daily cycles of net ecosystem CO2 exchange (NEE) and ecosystem respiration (Reco) were measured respectively with transparent and opaque cubic chambers of 60 cm length. Chamber measurements were performed on one collar in each of the 16 plots of the experiment (see Migliavacca et al. (2017)). In total, 1089 chamber measurements were carried out, with a median of 6 measurements per plot and campaign. The chambers were equipped with an infrared gas analyzer (LI-840, Li-Cor, Lincoln, NE, USA) to measure CO2 molar fractions; a quantum sensor (LI-190, Li-Cor, Lincoln, NE, USA) to measure photosynthetically active radiation (PAR); two temperature probes (type 107, Campbell Scientific, Logan, Utah, USA) to monitor soil  $(T_s)$  and air temperature  $(T_a)$ ; a soil moisture  $(SM_p)$  probe (Theta Probe ML2x, Delta-T Devices, Cambridge, UK); an infrared thermometer (IRTS-P, Apogee, UT, USA) to target canopy surface temperature  $(T_c)$ ; and an atmospheric pressure (P) sensor (CS100, Campbell Scientific, Logan, Utah, USA). NEE was computed as a function of the time rate of change of the measured CO<sub>2</sub> dry molar fraction using a flux-calculation algorithm implemented in the R Package 'respchamberproc' (Perez-Priego et al., 2015b). GPP was then computed by subtracting consecutive  $R_{\rm eco}$  and NEE measurements. Further details on the chambers design, acquisition and processing can be found in Perez-Priego et al. (2015a).

Measurements of sensible heat (H, W/m<sup>2</sup>), latent heat ( $\lambda E$ , W/m<sup>2</sup>),  $CO_2$  fluxes (µmol/m<sup>2</sup>/s), and friction velocity ( $u^*$ , m/s), as well as meteorological and soil properties were conducted at two near-by EC towers located in a non-fertilized area (Perez-Priego et al., 2017). The two EC systems are identical and consist of a three-dimensional sonic anemometer (R3-50, Gill LTD UK) and an infrared gas analyzer to measure dry mixing ratios of CO<sub>2</sub> and H<sub>2</sub>O (LI-7200, Licor Bioscience, Lincoln, USA).  $EC_{eco}$  measurement height was 15 m which corresponds to roughly 7 m above the mean tree canopy height (El-Madany et al., 2018). EC<sub>sub</sub> measured the fluxes of the herbaceous layer at a height of 1.6 m (Perez-Priego et al., 2017); only EC fluxes of this tower are of interest in this work. At  $EC_{eco}$ , shortwave incoming radiation ( $R_g$ ) was measured with a net radiometer (CNR4, Kipp and Zonen, Delft, Netherlands) at ~15 m. Also,  $T_a$  and relative humidity (rH) were measured with a combined Pt-100 temperature and capacitive humidity sensor (CPK1-5, MELA Sensortechnik, Germany) at 15 and 2 m, respectively.  $SM_{\rm p}$  (%) was measured at 4–5 cm below ground with 8 probes (ML2x, Delat-T Devices Ltd., Cambridge, UK).

Down-welling and up-welling TOC spectral radiances were recorded in each of the chamber collars at noon (  $\pm$  2 h), under clear sky conditions and right before the flux measurements. In total, 164 (noon) data were available: one per plot and campaign; some campaigns lasted more than one day, and some plots were repeated. The spectroradiometric system combined two field spectroradiometers (HR4000; OceanOptics, Dunedin, FL, USA). The first was a Visible and Near Infrared (VNIR, 400-1000 nm) sensor with Full Width at Half Maximum (FWHM)  $\sim$  1.5 nm. The second was a high spectral resolution spectroradiometer dedicated to SIF retrieval. In 2014 the SIF spectroradiometer featured FWHM ~0.1 nm and spectral range 700-800 nm, allowing the retrieval of SIF radiance in the observation direction in the  $O_2$ -A band ( $F_{760}^{\dagger}$ ). In 2015 this sensor was replaced by a similar SIF spectroradiometer (HR4000; OceanOptics, Dunedin, FL, USA) with a wider spectral range 650-840 nm (FWHM ~0.1 nm), allowing also the retrieval of SIF radiance in the observation direction in the O2-B band  $(F_{687}^{\uparrow})$ . Spectroradiometers were placed in a Peltier box, keeping the internal temperature at 25 °C to prevent dark current drift and changes in their spectral features. The system was controlled by the ad hoc software S3 (Meroni and Colombo, 2009). Five measurements per collar

were taken with 25° field of view optical fibers at nadir, ~110 cm above the ground. This ensured high spatial match between flux and spectral footprints. Down-welling radiances were measured sequentially to TOC up-welling radiances using a 99% reflective Spectralon® panel (Lab-Sphere, North Sutton, NH, USA). From the measured down and upwelling radiances, we computed Hemispherical-Conical Reflectance Factors (*HCRF*); also,  $F_{760}^{\dagger}$  and  $F_{687}^{\dagger}$  were retrieved using spectral fitting methods and a dedicated IDL code (ITTVIS IDL 7.1.1) (Meroni and Colombo, 2009). Further details can be found in Perez-Priego et al. (2015a) and Migliavacca et al. (2017).

Destructive sampling was carried out within the plot of each collar in quadrants (sample size n = 4), wherever vegetation presented similar conditions than the chamber collar. Samples were never acquired inside the collars in order to preserve them intact and to ensure the consistency of the spectral and chamber data time series. Therefore, some uncertainty related to the small-scale spatial heterogeneity of the herbaceous layer is still expected (Melendo-Vega et al., 2018; Vilar et al., 2016). These samples led to the estimation of *LAI*, leaf mass per area ( $C_m$ ), plant form abundances (grass, forbs and legumes), green fractions as well as carbon ( $C_{mass}$ ), phosphorus ( $P_{mass}$ ) and  $N_{mass}$  concentrations per mass (in %) using laboratory methods described in Perez-Priego et al., (2015a).

## 2.3. SCOPE model description and parameterization

SCOPE presents a modular architecture allowing the selection of different sub-models. In this work we inverted SCOPE v1.7, including the leaf RTM Fluspect (Fluspect-CX) (Vilfan et al., 2018), capable of reproducing xanthophyll cycle effects in leaf absorptance between 500 and 570 nm. These changes are propagated to TOC outgoing radiance. In the model, we selected fluorescence emission spectra from FluoWat leaf clip measurements (calc\_PSI = 0) (Vilfan et al., 2016); and a fluorescence model including sustained quenching (van der Tol et al., 2014) (Fluorescence\_model = 0). We also applied temperature correction to  $V_{\rm cmax}$  (apply\_T\_corr = 1) and defined soil heat flux (*G*) as a constant fraction of soil net radiation (soil\_heat\_method = 2).

SCOPE requires several input variables or drivers representing instantaneous meteorological conditions (e.g. air temperature, atmospheric pressure, wind speed, etc.), as well as spectral down-welling irradiance in the Visible-TIR domain. SCOPE also requires parameters describing vegetation biochemistry, structure and function such as pigment contents, leaf angle distribution (*LAD*), *LAI*,  $V_{cmax}$ , *m*, etc. We aim to retrieve these parameters from the inversion of the model.

## 2.3.1. Characterization of direct and diffuse illumination

SCOPE requires spectral diffuse and direct down-welling irradiances  $(E_{\rm dif}^{\downarrow}$  and  $E_{\rm dir}^{\downarrow}$ , respectively, W/m<sup>2</sup>/µm), whereas field spectroradiometers only measure total bottom of the atmosphere down-welling spectral irradiance ( $E_{tot}^{\downarrow}$ , W/m<sup>2</sup>/µm). In order to prescribe these quantities, we inverted the RTM 6S v2.1 (Vermote et al., 1997) against  $E_{tot}^{\downarrow}$ between 350 and 980 nm using a model emulator. First we generated a look-up table (LUT) with 1500 samples using the Python Py6S helper (Wilson, 2013) and Latin Hypercube Sampling (LHS). Next a neural network (NN) model was trained to predict  $E_{tot}^{\downarrow}$  from the atmospheric parameters using a modified version of SimpleR (Camps-Valls et al., 2012). 1000 samples were selected for training and 500 for validating the emulator. Then we retrieved atmospheric parameters minimizing the cost function in Eq. (1) using the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) algorithm (Hansen, 2006). Observed irradiances  $(E_{\lambda,obs}^{\downarrow})$  were resampled to meet center bands and bandwidth (2.5 nm) of the 6S predicted irradiances  $(E_{\lambda,\text{pred}}^{\downarrow})$  using spectral convolution (Damm et al., 2011). For each of the spectral observations, we used site coordinates and time stamps to compute solar angles using the algorithm described in (Reda and Andreas, 2004). Water vapor (H<sub>2</sub>O,  $g/m^2$ ), ozone (O<sub>3</sub>, cm·atm) and the aerosol optical thickness at 550 nm (AOT) were constrained for each of the following aerosol profiles (continental, maritime, urban, desert and biomass). The profile with the lowest error according to Eq. (1) was selected. From the retrieved parameters,  $E_{dir}^{\downarrow}$  and diffuse  $E_{dif}^{\downarrow}$  down-welling irradiances were computed with Py6S and the fraction of each component was used to derive more accurate direct and diffuse irradiances from  $E_{\lambda,obs}^{\downarrow}$  as the product of the fractions interpolated to the spectroradiometer bands and  $E_{\lambda,obs}^{\downarrow}$ .

$$\chi^2 = \sum_{\lambda=350}^{980} (E_{\lambda,\text{obs}}^{\downarrow} - E_{\lambda,\text{pred}}^{\downarrow})^2 \tag{1}$$

where  $\lambda$  stands for the wavelength in nm.

#### 2.3.2. Soil optical properties parameterization

Soil properties were determined inverting the brightness-shapemoisture (BSM) SCOPE sub-model model - described in Verhoef et al. (2018) - against bare soil HCRF measurements (HCRF<sub> $\lambda$  obs</sub>) acquired with an ASD Fieldspec® 3 (Analytical Spectral Devices, Boulder, CO, USA) in the range 400-2500 nm. The least square nonlinear curve-fitting optimization implemented in the Matlab<sup>™</sup> function LSONONLIN (MathWorks, Natick, MA, USA) minimized the cost function in Eq. (2). Spectral weights  $(w_{\lambda})$  improved the fit in the region covered by the sensor:  $w_{\lambda} = 1.00$  for  $\lambda \le 1000$  nm,  $w_{\lambda} = 0.15$  for  $\lambda > 1000$  nm and  $w_{\lambda} = 0.0$  within the atmospheric water absorption bands. We constrained soil brightness (B, -), spectral shape "latitude" (Lat, deg) and "longitude" (Lon, deg); soil moisture capacity (SMC, %), SM<sub>p</sub> (%) and the single water film optical thickness (film, -). Then for SCOPE inversion we combined SM<sub>p</sub> observations with the parametrized values of the B, Lat, Lon, SMC and film. This way SMp was the only parameter controlling the soil reflectance ( $\rho_{\lambda}$ ).

$$\chi^{2} = \sum_{\lambda=400}^{2500} w_{\lambda} \left( \frac{HCRF_{\lambda,\text{obs}} - \rho_{\lambda,\text{pred}}}{\sigma_{HCRF_{\lambda}}} \right)^{2}$$
(2)

where  $\rho_{\lambda, \text{ pred}}$  is the predicted soil reflectance and  $\sigma_{HCRF_{\lambda}}$  is the spectral uncertainty of  $HCRF_{\lambda,\text{obs}}$ .

#### 2.3.3. Soil resistances characterization

Soil boundary layer resistance ( $r_{\rm bs}$ , s/m) was computed directly from the  $u^*$  values internally calculated by SCOPE according to Monteith and Unsworth (2013) as  $r_{\rm bs} = 6.2u^{*0.67}$ . The soil resistance for evaporation from the pore space ( $r_{\rm ss}$ , s/m) was first parameterized using lysimeters data collected during the summer dry periods in 2015–2017, when grass was dry and evaporation was attributed to soil (Perez-Priego et al. (2017) and Appendix A). Then we fitted the empirical model in Eq. (3) between  $r_{\rm ss}$  and  $SM_{\rm p}$  measured at the EC towers; data were binned to percentile values to reduce noise. Finally, we predicted instantaneous  $r_{\rm ss}$  for each chamber measurement as a function of  $SM_{\rm p}$ observed at the EC site, but including an offset computed from the  $SM_{\rm p}$ chamber data in order to account for the generalized lower soil moisture in the SMANIE experiment.

$$r_{\rm ss} = a \cdot e^{(b \cdot SM_{\rm p})} + \frac{c}{SM_{\rm p}^2} \tag{3}$$

#### 2.4. SCOPE model inversion and uncertainty propagation

SCOPE was inverted using a multiple-constraint approach with two separated steps. This approach was used to assess the potential of *GPP* and SIF to retrieve plant biophysical and functional traits using them separately, as well as together. Moreover, we used an inversion not

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#### Table 1

Parameters estimated inverting SCOPE model, as well as the step of the inversion in which each parameter is retrieved.

Parameter	Symbol	Units	Step	Inversion bounds
Leaf chlorophyll content	$C_{\rm ab}$	µg/cm <sup>2</sup>	#1	[0, 100]
Leaf carotenoids content	$C_{\mathrm{ar}}$	µg/cm <sup>2</sup>	#1	[0, 40]
Senescent material	$C_{\rm s}$	-	#1	[0, 3]
Leaf water content	$C_{\rm w}$ ,	g/cm <sup>2</sup>	#1	$[6.3 \cdot 10^{-5}, 0.04]$
Leaf dry matter content	$C_{\rm dm}$	g/cm <sup>2</sup>	#1	[0.0019, 0.0165]
Leaf structural parameter	Ν	layers	#1	[1, 3.6]
Leaf area index	LAI	$m^2/m^2$	#1	[0, 8]
Leaf inclination distribution function	LIDFa	-	#1	$[-1, 1];  LIDF_{a} + LIDF_{b}  \le 1$
Bimodality of the leaf inclination	LIDFb	-	#1	
Maximum carboxylation capacity	V <sub>cmax</sub>	µmol/m²/s	#1 & #2	[0, 200]
Ball-Berry sensitivity parameter	m	-	#2	[0, 50]
Fluorescence quantum efficiency	$f_{ m qe}$	-	#1 & #2	[0,1]

including any of them as a reference. Hereafter, we refer to these inversion schemes as  $I_{GPP},\,I_{SIF},\,I_{GPP-SIF}$  and  $I_R,$  respectively. The parameters retrieved in each of the steps and the bounds imposed are presented in Table 1.

Fig. 1 summarizes the methodology proposed for the inversion of SCOPE. In the first step (Step#1), the biochemical ( $C_{ab}$ ,  $C_{ca}$ ,  $C_s$ ,  $C_w$ ,  $C_{dm}$ , N) and structural (*LAI*, *LDIF*<sub>a</sub>, *LDIF*<sub>b</sub>) parameters as well as  $V_{cmax}$  were constrained minimizing the prediction error of the near-simultaneous



Fig. 1. Schematic diagram of the SCOPE model inversion.

*HCRF* and *GPP* and/or  $F_{760}^{1}$  midday observations in each plot; I<sub>R</sub> used only *HCRF*. In the second step (Step#2), the functional parameters ( $V_{cmax}$  and m) were constrained minimizing the prediction errors of diel *GPP* estimates and/or midday  $F_{760}^{1}$  observations together with diel TIR radiance in the observation direction, assuming black body emissivity ( $L_{T,out,BB}$ ); I<sub>R</sub> used only  $L_{T,out,BB}$ . In Step#2,  $V_{cmax}$  previously retrieved ( $V_{cmax,S1}$ ) and its estimated uncertainty ( $\sigma_{V_{cmax,S1}}$ , this section) were used as a prior, where a minimum  $\sigma_{V_{cmax,S1}} = 5 \,\mu mol/m^2/s$  was imposed. EC tower micrometeorological data,  $SM_p$ , soil parameters, soil resistances,  $E_{dif}^{i}$  and  $E_{dir}^{i}$  were provided as forcing. Only chamber and proximal sensing observations constrained the inversion. Whenever  $F_{760}^{i}$  was used as a constraint (I<sub>SIF</sub> and I<sub>GPP-SIF</sub>),  $f_{qe}$  was also retrieved in both steps.

SCOPE was inverted using the numerical optimization algorithm in the Matlab<sup>m</sup> function LSQNONLIN. For both steps, the termination tolerance (*TolFun*) was set to  $10^{-9}$ . In Step#1, we minimized the following cost function (Eq. (4)):

$$\chi^{2} = \sum_{\lambda=400}^{930} \left( \frac{HCRF_{\lambda,\text{obs}} - HDRF_{\lambda,\text{pred}}}{\sigma_{HCRF_{\lambda}}} \right)^{2} + \left( \frac{GPP_{\text{noon,obs}} - GPP_{\text{noon,pred}}}{\sigma_{GPP}} \right)^{2} + \left( \frac{F^{\uparrow}_{760,\text{obs}} - F^{\uparrow}_{760,\text{pred}}}{\sigma_{F^{\uparrow}_{760}}} \right)^{2}$$

$$(4)$$

were  $\sigma_{GPP}$  is the *GPP* uncertainty as described in Perez-Priego et al. (2015a),  $\sigma_{F^{1}760}$  is the uncertainty in the  $F_{760}^{1}$  estimates and  $HDRF_{\lambda,\text{pred}}$  is the Hemispherical-Directional Reflectance Factor predicted by SCOPE. *HCRF* and *HDRF* were assumed to be comparable enough at nadir, reducing computation demand. Notice that whenever no specific type of reflectance factor is specified, RF is used through the manuscript.

In Step#2 we minimized the cost in Eq. (5) combining diel  $L_{T,out,BB}$ and the  $V_{cmax,S1}$  priors with either diel *GPP* (I<sub>GPP</sub>), noon  $F_{760}^{\dagger}$  (I<sub>SIF</sub>), diel *GPP* and noon  $F_{760}^{\dagger}$  (I<sub>SIF-GPP</sub>), or nothing else (I<sub>R</sub>). Predicted  $L_{T,out,BB}$  was calculated as the combination of SCOPE reflected and emitted radiances integrated in the 6–14 µm range, where the TIR sensors operate. Observed  $L_{T,out,BB}$  was computed from sensor surface temperature in the same spectral range.

$$\chi^{2} = \sum_{t=0}^{n} \left( \frac{GPP_{t,\text{obs}} - GPP_{t,\text{pred}}}{\sigma_{GPP}} \right)^{2} + \sum_{t=0}^{n} \left( \frac{L_{\text{T,out,BB}_{t,\text{obs}}} - L_{\text{T,out,BB}_{t,\text{pred}}}}{\sigma_{L_{\text{T,out}}}} \right)^{2} + \left( \frac{F^{\dagger}_{760,\text{obs}} - F^{\dagger}_{760,\text{pred}}}{\sigma_{F^{\dagger}_{760}}} \right)^{2} + \frac{V_{\text{cmax,S1}} - V_{\text{cmax,S2}}}{\max(\sigma_{V_{\text{cmax,S1}}}, 5)}$$
(5)

where  $\sigma_{L_{T, out}}$  is the  $L_{T, out, BB}$  uncertainty, t is each of the n diel observations and  $V_{cmax, S2}$  is the  $V_{cmax}$  retrieved in Step#2.

At each step, a Bayesian approach was used to estimate uncertainties in the constrained parameters as well as to predict uncertainties in the SCOPE model outputs. To do so, we used the method described in Omlin and Reichert (1999). For each observation, the Jacobian matrix produced parameter uncertainties and the covariance matrix. The covariance matrix was used to generate posterior distributions of the optimized parameters (Table 1). To avoid unrealistic values out of the parameter bounds, we used the truncated Normal and Student's t-distribution toolbox (Botev, 2017; Botev and Ecuyer, 2015). We used 200 realizations of the model to predict uncertainty distributions in the fluxes, TOC RF and SIF.

#### 2.5. Evaluation of the SCOPE inversion

The different inversion schemes tested in this work are evaluated against 1) inversion constraints (*GPP*,  $F_{760}^{+}$ , *HCRF* and  $L_{T,out,BB}$ ), 2)

direct measurement of retrieved parameters (e.g., *LAI*), 3) direct measurements of variables related with the estimated traits (e.g.,  $N_{\text{mass}}$ ), and 4) and quantities related to energy partitioning (*EF*).

LAI estimates were compared with values observed in the different plots. For the evaluation of the  $V_{\rm cmax}$  and m retrievals we did not use direct measurements of these parameters. The high biodiversity at the site hampered a representative scaling of leaf level gas exchange measurements at canopy level. Such exercise would require specie-based leaf level gas exchange and leaf area measurements in practice unaffordable; and even if feasible, the additive uncertainty associated to the scaling might become too large for the validation purposes. Nonetheless, there is a well-established relationship between  $V_{cmax}$  and foliar nitrogen (Ellsworth et al., 2004; Ouebbeman and Ramirez, 2016; Walker et al., 2014; Zhang et al., 2013). Therefore, we decided to evaluate whether  $V_{\rm cmax}$  estimates from inversion were related to  $N_{\rm mass}$ observations, as expected from literature (Walker et al., 2014); and to assess the consistency between the  $N_{\rm mass}$  observations -  $V_{\rm cmax}$  estimates relationship with other relationships reported in the literature from grasslands (e.g. Feng and Dietze (2013)). Similarly, since no direct  $C_{ab}$ measurements were available, we also evaluated it against  $N_{\text{mass}}$ (Houborg et al., 2013). The relationship between  $V_{\text{cmax}}$ ,  $C_{ab}$  and  $N_{\text{mass}}$  is expected to be robust for green vegetation. Therefore we accounted for the partitioning of N between green and senescent material by computing  $N_{\text{mass}}$  in the green leaves ( $N_{\text{mass,green}}$ ). To do so we used the relationship N<sub>mass</sub> - N<sub>mass,green</sub> observed at this site (Gonzalez-Cascon et al., 2019) and the observed green LAI fraction.

We used water and energy fluxes (e.g.  $\lambda E$ , H, etc.) as well as evaporative fraction ( $EF = \lambda E / (\lambda E + H)$ ) as independent observations to evaluate the performance and consistency of the different inversion schemes and the plausibility of m estimates. *EF* was chosen to evaluate if the partitioning of energy fluxes in the model runs for the C treatment was consistent with the ones measured in the nearby  $EC_{sub}$  station. We selected the *EF* rather than fluxes (H,  $\lambda E$ ) to ensure that energy partitioning was well described by the model and the estimated parameters, since biases in H and  $\lambda E$  could be induced by differences between SMANIE plots and the  $EC_{sub}$  footprint.

Moreover, we used  $F_{687}^{\dagger}$  for evaluation when available.  $F_{687}^{\dagger}$  was estimated only in the 2015 and 2016 campaigns, where a new SIF spectroradiometer covering this spectral range was used.

We used two-way analysis of variance (ANOVA) to assess the main effect -changes in mean- of treatments, campaigns and their interaction on the observed and retrieved parameters; and therefore to disentangle differences between treatments, independently of the seasonal variability. Also, parameter estimates were grouped per treatments according to the Tukey's Honest Significant Difference (HDS) test (Tukey, 1949). During evaluation, significance was described with the symbols for *p*-values  $0.05 \le p < 0.10$ ; and \* for p < 0.05.

#### 3. Results

## 3.1. Characterization of SCOPE inputs

Fig. 2a shows the simulated LUT and the NN-predicted  $E_{tot}^{\downarrow}$ ; while Fig. 2c shows the corresponding training and test errors. Errors are larger in the sharp absorption features of irradiance. Test mean error (*ME*), root mean square error (*RMSE*) and mean absolute (*MAE*) error (Richter et al., 2012) are -0.11, 9.24 and 6.20 W/m<sup>2</sup>µm, respectively; which are slightly lower than training errors (*ME*, *RMSE* and *MAE* are -0.01, 6.51 and 4.63 W/m<sup>2</sup>/µm, respectively). This suggests no training overfitting and sufficient accuracy and precision of prediction. Fig. 2b and d summarizes the inversion of 6S NN emulator against observations. They show observed and predicted  $E_{tot}^{\downarrow}$  as well as the error



fit, respectively. Uncertainties and model discrepancies produce errors larger than for training of the emulator:  $ME = 20.05 \text{ W/m}^2/\mu\text{m}$ ,  $RMSE = 49.41 \text{ W/m}^2/\mu\text{m}$ , and  $MAE = 39.21 \text{ W/m}^2/\mu\text{m}$ . Appendix B presents an example of the characterization of the atmospheric irradiance and the modeling of the direct and diffuse components (Fig. B.1a), as well as and the predicted diffuse-to-global radiation ratio (Fig. B.1b).

Bare soil *HCRF* inverted against the BSM model provides the following soil parameters: B = 0.921,  $Lat = 20.27^{\circ}$ ,  $Lon = 45.00^{\circ}$ , SMC = 43.29%, *film*: 0.012 and  $SM_{\rm p} = 12.71\%$ . Constrained *SMC* equals the 99.99% percentile of the  $SM_{\rm p}$  values registered by 8 soil moisture probes in the EC towers between January 2014 and January 2018. From the same probes,  $SM_{\rm p}$  interpolated at the time of the acquisition of the soil spectra ranges between 8.74% and 13.89% (mean,  $\mu = 10.20\%$ , standard deviation  $\sigma = 1.66\%$ ); which is very close to the retrieved  $SM_{\rm p}$ . For the 400–2400 nm spectral region, fit statistics were ME = -0.00%, RMSE = 0.04% and MAE = 0.03%.

We fitted a model describing the  $r_{\rm ss} - SM_{\rm p}$  relationship (Eq. (3)) with  $R^2 = 0.61$  and RMSE = 21.03 s/m. Uncertainties are large for  $SM_{\rm p} < 10\%$  where an exponential decay is found (Fig. C.1), as expected in sandy soils (Baldocchi et al., 2000).  $r_{\rm ss}$  values predicted from  $SM_{\rm p}$  and used in the inversion show a low median (3.91 s/m), but  $r_{\rm ss}$  sometimes reach the upper bounds set for this variable (50,000 s/m, according to Bayat et al. (2018)).

#### 3.2. Model inversion

Fig. 3a presents the observed Normalized Difference Vegetation Index (*NDVI*<sub>obs</sub>) -averaged per date and treatment-, representing both seasonality and fertilization effects. Fig. 3b–e summarize the temporal variability of the most relevant retrieved parameters grouped by treatment (~4 replicates each) together with  $C_{\rm s}$  (Fig. 3f), all of them estimated with the scheme I<sub>GPP</sub>. Analogously, Appendix D presents the results of the schemes I<sub>SIF</sub>, I<sub>GPP-SIF</sub> and I<sub>R</sub> in Figs. D.1, D.2 and D.3, respectively. As can be seen, estimated parameters are coherent with the seasonality represented by  $NDVI_{\rm obs}$ : the grassland development starts around March, peaks in April, and then starts the senescence phase due to water stress. Independent  $C_{\rm ab}$  and *LAI* observations follow the same trend (Luo et al., 2018; Melendo-Vega et al., 2018). **Fig. 2.** Simulated and NN-predicted total irradiance values (a). Test and fit errors of the 6S NN emulator. The mean ( $\mu$ ) and the standard deviation ( $\sigma$ ) of the error per band are also presented (c). Observed and NN-predicted total irradiance values (b). Fit errors in the inversion of the 6S NN emulator against observed irradiances. The mean ( $\mu$ ) and the standard deviation ( $\sigma$ ) of the error per band are also presented (d).



**Fig. 3.** Time series of observed Normalized Difference Vegetation Index (*NDVI*<sub>obs</sub>) averaged per campaign and treatment (a). Time series of retrieved key parameters  $C_{ab}$  (b), *LAI* (c),  $V_{cmax}$  (d), *m* (e) and  $C_s$  (f) for the inversion scheme I<sub>GPP</sub>. Parameters are presented per campaign and treatment: control (C), Nitrogen (N), Nitrogen plus phosphorous (NP) and phosphorous (P). Red lines separate campaigns corresponding to different years. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



**Fig. 4.** Distributions of the most relevant retrieved parameters grouped per treatment: control (C), N (N), N plus P (NP), and P (P). Results for  $I_{GPP}$ ,  $I_{SIF}$ ,  $I_{GPP-SIF}$  and  $I_R$  are respectively presented in each column from right to left.  $C_{ab}$  (a–d), *LAI* (e–h),  $V_{cmax}$  (i–l), *m* (m–p). Grey boxes represent  $V_{cmax,S1}$  (values constrained in Step#1) (i–l) or fixed *m* values in Step#1 (m–p). Tukey's honest significant difference groups are presented in each subplot.

The four inversion schemes show a good agreement between  $C_{\rm ab}$ and Cs with NDVIobs seasonality; whereas LAI seasonal variations are less pronounced. For I<sub>GPP</sub> (Fig. 3) and I<sub>GPP-SIF</sub> (Fig. D.2), C<sub>ab</sub> (b), LAI (c) and  $V_{\rm cmax}$  (d) increase during the growing season, peaking around April, and decrease during the dry period (May – July, depending on the year); whereas *m* values (e) are low for  $NDVI_{obs} < 0.31$ . As expected,  $C_{\rm s}$  (f) increases in the dry period. I<sub>SIF</sub> (Fig. D.1) and I<sub>R</sub> (Fig. D.3) show lower  $C_{ab}$  and  $C_s$  values than the other schemes, especially during the dry season. However, ISIF presents large intra-campaign variability for  $V_{\rm cmax}$  and *m*, which decouples these variables from phenology (Fig. D.1d-e). On the contrary, these variables show very little intra-campaign variability for I<sub>R</sub> (Fig. D.3d-e). In fact these estimates equal the starting points used for the inversions; which suggest that  $V_{cmax}$  and mhad little effect on the constraints used by this scheme.  $C_{\rm w}$  and  $C_{\rm dm}$  (not shown) are highly unconstrained in all the schemes since no information was used either in the Short Wave Infrared region or the Near Infrared (NIR) water absorption bands. Cw and Cdm show weak but

significant negative relationships with  $NDVI_{obs}$ ; which in the case of  $C_{dm}$  is agreement with previous observations in the site (Melendo-Vega et al., 2018; Vilar et al., 2016).

Fertilization with N and P increased foliar content of these elements where applied; and increases of  $C_{ab}$  and  $V_{cmax}$  related to foliar nitrogen were not only expected, but coherent with ancillary observations (e.g., *GPP*) and modeling exercises in previous works at this site (Migliavacca et al., 2017; Perez-Priego et al., 2015a). Fig. 4 presents the distributions per treatment of the most relevant parameters retrieved by each inversion scheme; informing therefore of the capability of each inversion scheme to reproduce expected vegetation responses to treatments. For all the inversion schemes, the highest  $C_{ab}$  estimates (Fig. 4a–d) are found in the N and NP treatments. I<sub>GPP</sub> and I<sub>GPP-SIF</sub> present higher values than I<sub>SIF</sub> and I<sub>R</sub>; however, two-way Tukey's HDS test only finds group differences for I<sub>SIF</sub> and I<sub>R</sub>. *LAI* estimates (Fig. 4e–f), show no strong differences between treatments nor inversion schemes. Both *LAI* observations and estimates do not show significantly different

#### Table 2

*p*-Values of the two-way analysis of variance (ANOVA) test corresponding to the effects treatments, campaigns and their interaction on the estimates of four parameters (chlorophyll, leaf area index, maximum carboxylation rate and Ball-Berry stomatal sensitivity). Results are presented for each of the inversion schemes. Symbol  $\cdot$  stands for 0.05  $\leq p < 0.10$ ; and symbol  $\cdot$  means p < 0.05.

	Treatment			Campaigr	Campaign				Interaction			
	C <sub>ab</sub>	LAI	V <sub>cmax</sub>	m	$C_{\rm ab}$	LAI	V <sub>cmax</sub>	m	$C_{\mathrm{ab}}$	LAI	V <sub>cmax</sub>	m
I <sub>GPP</sub> I <sub>SIF</sub> I <sub>GPP-SIF</sub> I <sub>R</sub>	0.08 <sup>*</sup> 0.04* 0.00* 0.00*	0.71 0.90 0.05' 0.00*	0.04* 0.00* 0.21 0.00*	0.56 0.55 0.83 0.38	0.00* 0.00* 0.00* 0.00*	0.00* 0.00* 0.00* 0.00*	0.00* 0.00* 0.00* 0.00*	0.00* 0.00* 0.00* 0.30	0.55 0.48 0.11 0.11	0.8 0.01* 0.92 0.45	0.55 0.22 0.15 0.02*	0.07 <sup>*</sup> 0.73 0.19 0.25

treatment groups; the strong treatment effects observed in exclusion cages (not shown) are likely minimized due to selective grazing of the cattle on the fertilized plots.  $V_{\rm cmax}$  estimates (Fig. 4i–l) quite vary between inversion schemes. I<sub>GPP</sub> and I<sub>GPP-SIF</sub> show the highest values for N

and NP. In  $I_{GPP-SIF}$  N and NP are grouped together; whereas in  $I_{GPP}$  only NP was placed in a different group. Contrarily,  $I_{SIF}$  shows the highest  $V_{cmax}$  in the C and P treatments, with no differences between groups. In the case of  $I_R$ , solutions stay almost at the starting points of the



**Fig. 5.** Evaluation of the inversion schemes  $I_{GPP}$ ,  $I_{SIF}$ ,  $I_{GPP-SIF}$  and  $I_R$  (columns from left to right, respectively). Predicted and observed variables used in the cost function during the inversion: *NDVI* (a–d), *GPP* (e–h),  $F_{fo0}^{+}$  (i–l), and  $L_{T,out,BB}$  (m–p). Predicted and observed variables not involved in the model constraint:  $F_{687}^{+}$  – in red - (i–l), *LAI* (q–t), and evaporative fraction (*EF*) summarizing the partition of water fluxes (u–y). *EF* is compared only for control plots against the fluxes of the nearby unfertilized subcanopy EC tower. Total Least Squares (Golub and Loan, 1980) was used to compute  $R^2$ , *RMSE*, offset and slope (orange line). The 1:1 line is also shown for comparison (black). Notice that spectral observation –and therefore retrieved parameters- are available only at noon, whereas several diel flux measurements were acquired per plot and campaign. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article.)



**Fig. 6.**  $N_{\text{mass,green}}$  vs.  $V_{\text{cmax}}$  retrieved in the second step of the inversion; results are compared with Feng and Dietze (2013) data and the same logarithmic function is fitted for both datasets for I<sub>GPP</sub> (a), I<sub>SIF</sub> (c), I<sub>GPP-SIF</sub> (e) and I<sub>R</sub> (g).  $N_{\text{mass,green}}$  vs. estimated  $C_{ab}$  for I<sub>GPP</sub> (b), I<sub>SIF</sub> (d), I<sub>GPP-SIF</sub> (f) and I<sub>R</sub> (h).. Vertical lines represent the 25%–75% confidence intervals of the estimated parameters. 95% confidence intervals for the fitted models are represented by dashed lines. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

inversion; which were set according to the relationship  $V_{\rm cmax}$ - $N_{\rm mass}$ used in Migliavacca et al. (2017); for this reason the highest values are found in N and NP treatments; which are grouped together. I<sub>R</sub> V<sub>cmax</sub> values are lower than those estimated by  $I_{GPP}$  and  $I_{GPP-SIF}$ . Fig. 4i–l show also  $V_{\text{cmax},S1}$  in grey boxes. Compared to Step#1, Step#2  $V_{\text{cmax}}$  values are 10.3% and 9.7.0% lower for  $I_{\text{GPP}}$  and  $I_{\text{GPP-SIF}}$ , respectively; and 1.9% higher in the case of  $I_{SIF}$ . As  $V_{cmax}$ , *m* estimates (Fig. 4m–p) also differ for each inversion scheme. IGPP and IGPP-SIF show higher values for N and for N and P than for the other treatments, respectively; whereas m estimates present lower values in NP, suggesting higher water use efficiency. Nonetheless, no different groups are found by the statistical analysis.  $I_{SIF}$  obtains the lowest *m* values, most often below the value used in Step#1 (m = 10), and sometimes close to 0. As occurred with  $V_{\rm cmax}$ , I<sub>R</sub> values do not move from the inversion starting point. Fig. 4m-p present the fix *m* value prescribed in Step#1 in grey; Step#2*m* in  $I_{GPP}$  and  $I_{GPP-SIF}$  is 13.0% and 11.6% larger than Step#1*m*, respectively; whereas m is 72.9% lower for  $I_{SIF}$ .

Table 2 shows the *p*-value of the treatment, campaign and interaction effects provided by the two-way ANOVA test. All the variable estimates present significant campaign effect but *m* in  $I_R$ , since it features

the same value. For all the inversion schemes,  $C_{\rm ab}$  estimates show significant treatment (p < 0.05 for al schemes but  $I_{\rm GPP}$  where p < 0.10), but no interaction effects. Significant treatment effects on *LAI* are observed for  $I_{\rm GPP-SIF}$  (p < 0.10) and  $I_{\rm R}$  (p < 0.05), and interaction effects for  $I_{\rm SIF}$  (p < 0.05).  $V_{\rm cmax}$  presents treatment effects for all the inversion schemes (p < 0.05) but for  $I_{\rm GPP-SIF}$ ; whereas for  $I_{\rm SIF}$  (p < 0.05) but for  $I_{\rm GPP-SIF}$ ; whereas for  $I_{\rm SIF}$   $V_{\rm cmax}$  shows interaction effects (p < 0.05). No treatment effects are found for *m*, but in  $I_{\rm GPP}$  *m* shows some interaction (p < 0.10).

## 3.3. Model inversion evaluation

Fig. 5a–p shows predicted and observed values of variables used in the cost functions of the SCOPE inversion (Eqs. (4)–(5)): Normalized Difference Vegetation Index (*NDVI*), *GPP*,  $F_{760}^{\dagger}$ , and  $L_{T,out,BB}$ . *NDVI* summarizes the fit of *HCRF* in Step#1. Additional statistics can be found in Table E.1 (Appendix E). For the inversion schemes I<sub>GPP</sub>, I<sub>SIF</sub>, I<sub>GPP-SIF</sub> and I<sub>R</sub>, *HCRF* in the spectral range 400–930 nm show *RMSE* = 0.029, 0.014, 0.028 and 0.014, respectively; and analogously *ME* = 0.004, 0.003, 0.003 and 0.003. However, the fit in absolute terms is better in the Visible (*RMSE* = 0.010, 0.004, 0.010, 0.004), which is underestimated (ME = -0.004, -0.000, -0.004, -0.000); than in the NIR region (RMSE = 0.043, 0.020, 0.041, 0.021), which results overestimated (ME = 0.015, 0.007, 0.013, 0.0078). I<sub>SIF</sub> and I<sub>R</sub> fit *NDVI* (Fig. 5a–d) and *HCRF* better than I<sub>GPP</sub> and I<sub>GPP-SIF</sub>; however these schemes largely underestimate *GPP* (Fig. 5.f,h), especially I<sub>SIF</sub>. On the contrary, I<sub>GPP</sub> and I<sub>GPP-SIF</sub> accurately fit *GPP* (Fig.5e,g).  $F_{760}^{+}$  (Fig.5gi–l) is well fitted in I<sub>SIF</sub> and I<sub>GPP-SIF</sub>; whereas it is overestimated by I<sub>GPP</sub>, (slope equal to 0.77) and precisely buy not so accurately predicted by I<sub>R</sub> (slope equal to 0.90).  $L_{T,out,BB}$  is similarly fitted by all the schemes (Fig. 5m–p); in all the cases the highest values are underestimated, and I<sub>SIF</sub>  $R^2$  is lower than for the other schemes.

Fig. 5 also shows the observed and predicted values of three variables not used in the cost function: *LAI*, *EF*, and  $F_{687}^{\dagger}$ . *LAI* (Fig. 5q–t) is acceptably estimated by I<sub>GPP</sub> and I<sub>GPP-SIF</sub> ( $R^2 = 0.41$ , 0.47; *RMSE* = 1.25, 1.19 m<sup>2</sup>/m<sup>2</sup>, respectively), although it results underestimated ( $ME = -0.49 \text{ m}^2/\text{m}^2$  in both cases). On the contrary I<sub>SIF</sub> and I<sub>R</sub> poorly predict *LAI* ( $R^2 = 0.01$  and 0.01, *RMSE* = 1.65 and 1.64 m<sup>2</sup>/m<sup>2</sup>; ME = -0.56 and  $-0.61 \text{ m}^2/\text{m}^2$ ).  $F_{687}^{\dagger}$  is underestimated by all the inversion schemes (Fig. 5i–l, in red), but with significant relationships (p < 0.05) of slopes equal to 5.4, 5.1, 5.3 and 4.4, respectively.

Fig. 5u–y present predicted and observed *EF*; I<sub>GPP</sub> and I<sub>GPP-SIF</sub> predict less biased *EF* than I<sub>SIF</sub> and I<sub>R</sub>, and consequently simulate energy partition more accurately. Also, I<sub>GPP</sub> and I<sub>GPP-SIF</sub> show closer agreement with observed fluxes than I<sub>SIF</sub> and I<sub>R</sub>. I<sub>GPP</sub>, I<sub>SIF</sub>, I<sub>GPP-SIF</sub> and I<sub>R</sub> predict  $\lambda E$  with *RMSE* = 86.8, 46.9, 85.7 and 56.8 W/m<sup>2</sup>, and  $R^2$  = 0.72, 0.74, 0.77 and 0.77, respectively. Similarly, *H* is predicted with *RMSE* = 83.9, 121.9, 88.3 and 105.1 W/m<sup>2</sup>, and  $R^2$  = 0.81, 0.62, 0.79 and 0.73, respectively. *RMSE* for *G* is close to 37 W/m<sup>2</sup> for all the schemes.

Fig. 6 presents the evaluation of  $C_{ab}$  and the functional traits ( $V_{cmax}$ , *m*) estimates with direct measurements of plant traits at canopy scale. The 25th and 75th percentiles of the predicted posterior uncertainties are also presented. Fig. 6a,d,g,j relate  $V_{\rm cmax}$  with  $N_{\rm mass,green}$  for  $I_{\rm GPP}$ ,  $I_{\rm SIF}$ , I<sub>GPP-SIF</sub> and I<sub>R</sub>, respectively; and compare these relationships against the one reported in the meta-analysis conducted by Feng and Dietze (2013) for grasses. For both datasets a logarithmic model is adjusted and the 95% confidence intervals of the fitted curves are presented. For IGPP, and  $I_{GPP-SIF}$ , the  $N_{mass,green}$ - $V_{cmax}$  relationship estimated after SCOPE inversion is consistent with that reported by Feng and Dietze (2013), but our estimates show lower V<sub>cmax</sub> for large N<sub>mass,green</sub> values. Contrarily,  $I_{SIF}$   $V_{cmax}$  shows non-positive relationship with  $N_{mass,green}$ ; whereas I<sub>R</sub> V<sub>cmax</sub> values are below the Feng and Dietze (2013) relationship, and are more uncertain than the estimates of other schemes. Fig. 6b,e,h,k compare  $C_{ab}$  with  $N_{mass,green}$ , all the inversion schemes present a saturating relationship.  $I_{GPP}$  and  $I_{GPP-SIF}$  show some high  $C_{ab}$ values for  $N_{\rm mass,green}$  < 2.0% during the dry period. On the contrary, I<sub>SIF</sub> and I<sub>R</sub> C<sub>ab</sub> estimates for this period are lower, and their relationships with  $N_{\text{mass,green}}$  are neater. Despite the differences in the dry period, the  $C_{\rm ab}$ - $N_{\rm mass,green}$  models of all the schemes are relatively similar, and these are even closer if values in the dry period are removed (not shown). Additionally, m is compared with values reported in the literature. For example the review of Miner et al., (2016) reports mean *m* values equal  $13.5 \pm 3.1$  (1 standard deviation) for a reduced dataset of C3 grasses (n = 5); and 10.4  $\pm -5$  for herbaceous annual species (n = 8). For IGPP, ISIF, IGPP-SIF and IR, the mean and 95% confidence intervals are respectively 11.3, [0.0, 32.9]; 5.3, [0.0, 40.0]; and 11.2, [0.4, 33.5]; and 10.0, [10.0, 10.0]. Estimated values are close to reported averages for I<sub>GPP</sub> and I<sub>GPP-SIE</sub>; whereas these are lower for I<sub>SIE</sub>, and I<sub>R</sub> shows the

starting values of the inversion. Distributions found in  $I_{GPP}$  and  $I_{GPP-SIF}$  are wider than in the literature; but also are the seasonality covered by our dataset and the number of species.

#### 4. Discussion

This work raised from the most recent efforts of the RS community to characterize the spatiotemporal variability of key plant functional traits by exploiting the increasingly rich RS data in coupled RTM and SVAT models (Bayat et al., 2018; Celesti et al., 2018; Dutta et al., 2019; Hu et al., 2018: van der Tol et al., 2016). Here, we have further developed a methodology to invert the SCOPE model with a multipleconstraint approach and assessed the importance of the different constraints (GPP and SIF, together with TIR and RF) in the retrieval. Our results suggest 1) that the inversion method proposed can provide robust estimates of biophysical and functional traits of vegetation (this means, coherent with seasonality, fertilization, observed biophysical parameters, fluxes, EF and N<sub>mass</sub>; as discussed in the following subsections), and is applicable on research sites monitored with eddy covariance systems and hyperspectral remote sensing data, and 2) that GPP is a better constraint of functional traits than monochromatic SIF. The additional contribution of this article to previous works can be summarized in four points: 1) the inversion method, 2) the comparison of GPP and SIF as constraints, 3) the use of pattern-oriented model evaluation and 4) the analysis the sources uncertainty.

#### 4.1. Inversion method

We separated the inversion of SCOPE model in two different steps; but unlike in former works (Bayat et al., 2018; Hu et al., 2018), we included constraints sensitive to plant functioning in all of them. Split model inversions have been already used in the literature in two ways: constraining different parameters in each step (Bavat et al., 2018; Hu et al., 2018; Migliavacca et al., 2009; Wutzler and Carvalhais, 2014), or tuning the same parameters in different steps (Peylin et al., 2016); here we combined both approaches. In Step#1, we jointly used midday biophysical (e.g., RF) and functional (e.g., GPP) constraints to optimize biochemical and structural traits together with  $V_{\rm cmax}$ . Since assimilation and transpiration are related,  $V_{\rm cmax}$  estimates depend on m, and therefore a second step was used to retrieve these two parameters constraining the model with diel functional constraints (e.g., GPP and TIR data). Simultaneous retrieval of all parameters led to equifinal results (not shown). Our results suggest that  $V_{\rm cmax}$  can be estimated in Step#1 and not strongly modified in Step#2 if an adequate guess on mis used in Step#1 (e.g. typified PFT values in LSM).  $V_{\rm cmax,S1}$  was biased respect to estimates in Step#2, but sensitivity to treatments and seasonality remained. With the adequate constraints, the method provided biophysical and functional parameters that are coherent with seasonality (e.g., Fig. 3) and fertilization. The analysis of fertilization effects is complex, and treatment differences shown in Fig. 4 and Table 2 are in part occluded by the fact that they are minimized when grass senesces. Statistical analyses carried out only on growing season data (not shown) revealed significant treatment effects on  $C_{ab}$ , LAI and  $V_{cmax}$ estimates, but not on m. The combination of biophysical and functional constraints in Step#1 improved the estimation of some biophysical parameters, such as LAI. Nonetheless, the use of diel information was still necessary to adequately estimate the functional traits (e.g.,  $V_{cmax}$ ) m). Additional tests using only midday data in Step#2 (not shown) provided  $V_{\rm cmax}$  values between Step#1 and Step#2 estimates, but in the overall, not as robust as those obtained using diel observations. This might be due to saturation in some of the physiological processes related to carbon fixation and stomatal closure during midday depression (Collatz et al., 1991; Frankenberg and Berry, 2018; Roessler and Monson, 1985; van der Tol et al., 2014). Saturation could make model outputs little sensitive to variation in some of the functional parameters, leading to equifinality and ill-posed solutions. Diel information is richer than midday observations since it comprehends vegetation function under different light saturation and water stress conditions; and therefore more robustly constrains functional traits.

In this work we proposed inverting SCOPE by means of numerical optimization (as in van der Tol et al. (2016)); which is time demanding when the full model is run. Former works used LUTs to speed up SCOPE inversion (Bayat et al., 2018; Hu et al., 2018); whereas the use of emulators has been limited so far to the inversion of the optical RTM (Verrelst et al., 2017). The emulation of different modules of SCOPE could facilitate the inversion of the model with imagery and large datasets.

## 4.2. Evaluation of the potential of GPP and SIF as functional constraints

Previous works have used combinations of constraints similar to the ones used in this work (RF, GPP, SIF and/or TIR radiance); but they used methodologies different to the one proposed here, and focused on the retrieval of vegetation parameters. Only Dutta et al., (2019) evaluated the effect of adding RF to the constraint imposed by carbon and water fluxes, concluding that RF improved their results. Our study compares for the first time the potential of GPP and SIF, in combination with optical hyperspectral and TIR data, to estimate functional parameters of vegetation. An inversion excluding GPP and SIF was used as a baseline for the evaluation of results.  $I_{GPP}$  and  $I_{GPP-SIF}$  presented the best estimates of functional traits such  $V_{cmax}$  and m; as well as some key biophysical traits, except some cases in the dry season. ISIF and IR weakly and very weakly constrained the functional traits; and failed to estimate LAI. We acknowledge that the comparison GPP vs. SIF was not totally balanced since we used diel GPP to invert SCOPE, whereas a single SIF value was available for the inversion. However,  $V_{cmax}$  estimates in Step#1 -where single values of GPP and/or SIF were used-, and tests performed using only midday data in Step#2 (not shown) were consistent with results of Step#2 (Fig. 4i-l); which suggests that GPP is a stronger constrain of functional parameters (e.g.,  $V_{cmax}$ ) than SIF.

The control of SIF on functional traits such as  $V_{\text{cmax}}$  and *m* has not been evaluated in former works inverting SCOPE against SIF (Celesti et al., 2018; Hu et al., 2018; van der Tol et al., 2016), since those focused on the estimation of parameters directly controlling SIF emission (e.g.  $f_{qe}$ ). Recent works have assimilated SIF in order to estimate  $V_{cmax}$ exclusively, obtaining better results than in this manuscript (Camino et al., 2019; Zhang et al., 2014b). In these works  $V_{\rm cmax}$  was constrained with SIF after the remaining biophysical parameters had been estimated, at the same time that no additional functional parameters such as  $f_{qe}$  or *m* were simultaneously involved in the cost function. We hypothesize that this method forced a univoque relationship between  $V_{\rm cmax}$  and SIF, allowing a successful retrieval of  $V_{\rm cmax}$  as long as the guess on the prescribed functional parameters ( $f_{qe}$  or m), was realistic. Our results show that midday  $F_{760}^{\dagger}$  weakly constrains  $V_{cmax}$ , and that solutions become ill-posed when additional functional parameters are simultaneously estimated. Also, it must be considered that SIF in Zhang et al. (2014b) features bi-weekly temporal resolution, so that the

information provided by these data might differ from the one contained by near-simultaneous datasets, as those presented in this manuscript. The weak constrain of  $F_{760}^{\uparrow}$  on  $V_{\rm cmax}$  and *m* that we found may be explained by the fact that  $V_{\rm cmax}$  is related to the dark reactions of photosynthesis whereas SIF is more closely related to the light reactions. Also, the link  $V_{\text{cmax}}$ -SIF is weak:  $V_{\text{cmax}}$  imposes a ceiling for photochemistry, but changes in fluorescence rate in response to saturating light are affected by the activation of alternative dissipation pathways such as non-photochemical quenching (Frankenberg and Berry, 2018; van der Tol et al., 2014), which can be enhanced at noon. In addition, the formal link between  $F_{760}^{\dagger}$  and *GPP* in the model is based on empirical relationships extrapolated from limited datasets; which might not be representative of the grassland under study. Another complementary hypothesis could be that the retrieval of  $f_{qe}$  against a single  $F_{760}^{\uparrow}$  observation is too loose and that multi-spectral or multi-temporal SIF data are needed to properly constraint this parameter. None of the inversion schemes accurately predicted  $F_{687}^{\uparrow}$ ; which could be in part explained by uncertainties in the retrieval of  $F_{687}^{\uparrow}$  related to i) assumptions on the shape of fluorescence emission (Cogliati et al., 2015), and ii) low signal-to-noise ration of the spectrometer used in this study (Julitta et al., 2016). Also, it could be possible that the fixed ratio between the  $f_{qe}$  of both photosystems was unrealistic. Hu et al. (2018) solved this problem constraining  $f_{\rm qe}$  parameters of each photosystem inverting SCOPE against diel cycles of  $F_{760}^{\uparrow}$  and  $F_{687}^{\uparrow}$ . In our case, the lack of reliable  $F_{687}^{\uparrow}$  data in all the campaigns prevented us from fully exploiting multi-spectral SIF.

I<sub>R</sub> relied on constraints similar to those used by Bayat et al. (2018); however, this scheme did not succeed to retrieve the functional traits. This could be explained by the reduced influence of these parameter on the outputs evaluated in Step#2 ( $L_{T,out,BB}$ ).  $V_{cmax}$  had no strong effect on RF in Step#1, and the response of TIR radiance to  $V_{cmax}$  and m in Step#2 was below the termination tolerance on the cost function in the first run of the inversion. Consequently I<sub>R</sub> functional traits remained at the initial values of Step#2. Bayat et al. (2018) relied on a LUT-based approach, and therefore wide ranges of parameter values were evaluated at once leading to different solutions. This suggests that global search methods might be more suitable than local optimization when only RF and TIR data are used to estimate  $V_{cmax}$  and m.

Our works suggests that the joint use of constraints on i) optical properties, ii) photosynthesis and iii) transpiration/evaporation, at least, allows obtaining reliable estimates of biophysical and functional traits. Such approach cannot rely exclusively on RS imagery, but could be applied at the growing EC network jointly with spectral and thermal data. This method would provide valuable information about the intra and inter PFT spatial and temporal dynamics of the functional traits at chamber/proximal sensing and EC site/RS scales. Such estimates could be further used for evaluation, cross-validation or modeling of LSM using different approaches.

#### 4.3. Pattern-oriented model evaluation of functional parameter estimates

In this work, we overcame the absence of direct measurements of the targeted functional traits using a pattern-oriented model evaluation strategy. This allowed us evaluating the suitability of the method developed as well as the potential of different sets of constraints to estimate plant functional traits. I<sub>GPP</sub> and I<sub>GPP-SIF</sub>  $V_{\rm cmax}$  positively related to  $N_{\rm mass,green}$ , following a curve close to relationships reported for grasses (Feng and Dietze, 2013); whereas I<sub>SIF</sub> estimates were unrelated to  $N_{\rm mass,green}$ . We also evaluated the consistency of  $C_{\rm ab}$  with  $N_{\rm mass,green}$ ; in

this case, all the inversion schemes provided expected positive saturating relationships.  $I_{GPP}$  and  $I_{GPP-SIF}$  presented too high  $C_{ab}$  values considering  $N_{mass,green}$  - during the dry period; suggesting that when *GPP* constrained the model,  $C_{ab}$  could result overestimated. This and other issues are discussed section 4.4.

An additional pattern that we analyzed to evaluate the consistency of the retrieved parameters is EF. This analysis revealed that IGPP and IGPP-SIF provided the most accurate and precise EF predictions; which suggests that the corresponding m estimates mimicked vegetation function most closely. Alternatively, m estimates could be evaluated using <sup>13</sup>C isotope discrimination, under certain assumptions (Medlyn et al., 2017).  $\lambda E$  and H were overestimated by all the inversion schemes (Table E.1): this could be in part explained by the differences in the radiative regime of the open experimental area and the EC<sub>sub</sub> footprint, more often shaded by tree crowns (e.g., up to a 60% of this footprint was shaded during the campaigns); however, EF seems to be robust to these differences. Patter-oriented model evaluation also showed that SIF in  $I_{GPP-SIF}$  slightly improved the estimation *EF* (and likely *m*) compared to I<sub>GPP</sub>. This seems in agreement with recent works exploring the relationships between SIF and transpiration (Alemohammad et al., 2017; Lu et al., 2018). On the other hand, the weak constrain if  $I_R$  and ISIF, led to noisier and more biased EF predictions, in part related with GPP underestimation (Fig. 5f,h). The evaluation of EF and the comparison with literature values suggests that  $I_{\mbox{\scriptsize SIF}}$  estimates were not realistic. These results open an interesting perspective to the use of combined flux observation and remote sensing products of RF (and SIF) for the parameterization as well as the evaluation of the stomatal slope m, a crucial parameters in LSM (e.g. Rogers et al. (2016)).

## 4.4. Sources of uncertainty

Different inversion schemes showed high uncertainty in the estimation of biophysical parameters traditionally retrieved from RTM inversion (e.g., LAI,  $C_{ab}$ ). This seems to be related with the inaccurate representation of the optical properties of the dry standing biomass, abundant in the grassland under study in certain periods of the year. Vilar et al. (2016) suggested that senescent material may hamper the estimation of key variables such as LAI using empirical parametric and non-parametric methods in the same study site. Melendo-Vega et al., (2018) related overestimation of NIR RF with the presence senescent material using PROSAIL and measured model parameters in the site. We hypothesize that this overestimation could have produced the underestimation of LAI in our study, since reduced LAI values would allow fitting low NIR RF during inversion. The use of GPP in Step#1 improved the estimation of LAI, which was likely due to the demand of suitable APAR levels for fitting GPP. In fact in Step #1, IGPP and IGPP-SIF predicted APAR values a 29.37% and 23.28% higher than  $I_R$  and  $I_{SIF}$ , respectively. These results might open the possibility of using precise estimates or observations of APAR to constrain biophysical and functional parameters; however, the potential of APAR to replace GPP needs to be explored in the future. On the other hand,  $I_{\mbox{\scriptsize GPP}}$  and  $I_{\mbox{\scriptsize GPP-SIF}}$  also provided high Cab values, especially in the dry season where the senescent LAI fraction peaks. We hypothesize that in this case, light saturation at midday allowed increasing Cab (and APAR) but not GPP, while improving the fitting of RF in the Visible bands. This likely compensated changes in other model parameters such as LAI. No strong differences were found in the parameters controlling LAD; however,  $I_{GPP}$  and  $I_{GPP-SIF}$  predicted canopies slightly less electrophile than the

other inversion schemes. These results suggest that exploiting biophysical and functional constraints simultaneously, as proposed here, can provide solutions more robust to observation uncertainties and model error. Nonetheless, this approach did not fully solve model representation problems. In addition, we must consider that SCOPE simulates homogeneous canopies where all the leaves present the same effective properties; whereas in reality, green and senescent leaves feature very different properties and processes. The effect of these discrepancies on the estimated parameters remains unknown. Further work is needed to improve representation of canopies mixing photosynthetic and senescent materials, ensuring robust estimates of plant biophysical and functional traits in ecosystems with large senescent fractions.

Additional sources of uncertainty can be related with the parametrization done before inversion. The large uncertainties in the fit of  $SM_{\rm p}$ - $r_{\rm ss}$  model might have had a strong effect on the predicted fluxes and therefore on the inversion. In order to understand the potential impact of these uncertainties, we propagated  $SM_{\rm p}$  uncertainties to predicted *GPP*,  $L_{\rm T,out,BB}$  and  $F_{760}^{\downarrow}$  (Appendix F). Small variations in  $SM_{\rm p}$ translated into large variability of  $r_{\rm ss}$  in dry conditions but also produced relatively small changes in the predicted fluxes, thus a low impact on the inversion is expected. Also, in the inversion of 6S some moderate uncertainties were found, especially within deep absorption features; however, these estimates were only used to describe the fractions of direct and diffuse  $E_{\rm tot}^{\downarrow}$ . These estimates are expected to be more accurate than the fractions computed by default by SCOPE, according to some standard atmospheric transfer functions; therefore the impact of inversion uncertainties should be small.

## 5. Conclusions

The multiple-constraint inversion of coupled RTM and SVAT models, such as SCOPE, requires information on i) biophysical properties, ii) photosynthesis, and iii) transpiration/evaporation in order to provide reliable estimates of biophysical and functional traits of vegetation (e.g.  $V_{cmax}$ , m,  $C_{ab}$  and LAI). Whereas hyperspectral RF and diel TIR information can be used as constraints of i) and iii); GPP is a stronger constraint of ii) than monochromatic SIF, indicating that the use of SIF alone might not be enough to retrieve  $V_{cmax}$ . The simultaneous combination constraints on vegetation biochemistry and structure (e.g., RF) and function (e.g., GPP) provides more robust estimates of biochemical and functional parameters than the separated retrieval of each type of trait. We propose a method that can be exploited at EC sites to improve the characterization of the spatio-temporal variability of key functional traits by combining ground GPP and TIR time series with hyperspectral RS. This information is nowadays needed to improve the parameterization of LSM predicting Carbon cycle at global scale. In this context, we also proved the potential of pattern-oriented model evaluation approach to assess the suitability of models, inversion methods and constraints.

Further work is needed test the proposed method at eddy covariance sites and with satellite information, and to develop methods that successfully exploit SIF to constrain parameters related with photosynthetic activity. This is critical for the exploitation of the RF, SIF and TIR datasets provided by the up-coming FLuorescence EXplorer (FLEX), in tandem with Sentinel-3 (Drusch et al., 2017). Also, new models should be adapted to better represent processes in ecosystems featuring senescent material, such as the widely distributed semi-arid grasslands.

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## Appendix A. Computation of soil resistance for evaporation from the pore space

Soil resistance for evaporation from the pore space (r<sub>ss</sub>) was computed according to Mahfouf and Noilhan (1991) as described in Eq. (A.1)

$$r_{ss} = \frac{\rho C_p}{\gamma} \frac{e_{sat} - e_a}{\lambda E_{soil}} - r_{bs}$$
(A.1)

where  $r_{\rm bs}$  is the soil boundary layer resistance (s/m),  $\rho$  is air density (kg m<sup>-3</sup>),  $C_{\rm p}$  is the specific heat capacity (J kg<sup>-1</sup> K<sup>-1</sup>),  $\gamma$  is the psychrometric constant (kPa k<sup>-1</sup>),  $e_{\rm sat}$  and  $e_{\rm a}$  are the saturated and ambient water vapor pressure (kPa) of soil air pore spaces, respectively, and  $\lambda E_{\rm soil}$  (W m<sup>-2</sup>) is the latent heat flux measured by the lysimeters.  $e_{\rm sat}$  was calculated as a function of soil temperature, whereas  $e_{\rm a}$  was computed according to thermodynamic principles as a function of Eq. A.2, the relative humidity of the soil pores ( $\varphi$ ).

$$\varphi = e_a \left(\frac{g \,\psi}{R_{\rm tor} \, T_{\rm s}}\right) \tag{A.2}$$

where g is the gravitational acceleration (9.81 m s<sup>-2</sup>),  $\psi$  is the matric soil potential (water column, m),  $R_w$  is the water vapor gas constant (461.5 J kg<sup>-1</sup> k<sup>-1</sup>) and  $T_s$  is soil temperature expressed in K.  $\Psi$  was measured using tensiometers (Full Range Tensiometer, Umwelt-Geräte-Technik GmbH, Müncheberg, Germany).

#### Appendix B. Example of the inversion of 6S and SCOPE models on spectral variables



**Fig. B.1.** Example of the VNIR observed down-welling and up-welling radiances together with the predicted global, direct and diffuse down-welling radiances from the inversion of the 6S model. Irradiances are transformed to radiances (L) as  $E / \pi$ . Notice that here predicted 6S radiances present a lower spectral resolution than the measurements (a). Observed and predicted reflectance factors corresponding to the left panel of this figure as well as the predicted diffuse-to-global radiation ratio (b).



## Appendix D. Most relevant SCOPE parameter estimates



**Fig. D.1.** Time series of observed Normalized Difference Vegetation Index ( $NDVI_{obs}$ ) averaged per campaign and treatment (a). Time series of retrieved key parameters  $C_{ab}$  (b), LAI (c),  $V_{cmax}$  (d), m (e) and  $C_s$  (f) for the inversion scheme  $I_{SIF}$ . Parameters are presented per campaign and treatment: control (C), Nitrogen (N), Nitrogen plus Phosphorous (NP) and Phosphorous (P). Red lines separate campaigns corresponding to different years.



**Fig. D.2.** Time series of observed Normalized Difference Vegetation Index ( $NDVI_{obs}$ ) averaged per campaign and treatment (a). Time series of retrieved key parameters  $C_{ab}$  (b), LAI (c),  $V_{cmax}$  (d), m (e) and  $C_s$  (f) for the inversion scheme  $I_{GPP-SIF}$ . Parameters are presented per campaign and treatment: control (C), Nitrogen (N), Nitrogen plus Phosphorous (NP) and Phosphorous (P). Red lines separate campaigns corresponding to different years.



**Fig. D.3.** Time series of observed Normalized Difference Vegetation Index ( $NDVI_{obs}$ ) averaged per campaign and treatment (a). Time series of retrieved key parameters  $C_{ab}$  (b), LAI (c),  $V_{cmax}$  (d), m (e) and  $C_s$  (f) for the inversion scheme I<sub>R</sub>. Parameters are presented per campaign and treatment: control (C), Nitrogen (N), Nitrogen plus Phosphorous (NP) and Phosphorous (P). Red lines separate campaigns corresponding to different years.

## Appendix E. Comparison of different inversion schemes

Table E.1 summarizes the performance of different inversion schemes tested to retrieve biophysical and functional parameters of the SCOPE model. We compare the three inversion schemes described in this manuscript ( $I_{GPP}$ ,  $I_{SIF}$ ,  $I_{GPP-SIF}$  and  $I_R$ ). The table shows  $R^2$ , *RMSE*, *RRMSE*, *ME*, *MAE*, posterior uncertainties ( $U_{posterior}$ ), slope and offset obtained with each of the schemes comparing predicted and observed: *LAI*,  $C_{ab}$ , *HCRF*,  $L_{T,out,BB}$ ,  $F_{687}^{\dagger}$ ,  $F_{760}^{\dagger}$ , *GPP*,  $\lambda E$ , *H*, *G* and *EF* analogously to Fig. 5. Total Least Squares (Golub and Loan, 1980) is used in the comparisons. In addition, for *LAI*,  $C_{ab}$  and *m*, statistics for the models fit to the relationships  $N_{mass,green}$ - $V_{cmax}$ ,  $N_{mass,green}$  -  $C_{ab}$  and  $\Delta^{13}$ C-*m* are presented.

## Table E.1

Performance of the inversion of SCOPE using different inversion schemes.

	$\mathbb{R}^2$	RMSE	RRMSE	MAE	ME	Uposterior	Slope	Offset
LAI								
I <sub>GPP</sub>	0.41	1.25	44.31	0.93	-0.49	0.24	2.22	-2.34
I <sub>SIF</sub>	0.01	1.65	58.85	1.29	-0.56	0.22	27.32	-58.44
I <sub>GPP-SIF</sub>	0.47	1.19	42.44	0.89	-0.49	0.23	1.92	-1.66
I <sub>R</sub>	0.01	1.64	58.43	1.3	-0.61	0.17	22.87	- 47.58
C .								
LCDD	0.16	15.00	64.1	10.84	0.00	12.21	-	-
ISTE	0.31	9.00	54.14	7.20	0.00	7.21	-	-
I <sub>GPP-SIF</sub>	0.20	16.45	65.76	12.00	0.00	12.61	-	-
IR	0.34	8.40	51.39	6.82	0.00	0.73	-	-
17								
V <sub>cmax</sub>	0.25	30.85	43 71	24.03	0.00	1.67	_	_
IGPP	0.25	71.93	127.04	57.5	0.00	0.91	_	_
LCDD GIE	0.30	29.48	38.95	24.31	0.00	1 69	_	_
Ip	0.31	7.66	23.70	5.79	0.00	43.42	-	-
-ĸ								
m	0.10	4.07	10.1.6	0.07	0.00	4 5 1		
I <sub>GPP</sub>	0.12	4.37	42.16	3.3/	0.00	4.51	-	-
1 <sub>SIF</sub>	0.12	2.48	09.77	1.94	0.07	10.21	-	-
I <sub>GPP-SIF</sub>	0.13	3.76	37.58	2.75	0.00	4.08	-	-
IR	0.00	0.00	0.00	0.00	0.00	15.05	-	-
GPP								
$I_{GPP}$	0.90	2.11	21.92	1.55	0.04	1.23	0.98	0.12
I <sub>SIF</sub>	0.17	9.82	102.71	8.00	-7.78	2.50	2.73	4.69
I <sub>GPP-SIF</sub>	0.89	2.20	22.87	1.61	0.02	1.23	0.97	0.25
$I_R$	0.62	5.64	58.76	4.13	- 3.68	1.00	2.09	-2.75
R								
I <sub>GPP</sub>	0.95	0.03	18.68	0.02	0.00	0.03	0.93	0.01
I <sub>SIF</sub>	0.99	0.01	8.73	0.01	0.00	0.03	0.97	0.00
I <sub>GPP-SIF</sub>	0.96	0.03	17.7	0.02	0.00	0.03	0.93	0.01
I <sub>R</sub>	0.99	0.01	9.01	0.01	0.00	0.01	0.96	0.00
$L_{T,out,BB}$								
$I_{GPP}$	0.83	8.72	14.96	7.23	-7.17	3.98	1.57	-21.79
I <sub>SIF</sub>	0.75	7.82	13.43	5.92	-5.69	6.13	1.45	-18.05
I <sub>GPP-SIF</sub>	0.82	8.67	14.89	7.09	-7.03	4.32	1.59	-23.39
$I_R$	0.79	8.02	13.76	6.41	-6.2	1.96	1.46	-17.96
$\lambda E$								
IGPP	0.72	86.79	104.56	69.6	60.36	19.35	0.65	-10.86
I <sub>SIF</sub>	0.74	46.87	54.02	31.70	16.45	42.98	0.95	-10.85
I <sub>GPP-SIF</sub>	0.77	85.66	103.19	67.68	62.49	19.06	0.66	-13.21
I <sub>R</sub>	0.77	56.8	68.43	43.75	39.02	60.7	0.91	-28.31
Н								
ICER	0.81	83.94	94.43	67.73	67.16	22.57	0.69	-19.39
ISIF	0.62	121.89	146.94	103.36	103.03	38.97	0.62	- 32.34
I <sub>GPP-SIF</sub>	0.79	88.29	99.33	70.05	68.4	22.2	0.65	-14.08
IR	0.73	105.11	118.25	87.8	87.51	49.67	0.67	-29.47

(continued on next page)

#### Table E.1 (continued)

	$\mathbb{R}^2$	RMSE	RRMSE	MAE	ME	Uposterior	Slope	Offset
G								
U I	0.79	26.27	E4 20	20.21	10 76	6.95	1.02	20.06
1GPP	0.70	20.37	59.30	29.21	- 18.70	0.25	1.92	- 20.90
I <sub>SIF</sub>	0.69	38.81	59.79	30.21	- 20.48	8.11	2.07	- 22.12
I <sub>GPP-SIF</sub>	0.75	36.79	55.00	29.47	-18.88	6.39	1.90	- 19.54
I <sub>R</sub>	0.77	37.87	56.61	30.49	-21.02	4.22	1.95	-17.81
EF								
I <sub>GPP</sub>	0.56	0.17	36.4	0.13	-0.01	0.47	1.23	-0.10
I <sub>SIF</sub>	0.51	0.24	47.97	0.19	-0.16	0.29	1.77	-0.10
I <sub>GPP-SIF</sub>	0.67	0.15	30.94	0.12	0.00	0.48	1.20	-0.09
I <sub>R</sub>	0.59	0.18	37.48	0.14	-0.07	0.30	1.65	-0.20
$F_{760}^{\dagger}$								
I <sub>GPP</sub>	0.61	0.27	55.11	0.20	0.13	0.11	0.77	0.01
I <sub>SIF</sub>	1.00	0.02	3.67	0.00	0.00	0.15	1.02	-0.01
I <sub>GPP-SIF</sub>	1.00	0.02	4.36	0.01	0.00	0.39	1.02	-0.01
I <sub>R</sub>	0.71	0.19	38.53	0.15	0.01	0.01	0.90	0.04
$F_{687}^{\dagger}$								
I <sub>GPP</sub>	0.37	0.52	100.45	0.39	0.17	0.06	5.42	-1.76
I <sub>SIF</sub>	0.24	0.53	101.52	0.42	0.15	0.19	5.18	-1.51
I <sub>GPP-SIF</sub>	0.33	0.50	96.23	0.40	0.08	0.14	5.33	-1.24
I <sub>R</sub>	0.45	0.50	95.53	0.35	0.15	0.01	4.44	-1.27

## Appendix F. Analysis of error propagation in soil water content

Eq. (3) describes the model fitted to predict  $r_{ss}$  data as a function of  $SM_p$ . The overall RMSE = 21.03 s/m is mainly explained by the fit errors in the steepest part of the curve ( $SM_p < 10\%$ ) and the noisy nature of the  $r_{ss}$  observations (Fig. C.1). RMSE = 15.66 s/m for  $SM_p > 10\%$  and RMSE = 55.99 s/m for  $SM_p < 10\%$ . However in this region, the slope of the function ( $dr_{ss}/dSM_p$ , in m/s / 100·m<sup>3</sup>/m<sup>3</sup>) increases rapidly from -0.96 at  $SM_p = 10.0\%$  to -2.79 at  $SM_p = 7.5\%$  to -12,630.9 at  $SM_p = 5.0\%$ . Therefore model fit as well as  $SM_p$  estimation errors might lead to large uncertainties in  $r_{ss}$  under very dry conditions.

To understand the impact of  $r_{ss}$  uncertainties, we simulated diel *GPP*,  $L_{T,out,BB}$  and  $F_{760}^{\dagger}$  at the each solution of the I<sub>GPP</sub> scheme, but adding an increment of  $\pm 0.50\%$  to the  $SM_p$ . Shifted  $SM_p$  values were used to predict  $r_{ss}$  and this way the change in  $SM_p$  propagated to variables used to constraint the parameters. Fig. F.1 shows the differences ( $\Delta$ ) induced by these variations in  $SM_p$  on  $r_{ss}$ , *GPP*,  $L_{T,out,BB}$  and  $F_{760}^{\dagger}$ . As can be seen, small changes in SM produce large variations in on  $r_{ss}$ . However, these propagate in the shape of small changes in for the remaining variables. Changes in  $SM_p$  values lead to negligible variations for most of the observed  $SM_p$  range. The largest uncertainties occurred within the  $SM_p$  range 2%-4%, and become again negligible for lower values (due to the upper bound of 50.000 s/m). Additional simulations (not shown), reveal that predicted fluxes are most sensitive to changes in  $r_{ss}$  in a relatively small range of values of this variable, out of which fluxes show low sensitivity. In general, the effects of the simulated  $SM_p$  are relatively small when compared to fit errors reported in Table E.1, but errors in the estimation of  $SM_p$  should still be a source of uncertainty, with effects on the inversion difficult to predict.



**Fig. F.1.** Variation ( $\Delta$ ) of  $\pm$  0.5% shifts in soil moisture content ( $SM_p$ ) on: soil resistance for evaporation from the pore space ( $r_{ss}$ , a), gross primary production (GPP, b), emitted thermal radiance ( $L_{T,out,BB}$ , c) and emitted sun induced fluorescence in the O<sub>2</sub>-A band ( $F_{760}^{\dagger}$ , d) predicted for the solutions of the inversion scheme I<sub>GPP</sub>. Data are binned in ranges of  $SM_p$  equal to 1%.

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