

1 **senSCOPE: Modeling radiative transfer and biochemical processes in** 2 **mixed canopies combining green and senescent leaves with SCOPE**

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23 **Abstract.**

24 Semi-arid grasslands and other ecosystems combine green and senescent leaves featuring different
25 biochemical and optical properties, as well as functional traits. Knowing how these properties vary is
26 necessary to understand the functioning of these ecosystems. However, differences between green and
27 senescent leaves are not considered in recent models representing radiative transfer, heat, water and
28 CO₂ exchange such as the Soil-Canopy Observation of Photosynthesis and Energy fluxes (SCOPE).
29 Neglecting the contribution of senescent leaves to the optical and thermal signal of vegetation limits the
30 possibilities to use remote sensing information for studying these ecosystems; as well as neglecting their

31 lack of photosynthetic activity increases uncertainty in the representation of ecosystem fluxes. In this
32 manuscript we present senSCOPE as a step towards a more realistic representation of mixed green and
33 senescent canopies. senSCOPE is a modified version of SCOPE model that describes a canopy
34 combining green and senescent leaves with different properties and function. The model relies on the
35 same numerical solutions than SCOPE, but exploits the linear nature of the scattering coefficients to
36 combine optical properties of both types of leaf. Photosynthesis and transpiration only take place in
37 green leaves; and different green and senescent leaf temperatures are used to close the energy balance.
38 Radiative transfer of sun-induced fluorescence (SIF) and absorptance changes induced by the
39 xanthophyll cycle action are also simulated. senSCOPE is evaluated against SCOPE both using
40 synthetic simulations, forward simulations based on observations in a Mediterranean tree-grass
41 ecosystem, and inverting dataset of ground measurements of reflectance factors, SIF, thermal radiance
42 and gross primary production on a heterogeneous and partly senescent Mediterranean grassland. Results
43 show that senSCOPE outputs vary quite linearly with the fraction of green leaf area, whereas SCOPE
44 does not respond linearly to the effective leaf properties, calculated as the weighted average of green
45 and senescent leaf parameters. Inversion results and pattern-oriented model evaluation show that
46 senSCOPE improves the estimation of some parameters, especially chlorophyll content, with respect
47 SCOPE retrievals during the dry season. Nonetheless, inaccurate knowledge of the optical properties of
48 senescent matter still complicates model inversion. senSCOPE brings new opportunities for the
49 monitoring of canopies mixing green and senescent leaves, and for improving the characterization of the
50 optical properties of senescent material.

51 **1 Introduction**

52 Consistent monitoring of relevant vegetation properties is an essential step towards understanding the
53 response of vegetation function (e.g., photosynthesis, transpiration) to changes in environment. Among
54 others, photosynthetic performance and water use efficiencies are key elements to predict and
55 understand vegetation responses to the climate change scenarios (e.g., elevated atmospheric CO₂
56 concentration, higher temperatures and altered water regimes) (IPCC 2014). However, current Land

57 Surface Models (LSM) predictions of these fluxes include large uncertainties (Friedlingstein et al.
58 2014); partly due to inadequate representation of different processes as well as to the lack of knowledge
59 of functional parameters describing plant function (e.g., maximum carboxylation rate (V_{cmax}), maximum
60 electron transport rate (J_{max}) or the Ball-Berry stomatal sensitivity (m)) (Rogers 2014; Rogers et al.
61 2016; Schaefer et al. 2012). Recent efforts of the Remote Sensing (RS) community have focused on the
62 estimation of these parameters either using statistical approaches (Serbin et al. 2015; Silva-Perez et al.
63 2018), or combining Radiative Transfer Models (RTM) with Soil-Vegetation-Atmosphere Models
64 (SVAT) (Bayat et al. 2018; Camino et al. 2019; Dutta et al. 2019; Pacheco-Labrador et al. 2019; Zhang
65 et al. 2014; Zhang et al. 2018), notably using the Soil-Canopy Observation Photosynthesis and Energy
66 fluxes (SCOPE) model (van der Tol et al. 2009).

67 SCOPE represents radiative transfer of optical and thermal infrared radiation (TIR), in a homogeneous
68 1-D canopy, which is coupled with an energy balance and a photosynthesis models predicting heat and
69 water fluxes and carbon assimilation. SCOPE also propagates leaf level sun-induced chlorophyll
70 fluorescence (SIF) emission and absorptance changes related with the activation of the xanthophyll
71 cycle (Vilfan et al. 2018) to top of the canopy radiances. SCOPE uses Fluspect to model leaf optical
72 properties (Vilfan et al. 2016; Vilfan et al. 2018) and combines 4 different canopy RTM representing
73 outgoing radiation (RTM_o), SIF (RFM_f , (van der Tol et al. 2016)), TIR emission (RTM_t) and
74 xanthophyll absorption (RTM_z , (Vilfan et al. 2018)) that rely on the four stream SAIL extinction and
75 scattering coefficients model (Verhoef 1984). In addition, Yang and colleagues (2017) developed
76 mSCOPE, an extension of SCOPE that uses a different numerical solution of the radiative transfer
77 problem to represent 1-D but vertically heterogeneous canopies.

78 A current limitation of SCOPE is the lack of representation of within-canopy heterogeneity of
79 vegetation properties, and specifically the separation of green and senescent leaves, which feature large
80 differences in biophysical properties and function. When leaves senesce, flavonoids undergo enzymatic
81 oxidation processes within the leaf producing diverse semiquinones and quinones which can suffer non-
82 enzymatic secondary reactions with phenols, amino acids and proteins or other polyphenols (Pourcel et
83 al. 2007; Taranto et al. 2017). The result is a heterogeneous mixture of complex brown polymers,

84 difficult to characterize *in vivo* and responsible of the yellow and brown tones that these leaves exhibit
85 (Guyot et al. 1996; Pourcel et al. 2007). The characterization of the optical properties of these
86 “senescent” or “brown” pigments of leaves were addressed by Jacquemoud (1988) using albino corn
87 leaves; however, the authors stated that the characterization had to be improved. In fact, the absorption
88 coefficients currently used by Prospect are usually attributed to F. Baret, via personal communication
89 (e.g., (Féret 2009)). Thus, the characterization of senescent pigments is not as thoroughly documented
90 as for other pigments (Feret et al. 2008; Féret et al. 2017; Jacquemoud and Baret 1990; Vilfan et al.
91 2018), and their concentration is presented in arbitrary units due to the measurement technique used in
92 their determination (Jacquemoud 1988). Also, when leaves further degrade their color changes (Kidnie
93 et al. 2015), and some of their optical properties might vary with respect to those characterized and used
94 by leaf-level RTM. For example, Melendo-Vega et al, (2018) suggested that overestimation of near
95 infrared reflectance factors in a semi-arid grassland could be related to senescent material, and that this
96 effect increased with its longevity.

97 Commonly used models such as PROSAIL (Jacquemoud et al. 2009), or more recently SCOPE, allocate
98 all the pigments in a unique “effective” according to the averaged concentrations of the different leaves
99 of the canopy. However, this approach does not adequately represent mixed canopies with varying
100 fractions of green and senescent leaves. The presence of non-photosynthetic elements in the canopy has
101 been already addressed in turbid medium RTM (Bach et al. 2001; Braswell et al. 1996; Wenhan 1993)
102 and used to improve the estimation of biophysical parameters such as leaf area index (*LAI*) or
103 chlorophyll concentration (C_{ab}) or the fraction of absorbed photosynthetically active radiation (Houborg
104 and Anderson 2009; Houborg et al. 2009; Houborg and McCabe 2016; Wenhan 1993). However,
105 senescent and green leaves do not only feature different optical properties, but also different
106 physiological processes. For example, senescent leaves present little or no chlorophyll content
107 (Hörtensteiner 2006; Whitfield and Rowan 1974) so that they do not assimilate CO₂ through
108 photosynthesis. Also, senescent leaves do not transpire water and lack of stomatal regulation. Senescent
109 leaves can pose problems for the retrieval of biophysical variables if not adequately represented (Bacour
110 et al. 2002; Houborg and Boegh 2008; Wang et al. 2005). Analogously, inadequate representation of

111 green and senescent leaf pools could also potentially induce uncertainties in the simulation of processes
112 at canopy scale related to photosynthesis and transpiration. Finally, given that SCOPE is now widely
113 used for retrieval of functional properties (Bayat et al. 2018; Camino et al. 2019; Dutta et al. 2019;
114 Pacheco-Labrador et al. 2019; Zhang et al. 2014; Zhang et al. 2018), these uncertainties can propagate
115 in the estimated parameters (Pacheco-Labrador et al. 2019). This fact may limit the application of recent
116 approaches combining RTM and SVAT models for the study of canopies or ecosystems featuring large
117 fractions of dry leaves (in particular in grasslands or semi-arid ecosystems) or for the monitoring of
118 vegetation health, crop productivity and phenology.

119 Senescent material is present in all vegetation, and for a remote sensing perspective is very critical for
120 annual plants such as grasslands (Houborg et al. 2009; Melendo-Vega et al. 2018), which cover about
121 40% of the Earth's terrestrial surface (Anderson 2006). Grassland's phenology and function are strongly
122 governed by water availability, temperature, herbivory, fire, nitrogen deposition or CO₂ concentration
123 increase (Anderson 2006; Cleland et al. 2006; Figueroa and Davy 1991; Luo et al. 2018; Migliavacca et
124 al. 2011; Richardson et al. 2013). Green plants transit to senescent, recently dead, and long-term dead
125 plants, each of them featuring different biophysical and optical properties (Kidnie et al. 2015). This
126 transition varies with meteorology (Ren and Zhang 2018), biophysical properties (Henry et al. 2008;
127 Sanaullah et al. 2010; Yuan and Chen 2009), plant functional types (Henry et al. 2008) and changes for
128 different parts of the plant (Henry et al. 2008; Koukoura et al. 2003). Usually, even in grasses, leaves
129 fall while stems stay longer and degrade more slowly due to differences in biochemical composition.
130 Therefore, in multi-species grasslands senescence and degradation can take place at different rates and
131 periods, increasing the variability of surface biophysical and optical properties as well as the complexity
132 of modeling and characterization. In fact, senescent material and litter are nowadays considered a
133 challenge for the estimation of biophysical properties in semi-arid grasslands (He and Mui 2010).

134 In this work, we present senSCOPE, a modified version of the SCOPE model that separates RTM and
135 physiological processes (photosynthesis and transpiration) for green and senescent leaves. senSCOPE
136 aims at improving the representation of radiative transfer and physiology in senescent canopies. The
137 model is then evaluated in three ways:

138 1) We run a sensitivity analysis comparing forward simulations of SCOPE and senSCOPE under
139 different meteorological conditions and under different combinations of vegetation parameters for
140 different abundances of senescent leaves.

141 2) We use observations of model parameters and meteorological data at ecosystem scale to predict
142 fluxes and compare them with EC data.

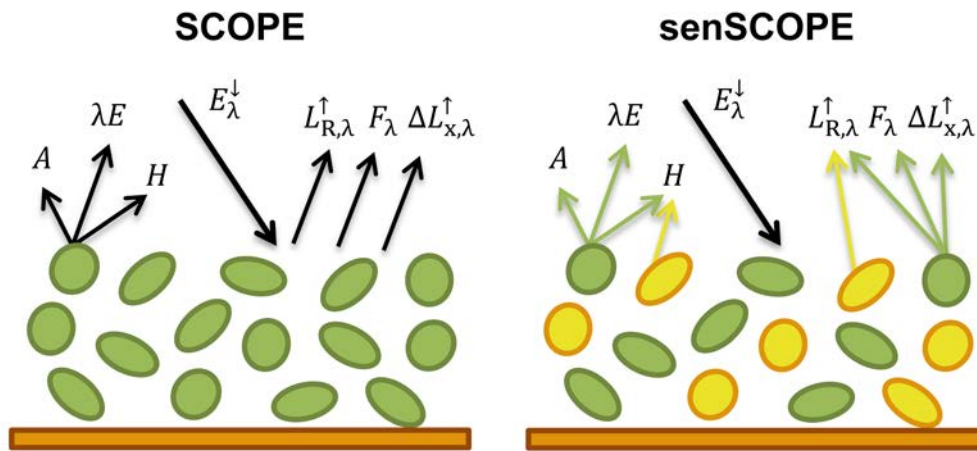
143 3) We invert SCOPE and senSCOPE against the same dataset of ground observations of carbon
144 fluxes, reflectance factors (R), SIF and TIR radiance used by Pacheco-Labrador et al, (2019) for
145 comparison.

146 As in the former work, functional and biophysical model parameters are estimated by inverting SCOPE
147 against different combinations of the abovementioned variables sampled at plot scale in a
148 Mediterranean grassland. New inversion boundaries are used according to observations of some of the
149 parameters in the site. Results of both inversions are compared and evaluated using pattern-oriented
150 model evaluation approach (Pacheco-Labrador et al. 2019).

151 **2. Description of senSCOPE**

152 The model senSCOPE extends the 1-D model SCOPE to describe homogeneous canopies combining
153 green and senescent leaves randomly mixed. Fig. 1 summarizes the conceptual differences between
154 SCOPE and senSCOPE. Green leaves contain chlorophylls and other photosynthetic pigments that
155 allow them to photosynthesize; and regulate their temperature via transpiration. In contrast, senescent
156 leaves only contain senescent pigments and neither photosynthesize nor transpire. These leaves present
157 some microbial activity related to its degradation, and superficial water (e.g., intercepted rainfall) can
158 evaporate from their surface; however these processes are not represented neither by SCOPE nor
159 senSCOPE. In senSCOPE, the leaf RTM Fluspect (Vilfan et al. 2016; Vilfan et al. 2018) simulates
160 reflectance, transmittance and, in the case of green leaves, also fluorescence according to the
161 biochemical and structural properties of each leaf type. Canopy RTM₀ implemented in SCOPE (van der
162 Tol et al. 2009) is modified to separately compute the radiation absorbed by each leaf type; and the

163 energy balance model is customized to account for the presence of leaves that neither photosynthesize
164 nor transpire. Since green and senescent leaves feature different radiative balances, a modified RTM_t
165 model quantifies thermal emission of each of these two leaf types separately and combines them
166 according to the corresponding fractions of leaf area (f); then the model calculates scattering and
167 absorption of this diffuse flux. Eventually, fluorescence emission and optical changes induced by the
168 activation of the xanthophyll cycle in the green leaves is propagated to top of canopy (TOC) radiances
169 and R using the RTM_f (van der Tol et al. 2016) and RTM_z (Vilfan et al. 2018) models already
170 implemented in SCOPE. Both models are coded in Matlab (Matwoks Inc., Natick, MA, USA).



171

172 **Figure 1. Conceptual differences between SCOPE and senSCOPE models. Green and yellow colours**
173 **correspond to green and senescent leaves, respectively. Black arrows show processes featured by all leaves;**
174 **whereas coloured arrows refer to processes featured only for a given type of leaf. The scheme represents**
175 **assimilation (A), latent (λE) and sensible heat (H) fluxes, incoming spectral irradiance (E_i), reflected**
176 **spectral radiance ($L_{R,\lambda}$), emitted fluorescence radiance (F_i) and changes in $L_{R,\lambda}$ due to activation of**
177 **xanthophyll cycle ($\Delta L_{x,\lambda}$)**

178 senSCOPE relies on the same solution of the radiative transfer problem implemented in SCOPE, since it
179 exploits the linear nature of the single leaf scattering efficiency factors (Verhoef 1984) to combine the
180 optical properties of green and senescent leaves in an “averaged” leaf. This is simple if leaf angle
181 distribution is assumed the same for both types of leaves. The main advantage of this approach is that it
182 allows representing physiological processes separately in each leaf type. This is important since
183 photosynthesis and transpiration are non-linearly related with radiation and leaf temperature, and

184 therefore might not be adequately represented by a model featuring a unique leaf type characterized by
185 the “averaged parameters” of photosynthetic and non-photosynthetic leaves.

186 senSCOPE requires a larger number of parameters than SCOPE, since two different leaves must be
187 described, as well as their respective area fractions. Alternatives to minimize the number of parameters
188 and simplify the application of the model in inverse problems are presented in Sect. 3.2.2 and discussed
189 later.

190 **2.1 Radiation Fluxes**

191 As SCOPE, senSCOPE relies on SAIL 4-stream theory that can be summarized by a system of four
192 linear equations describing the radiative transfer of the solar direct flux (E_s), the downward diffuse flux
193 (E^-), the upward diffuse flux (E^+), and the flux in the observation direction (E_o).

$$194 \quad \frac{dE_s}{Ldx} = kE_s, \quad (1a)$$

$$195 \quad \frac{dE^-}{Ldx} = -sE_s + aE^- - \sigma E^+, \quad (1b)$$

$$196 \quad \frac{dE^+}{Ldx} = -s'E_s + \sigma E^- - aE^+, \quad (1c)$$

$$197 \quad \frac{dE_o}{Ldx} = wE_s + vE^- + v'E^+ - KE_o, \quad (1a)$$

198 In this system, x represents the vertical relative height within the canopy ($x = 0$ for top, $x = -1$ for
199 bottom), and L represents the Leaf Area Index (also LAI). The remaining variables are the SAIL
200 coefficients defined for first time by Verhoef (1984). k and K are the extinction coefficients in the solar
201 and observation directions, respectively. They depend on the sun-view geometry, LAI and the leaf angle
202 distribution (LAD); and they are therefore independent of leaf optical properties. s , a , σ , s' , w , v and v'
203 are the scattering coefficients depending on sun-view geometry, canopy structure and leaf optical
204 properties. These coefficients define the relationship between a given incident flux (E_1) and a given
205 scattered flux (E_2) in the canopy, and they are computed by integrating single-leaf scattering efficiency
206 factors (Q_{sc}) that represent the analogous relationship for individual leaves. The scattering coefficient

207 (b) corresponding to all the leaves of given zenith inclination angle (θ_1) can be defined as (Verhoef
208 1984):

$$209 \quad b(\theta_1) = \frac{L'}{2\pi} \int_0^{2\pi} Q_{sc}(E_1, E_2) d\varphi_1, \quad (2)$$

210 where L' is the LAI contained in a horizontal layer of the canopy of width dx and φ_1 is the leaf azimuth
211 angle.

212 As in SCOPE, senSCOPE solves the radiative transfer problem numerically, defining a discrete number
213 of canopy layers and leaf angles. $Q_{sc}(E_1, E_2)$ are defined assuming that individual leaves are Lambertian
214 diffusors of known hemispherical reflectance (ρ) as and hemispherical transmittance (τ). ρ and τ are
215 predicted in SCOPE by Fluspect (Vilfan et al. 2016). For each pair of incident and scattered fluxes,
216 $Q_{sc}(E_1, E_2)$ is defined as a linear combination of ρ and/or τ weighted by spectrally invariant factors
217 determined by the geometry of the leaf, or more specifically, the projection of the leaves with respect to
218 the incident flux (E_1) and the downward (-) or upward (+) scattered flux (E_2). As proposed by Bach et
219 al, (2001), senSCOPE exploits this linear nature of Q_{sc} to combine the ρ and the τ of green and
220 senescent leaves into an averaged factors; weighted by their corresponding fractions of leaf area (Eq. 3
221 and 4). This approach allows applying the solution already proposed by van der Tol et al., (2009) for the
222 linear system shown in Eq. 1a-d.

$$223 \quad \rho = f_{\text{green}}\rho_{\text{green}} + (1 - f_{\text{green}})\rho_{\text{senes}}, \quad (3)$$

$$224 \quad \tau = f_{\text{green}}\tau_{\text{green}} + (1 - f_{\text{green}})\tau_{\text{senes}}, \quad (4)$$

225 where subscripts “green” and “senes” indicate the type of leaf. Notice that the weighted average of ρ
226 and τ is not equivalent to the factors predicted for a weighted average of the leaf parameters.

227 This approach is suitable to represent the radiative transfer of a canopy of homogeneously mixed green
228 and senescent leaves. In order to represent physiological processes for each leaf type separately, it is
229 necessary differentiating the amount total radiation absorbed by each leaf type, and the
230 photosynthetically active radiation (PAR) absorbed by chlorophyll ($E_{\text{ap,Chl}}$). SCOPE quantifies $E_{\text{ap,Cab}}$
231 (W m^{-2}) using the relative absorption of this pigment respect to the remaining total absorption in the leaf

232 in each spectral band ($k_{\text{Chl,rel}}$). $E_{\text{ap,Chl}}$ is computed for the direct ($E_{\text{ap,Chl,dir}}$) and the diffuse irradiances
 233 ($E_{\text{ap,Chl,dif}}$) as follows:

$$234 \quad E_{\text{ap,Chl,dir}} = f_{\text{green}} \int_{\lambda=400}^{\lambda=700} k_{\text{Chl,rel,green}}(\lambda) E_{\text{sun}}(\lambda) [1 - \rho_{\text{green}}(\lambda) - \tau_{\text{green}}(\lambda)] d\lambda, \quad (5)$$

$$235 \quad E_{\text{ap,Chl,dif}}(x) = f_{\text{green}} \int_{\lambda=400}^{\lambda=700} k_{\text{Chl,rel,green}}(\lambda) [E^-(x, \lambda) + E^+(x, \lambda)] [1 - \rho_{\text{green}}(\lambda) - \tau_{\text{green}}(\lambda)] d\lambda, \quad (6)$$

236 where λ is the wavelength and $k_{\text{Chl,rel,green}}$ is $k_{\text{Chl,rel}}$ in the green leaves. These quantities are calculated
 237 from the upward and downward fluxes without modifying the transfer of radiation. Since senSCOPE
 238 defines senescent leaves as containing no chlorophyll, $k_{\text{Chl,rel}} = 0$ in senescent leaves and for this reason,
 239 absorbed PAR used to simulate photosynthesis in sunlit ($E_{\text{ap,Chl,u}}$) and shaded leaves ($E_{\text{ap,Chl,h}}$) per total
 240 leaf area of the mixed canopy scales with f_{green} . Shaded leaves (subscript ‘h’) are only illuminated by
 241 diffuse light (Eq. 7); whereas Eq. 5 and 6 must be combined to get $E_{\text{ap,Chl}}$ in the sunlit leaves ($E_{\text{ap,Chl,u}}$,
 242 subscript ‘u’) (Eq. 8).

$$243 \quad E_{\text{ap,Chl,h}}(x) = E_{\text{ap,Chl,dif}}(x), \quad (7)$$

$$244 \quad E_{\text{ap,Chl,u}}(x, \theta_1, \varphi_1) = |f_s(x, \theta_1, \varphi_1)| E_{\text{ap,Chl,dir}} + E_{\text{ap,Chl,dif}}(x), \quad (8)$$

245 where f_s is a geometric factor accounting for the projection of each leaf towards the sun.

246 Total absorbed radiation is used to compute the radiation budget in the canopy and determines leaf
 247 temperature, which has implications for photosynthesis and transpiration, and must therefore be
 248 computed separately for each leaf type. Total absorbed radiation is computed by SCOPE similarly as in
 249 Eq. 5-8, but integrating the fluxes in the full spectral domain (e.g., 400-50.000 nm):

$$250 \quad E_{a,i,dir} = f_i \int_{\lambda=400}^{\lambda=50000} E_{\text{sun}}(\lambda) [1 - \rho_i(\lambda) - \tau_i(\lambda)] d\lambda, \quad (9)$$

$$251 \quad E_{a,i,dif}(x) = f_i \int_{\lambda=400}^{\lambda=50000} [E^-(x, \lambda) + E^+(x, \lambda)] [1 - \rho_i(\lambda) - \tau_i(\lambda)] d\lambda, \quad (10)$$

$$252 \quad E_{a,i,h}(x) = E_{a,i,dif}(x) \quad (11)$$

$$253 \quad E_{a,i,u}(x, \theta_1, \varphi_1) = |f_s(x, \theta_1, \varphi_1)| E_{a,i,dir} + E_{a,i,dif}(x), \quad (12)$$

254 Where subscript “i” now stands for either ‘green’ or ‘senescent’.

255 2.2 Energy balance

256 As in SCOPE, energy balance is closed iteratively by modifying canopy and soil temperatures until the
257 following is met for the soil and for all leaf angles and layers separately:

$$258 |R_n - H - \lambda E - G| < \varepsilon_{\text{threshold}}, \quad (13)$$

259 where R_n is net radiation, H is latent heat flux, λE is energy heat flux, G is soil heat flux and $\varepsilon_{\text{threshold}}$ is a
260 predefined threshold for the accepted energy balance closure error ($\varepsilon_{\text{threshold}}$), all in W m^{-2} .

261 senSCOPE addresses the energy balance separating the processes occurring in green and senescent
262 leaves, where only the first are assumed to photosynthesize and transpire. Therefore, $\varepsilon_{\text{ebal}}$ is separated
263 into the following elements (Eq. 14):

$$264 R_{n,\text{green}} - R_{n,\text{senes}} - R_{n,\text{soil}} - H_{\text{green}} - H_{\text{senes}} - H_{\text{soil}} - \lambda E_{\text{green}} - \lambda E_{\text{soil}} - G = \varepsilon_{\text{ebal}}, \quad (14)$$

265 where the subscript “soil” refers to soil fluxes, and only green leaves and soil contribute to λE .
266 However, notice that similarly as in SCOPE, the energy balance is separately closed for soil and for all
267 leaf angles, layers and leaf types.

268 In order to compute R_n , the contribution of thermal emission must be added to the absorbed radiation
269 calculated in Sect. 2.1. senSCOPE separately represents the temperatures of green and senescent leaves
270 ($T_{c,\text{green}}$, $T_{c,\text{senes}}$, respectively) since they absorb radiation cool down differently. Distinguishing these
271 temperatures has an impact on the calculation of photosynthesis, which is temperature dependent.
272 Consequently, black-body thermal emission (H_c) is different for each leaf type ($H_{c,\text{green}}$, $H_{c,\text{senes}}$); and the
273 on-sided black-body thermal emission of all leaves is computed as a linear combination of the emission
274 of each leaf type in the canopy:

$$275 \varepsilon H_c = f_{\text{green}} \varepsilon_{\text{green}} H_{c,\text{green}}(T_{c,\text{green}}) + (1 - f_{\text{green}}) \varepsilon_{\text{senes}} H_{c,\text{senes}}(T_{c,\text{senes}}), \quad (15)$$

276 where ε is the emissivity, and equals absorptance ($1 - \rho - \tau$) according to Kirchhoff’s Law. The propagation
277 of emitted radiation by leaves and soil through the canopy is calculated using the averaged layer
278 properties as in the original SCOPE. In order to quantify the net thermal radiation (emitted minus

279 absorbed) ($R_{n,t}$) senSCOPE calculates the amount of energy absorbed by each leaf type using their
280 respective emissivity:

$$281 \quad R_{n,t,green} = [E^- + E^+ - 2H_{green}] \varepsilon_{green} f_{green} , \quad (16)$$

$$282 \quad R_{n,t,senes} = [E^- + E^+ - 2H_{senes}] \varepsilon_{senes} (1 - f_{green}) , \quad (17)$$

283 where E^- and E^+ are the diffuse emitted fluxes. $R_{n,t}$ of sunlit and shaded leaves is computed
284 separately. These are energy fluxes per total (senescent plus green) leaf surface area. Therefore, canopy
285 net radiation is computed as the addition of E_a and $R_{n,t}$; and $R_{n,t} = R_{n,t,green} + R_{n,t,senes}$ without the need to
286 further weight by fraction.

287 Aerodynamic resistances are computed as in SCOPE for the whole mixed canopy, since they depend on
288 meteorology and canopy structure. Consequently water and heat fluxes (H_{green} , H_{senes} and λE_{green}) in
289 senSCOPE are computed with an identical representation of resistances as in SCOPE, but with leaf
290 temperatures differentiated per leaf type. These fluxes are defined per unit of leaf-type surface, and need
291 to be scaled to the fraction of LAI represented by each leaf type in the mixed canopy. Eventually,
292 senSCOPE iteratively resolves six temperatures: sunlit and shaded green leaves ($T_{c,u,green}$, $T_{c,h,senes}$),
293 sunlit and shaded senescent leaves ($T_{c,u,senes}$, $T_{c,h,usenes}$), and both sunlit and shaded soil ($T_{s,u}$, $T_{s,h}$).

294 **2.3 Photosynthesis**

295 In senSCOPE, only green leaves photosynthesize and transpire. Photosynthesis is driven by the PAR
296 absorbed by chlorophyll ($APAR_{Chl}$; which equals $E_{ap,Chl}$ transformed from $W m^{-2}$ to $\mu mol m^{-2} s^{-1}$). The
297 absorbed PAR by chlorophyll in green leaves per unit green leaf area is $E_{ap,Chl,green} = E_{ap,Chl} / f_{green}$. Other
298 area-based inputs such as maximum carboxylation rate V_{cmax} [$\mu mol m^{-2} s^{-1}$], as well as model outputs
299 (e.g., internal CO_2 concentration, C_i [$\mu mol m^{-3}$]) refer to green leaves only. Assimilation (A_c) is
300 therefore initially computed per unit green leaf area. The stomatal conductance (r_{cw}) as output of the
301 leaf biochemical model is further used to calculate the transpiration of green leaves λE_{green} , also per unit
302 green leaf area. Consequently, both fluxes first calculated per unit green leaf area, and later scaled with
303 f_{green} .

304 **2.4 Fluorescence**

305 SCOPE computes leaf level fluorescence emission using three main elements: incident irradiance in the
306 excitation range 400-750 nm, excitation-fluorescence (E-F) matrices ($M(\lambda_e, \lambda_f)$ and $M'(\lambda_e, \lambda_f)$ for
307 backwards and forward fluorescence, respectively), and the amplification factors Φ'_f which are
308 provided by the biochemical model for sunlit and shaded leaves. E-F matrices represent the excitation
309 of chlorophyll and the radiative transfer of incident and re-emitted radiation inside the leaf (Vilfan et al.
310 2016). In senSCOPE the leaf fluorescence emission is only calculated for green leaves, because for
311 senescent leaves, the E-F matrices equal zero. Then the emission is scaled with f_{green} .

$$312 E_1^f = f_{\text{green}} \cdot \Phi'_f \cdot [(M'_{\text{green}}(\lambda_e, \lambda_f) + M_{\text{green}}(\lambda_e, \lambda_f))] \otimes E, \quad (18)$$

313 Leaf level fluorescence emission is then propagated to top of the canopy combining the same radiative
314 transfer approach used by SCOPE and the averaged leaf optical properties (ρ and τ) for the mixed
315 canopy.

316 **2.5 Xanthophyll cycle**

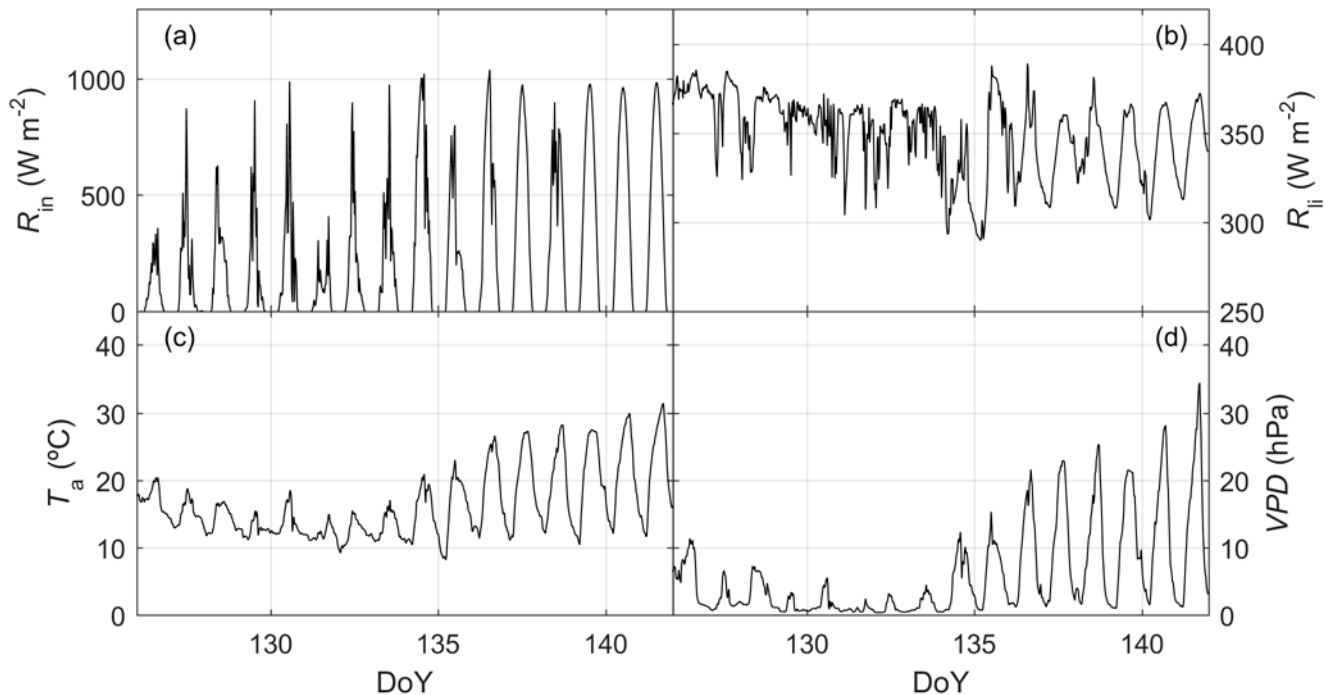
317 A recent version of SCOPE incorporates Fluspect-CX (Vilfan et al. 2018), a leaf RTM that simulates
318 the variations in leaf optical properties induced by the activation of the xanthophyll cycle for
319 photosynthetic down-regulation-, and propagates these variations from leaf to canopy level radiances.
320 Changes in leaf optical properties are computed after photosynthesis, as a function of the rate
321 coefficient for non-photochemical quenching (K_n) provided by the biochemical module. This rate serves
322 as a scaling factor of leaf ρ and τ between two extreme cases of with completely activated and
323 completely deactivated xanthophyll cycle. In senSCOPE, senescent leaves show no carotenoids, no
324 xanthophyll cycle and no related changes in optical properties; for this reason, the extreme cases
325 calculated on the averaged ρ and τ simulate only variations induced by the green leaves. K_n is a rate
326 defining the probability of the different fates of photons exciting chlorophyll, therefore, and similarly to
327 Φ'_f , it does not require additional correction. Therefore, senSCOPE uses the same radiative transfer
328 functions than SCOPE for the propagation of signals related with the xanthophyll cycle.

329 3. Methods

330 3.1 Comparison with SCOPE model. Sensitivity analysis

331 In order to evaluate the differences between senSCOPE and the original model SCOPE (van der Tol et
332 al. 2009), we run two different series of forward simulations modifying separately meteorological
333 variables (F_{meteo}) and vegetation properties (F_{veg}). Eleven different canopies with f_{green} ranging between
334 0.0 and 1.0 with steps of 0.1 were simulated. As input to SCOPE we used weighted averages of the leaf
335 parameters of each leaf type; similarly as field leaf measurements would be averaged to calculate
336 canopy mean values.

337 In order to provide realistic meteorological forcing in the simulations F_{meteo} , we used actual
338 measurements acquired in the research site of Majadas de Tiétar between 5th and the 20th May 2016
339 (day of the year (DoY) 126 and 141, respectively). Fig. 2 summarizes this dataset.



340

341 **Figure 2. Short wave (a) and long wave incoming radiation (b), air temperature (c) and vapour pressure**
342 **deficit (d) recorded in Majadas de Tiétar between the 5th and the 20th May 2019 (DoY 126 and 141,**
343 **respectively) used in the forward simulation F_{meteo} .**

344 Short wave incoming radiation (R_{in} , W m^{-2}), long wave incoming radiation (R_{li} , W m^{-2}), air temperature
345 (T_{a} , $^{\circ}\text{C}$), atmospheric vapour pressure (e_{a} , hPa), wind speed (u , m s^{-1}), air pressure (p , hPa) and soil
346 moisture (SM_{p} , % volume) were provided by a sub-canopy eddy covariance station at 1.6 m height
347 (detailed description of the system can be found in El-Madany et al, (2018) and Perez-Priego et al,
348 (2017)). Vapour pressure deficit (VPD , hPa) was calculated from T_{a} and e_{a} ; also, soil resistance for
349 evaporation from the pore space (r_{ss} , s m^{-1}) was estimated as a function of using SM_{p} the model SCOPE
350 v1.73. Sun zenith (θ_{s}) and azimuth (φ_{s}) angles were computed from timestamps and site location. In the
351 F_{meteo} runs, only the abovementioned variables were modified; leaf and canopy properties were kept
352 constant for the different f_{green} levels tested. Only daytime data ($\theta_{\text{s}} < 85.0$ deg) were used in the
353 simulation; which equals 422 runs per model and f_{green} level.

354 F_{veg} represented varying vegetation properties under constant meteorological conditions. To do so, we
355 selected midday conditions of the 18th May 2019 (DoY 139). A look up table with 500 samples of C_{ab} ,
356 carotenoids concentration (C_{ca}), V_{cmax} , Fluorescence quantum efficiency (f_{qe}), m and LAI was generated
357 using Latin Hypercube Sampling (McKay et al. 1979). C_{ca} and V_{cmax} were constrained as a function of
358 C_{ab} mimicking the relationships (linear function and noise) reported in Sims and Gamon (2002) and
359 Croft et al, (2017), respectively. Table 1 shows the ranges of variation generated for each parameter
360 varying in each F_{veg} simulation. Additionally, a smaller dataset was generated modifying only LAI or
361 C_{ab} (and V_{cmax} and C_{ca} as a function of these) to illustrate an example of the response of models to these
362 parameters. Several model outputs and internal parameters were evaluated. Moreover, we also
363 compared the predicted underlying water use efficiency ($uWUE$, Eq. 19):

$$364 \quad uWUE = \frac{A}{\lambda E_{\text{c}}} \sqrt{VPD}, \quad (19)$$

365 where λE_{c} is the canopy λE , excluding evaporation from the soil.

366

367

368 **Table 1. Vegetation parameters used in the forward simulation F_{veg} .**

Parameter	Symbol	Units	Range
Leaf chlorophyll content	C_{ab}	$\mu\text{g cm}^{-2}$	[0.13, 99.98]
Leaf carotenoids content	C_{ca}	$\mu\text{g cm}^{-2}$	[0.02, 37.26]
Maximum carboxylation capacity	V_{cmax}	$\text{mmol m}^{-2} \text{s}^{-1}$	[0.40, 162.78]
Ball-Berry sensitivity parameter	m	-	[0.05, 39.98]
Fluorescence quantum efficiency	f_{qe}	-	[0.01, 0.03]
Leaf area index	LAI	$\text{m}^2 \text{m}^{-2}$	[0.00, 7.99]

369

370 The MatlabTM Profiler (Matwoks Inc., Natick, MA, USA) was used to evaluate the computing time and
371 number of calls of the different functions of each model used during these simulations in each run.
372 These metrics, together with the total computation time and the number of unsuccessful runs -where the
373 energy balance does not succeed to converge to a solution-, were used to compare models'
374 performances.

375 **3.2 Comparison with SCOPE model. Forward simulation with observational datasets**

376 SCOPE and senSCOPE were also run forward using observational datasets from the study site of
377 Majadas de Tiétar, Cáceres, Spain (39° 56' 24.68"N, 5° 45' 50.27"W). Observations -and when missing
378 estimates- of vegetation properties and forcing variables integrated at ecosystem scale were used to run
379 both models. Predicted fluxes and reflectance factors where compared with EC observations and
380 hyperspectral airborne imagery.

381 3.2.1 Study site and datasets

382 The study site is located in the experimental station of Majadas de Tiétar. It is a managed tree-grass
383 ecosystem combining sparse trees (*Quercus ilex* L. subsp. *ballota* [Desf.] Samp) and a highly diverse
384 herbaceous cover combining numerous species of three main functional plant forms: grasses, forbs and
385 legumes. The climate is continental Mediterranean so that the grassland shows a strong seasonality
386 initiated by greening phase around April, followed by a dry season that starts between May and June, a
387 second re-greening driven by autumn rains, and a dormant phase during winter (El-Madany et al. 2018).
388 The grassland phenology and functioning strongly responds to light and temperature in spring and to
389 water availability in late spring-summer and in autumn (Luo et al. 2018). Several species grow and
390 senesce at different times, usually, in early spring senescent material remnant from the winter is already
391 present, then new material is also generated during spring, where f_{green} can already be already as low as
392 ~ 0.7 (Melendo-Vega et al. 2018).

393 In this site, three EC towers monitor three areas of the same ecosystem, one of them fertilized with
394 nitrogen (N) and another one with N plus phosphorous (P), and the control one with no fertilization.
395 These towers include also eddy covariance systems around 15 m above the ground, providing
396 ecosystem-level measurements of carbon and water fluxes. Three sub-canopy towers monitor grassland
397 fluxes ~ 1.6 m aboveground. Details of the instrumentation and the manipulation can be found in El-
398 Madany et al, (2018) and Perez-Priego et al, (2017). Also, a series of airborne campaigns with the
399 Compact Airborne Spectrographic Imager CASI-1500i (Itres Research Ltd., Calgary, AB, Canada),
400 operated by the Instituto Nacional de Técnica Aeroespacial (INTA) were conducted between 2012 and
401 2017. From a total of 17 images, a R of the footprint of each EC tower and campaign was extracted.
402 Details of methods and data processing can be found in Pacheco-Labrador et al., (2017). Additionally,
403 in each of the airborne campaigns, destructive sampling of vegetation provided estimates of ecosystem
404 LAI , f_{green} , C_{dm} , C_{w} , Nitrogen concentration (N_{mass}) and/or C_{ab} and C_{ca} . Further information on protocols
405 and methods can be found in Melendo-Vega et al., (2018), Gonzalez-Cascon et al., (2017) and
406 (Gonzalez-Cascon and Martin 2018).

407 **3.2.2 senSCOPE and SCOPE. Forward simulation and evaluation**

408 Observed/estimated forcing variables and vegetation properties were used to predict fluxes and
409 reflectance factors ± 1 day around each flight campaign in each EC tower during daytime. Since no field
410 observations of all the vegetation parameters were available, some of them had to be estimated. When
411 missing, C_{ab} and C_{ca} were estimated from their relationship with N_{mass} observed in the site. Also V_{cmax}
412 was estimated as a function of N_{mass} in the green leaves ($N_{mass,green}$) following the relationship in Feng
413 and Dietze (2013), and assumed $45 \mu\text{mol m}^{-2} \text{s}^{-1}$ for tree leaves. A constant m parameter of 10 was
414 assumed, N and LAD were assumed 1.5 and spherical, respectively. C_s was estimated from the
415 remaining leaf parameters inverting the statistical model described section 3.3.2 and in Appendix A.
416 Soil reflectance was determined by SM_p and the parameters estimated by inversion of the BSM model
417 (Verhoef et al. 2018) in Pacheco-Labrador et al (2019). Also, r_{ss} was estimated as function of SM_p
418 using the model in Pacheco-Labrador et al (2019).

419 Then, we evaluated the capability of both models to predict GPP , λE , R_n , G , and H comparing SCOPE
420 and senSCOPE predictions with EC fluxes in the site. We also evaluated model performance and
421 structure using predicted fluxes and computing quantities that describe energy partitioning, the
422 evaporative fraction (Eq. 20)

$$423 \quad EF = \frac{\lambda E}{\lambda E + H}, \quad (20)$$

424 where λE and H are the total latent heat sensible heat fluxes, respectively.

425 Emitted irradiance in the TIR (E_t) was compared with net radiometer measurements in the EC towers
426 (CNR4, Kipp and Zonen, Delft, Netherlands); also R were compared with those of the imagery at the
427 time of the overpass.

428 **3.3 Comparison with SCOPE model. Inversion on observational datasets**

429 In order to assess the impact of accounting for senescence material during the estimation of key
430 biophysical (e.g., LAI , C_{ab}) and functional (e.g., V_{cmax} , m) vegetation parameters, we compared the
431 parameter estimates and posterior predictions resulting from the inversion of both models against real

432 observations in a Mediterranean grassland in the context of a nutrient manipulation experiment with N
433 and P, featuring f_{green} between 0.05-1. In this work, we inverted SCOPE and senSCOPE using the
434 inversion method and approaches proposed in Pacheco-Labrador et al. (2019).

435 **3.3.1 Study site and datasets**

436 The inversion the models is tested using field observations from the understory grass layer of the site of
437 Majadas de Tiétar, Cáceres, Spain, acquired in the context of the Small-scale MANipulation
438 Experiment (SMANIE) (Perez-Priego et al. 2015). This manipulation nutrient experiment was
439 performed in an open area to minimize the effect of trees. The experimental design consisted of 4
440 blocks (4 replicates each) with N, P, both (NP) additions, and the control treatment (C, not fertilized).
441 As a result of the fertilization, N, NP and P treatments induced changes in plant community, plant
442 structure and function (Martini et al. 2019; Migliavacca et al. 2017; Perez-Priego et al. 2015). 9 field
443 campaigns took place between 2014-2016 covering spring and early summer. In each block, midday
444 measurements were carried out in two different collars with a dual spectroradiometric system providing
445 hyperspectral R and SIF estimates in the O₂-A (F_{760}) and the O₂-B (F_{687} , not in all the campaigns).
446 Diurnal time course of TIR up-welling radiance (L_t) and GPP was determined using gas exchange
447 chambers from sunrise to sunset. Fluxes were collected quasi-simultaneously in the same collars of the
448 radiometric measurements at midday. The mismatch between the radiometric and chamber
449 measurements was minimum. Moreover, destructive sampling near by the collars provided estimates of
450 plant traits (f_{green} , LAI , and nitrogen concentration N_{mass}). Additional information about instrumentation,
451 sampling methods and data processing can be found elsewhere (Martini et al. 2019; Migliavacca et al.
452 2017; Pacheco-Labrador et al. 2019; Perez-Priego et al. 2015).

453 **3.2.2 senSCOPE and SCOPE. Inversion and evaluation**

454 We inverted senSCOPE and SCOPE using the same datasets and methodology described for the
455 inversion of SCOPE in Pacheco-Labrador et al. (2019). Observations of R and L_t , F_{760} and/or GPP were
456 used to estimate LAI , C_{ab} , V_{cmax} , m and other biophysical parameters (Table 2) using an innovative
457 methodology that combined biophysical and functional constraints in two different steps. Three

458 different sets of constraints (inversion schemes) were tested, each combined in the first step of the
 459 inversion (Step#1), noon R with noon GPP (I_{GPP}), noon GPP and F_{760} ($I_{GPP-SIF}$), or nothing else (I_R).

460 **Table 2. Parameters estimated inverting senSCOPE model**

Parameter	Symbol	Units	Step	Inversion bounds
Leaf chlorophyll content	C_{ab}	$\mu\text{g cm}^{-2}$	#1	[0, 100]
Leaf carotenoids content	C_{ca}	Mg cm^{-2}	#1	[0, 40]
Senescent material	C_s	-	#1	[0, 7.5]
Leaf water content	C_w	g cm^{-2}	#1	$[6.3 \cdot 10^{-5}, 0.06]$
Leaf dry matter content	C_{dm}	g cm^{-2}	#1	[0.0019, 0.03]
Leaf structural parameter	N	Layers	#1	[1, 3.6]
Leaf area index	LAI	$\text{m}^2 \text{m}^{-2}$	#1	[0, 8]
Leaf inclination distribution function	$LIDF_a$	-	#1	[-1, 1]; $ LIDF_a + LIDF_b \leq 1$
Bimodality of the leaf inclination	$LIDF_b$	-	#1	
Maximum carboxylation capacity	V_{cmax}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	#1 & #2	[0, 200]
Ball-Berry sensitivity parameter	m	-	#2	[0, 50]
Fluorescence quantum efficiency	f_{qe}	-	#1 & #2	[0,1]

461

462 In Step#1 biophysical parameters of the SCOPE model and a first guess of V_{cmax} were estimated.
 463 Uncertainties were estimated using a Bayesian approach (Omlin and Reichert 1999). Then, in a second
 464 step (Step#2) the guess of V_{cmax} was used as a prior and diel cycles of L_t combined with diel GPP (I_{GPP}),
 465 diel GPP and noon F_{760} ($I_{GPP-SIF}$), or only diel L_t (I_R) were used to estimate the functional parameters
 466 V_{cmax} and m . f_{qe} was estimated in both steps in the schemes I_{SIF} and $I_{GPP-SIF}$. Also, pattern-oriented model
 467 evaluation was used to assess the results of the different schemes. Unlike the previous work, this time

468 we increased the inversion bounds (Table 2) for C_{dm} and C_w according to observed distributions in the
469 site (Martín et al. 2019; Melendo-Vega et al. 2018). Also, since previous works found problems to
470 cover the range of R in the near infrared, C_s upper bound was raised up to 7.5 a.u.; a value that allowed
471 covering the low R values found in dry periods in the ecosystem (Martín et al. 2019). The multiple
472 constraint inversion approach proposed in Pacheco-Labrador et al. (2019) provided coherent parameter
473 estimates when GPP constrained the inversion (I_{GPP} and $I_{GPP-SIF}$) using SCOPE; however, uncertainties
474 in part related to the presence of senescent materials biased the estimation some of the parameters,
475 notably C_{ab} during the dry season. In all the cases senescent material also was suspected to induce
476 underestimation of LAI .

477 We used the same methodology to invert senSCOPE on the same datasets in order to compare the
478 results provided by both models and to understand the suitability of using senSCOPE in environments
479 featuring large fractions of senescent leaves. However, in the case of senSCOPE, 6 leaf parameters of
480 two different leaf types must be estimated (Table 2). In order limit the number of free parameters in the
481 inversion, we applied the following constraints: We assumed that green leaves presented no senescent
482 pigments ($C_s = 0$) whereas senescent leaves only presented senescent pigments ($C_{ab} = C_{ca} = 0$). We also
483 assumed that the mesophyll parameter (N) and dry matter content (C_{dm}), were the same for both types of
484 leaves, whereas that water content (C_w) of green leaves was four times higher than senescent C_w (Kidnie
485 et al. 2015). This allowed us reducing the degrees of freedom by 6. We assumed that average leaf
486 parameters (X) could be computed as a linear combination of the parameters of each leaf type (X_{green} and
487 X_{senes}) as in Eq. 21:

$$488 \quad X = X_{green} \cdot f_{green} + X_{senes} \cdot (1 - f_{green}), \quad (21)$$

489 Given the constrains imposed on leaf parameters, we could directly optimize the leaf averaged
490 parameters in the inversion, similarly as parameters are retrieved in the inversion of SCOPE (Pacheco-
491 Labrador et al. 2019). To do so, X_{green} or X_{senes} are internally calculated solving them from Eq. 21; which
492 is possible in all the cases since at least the value one of them together with f_{green} are known: Either they
493 are equal, 0, or their ratio has been prescribed. senSCOPE includes the additional parameter f_{green} ; in
494 order to reduce equifinality and as well as the number of parameters to estimate we prescribed f_{green} by

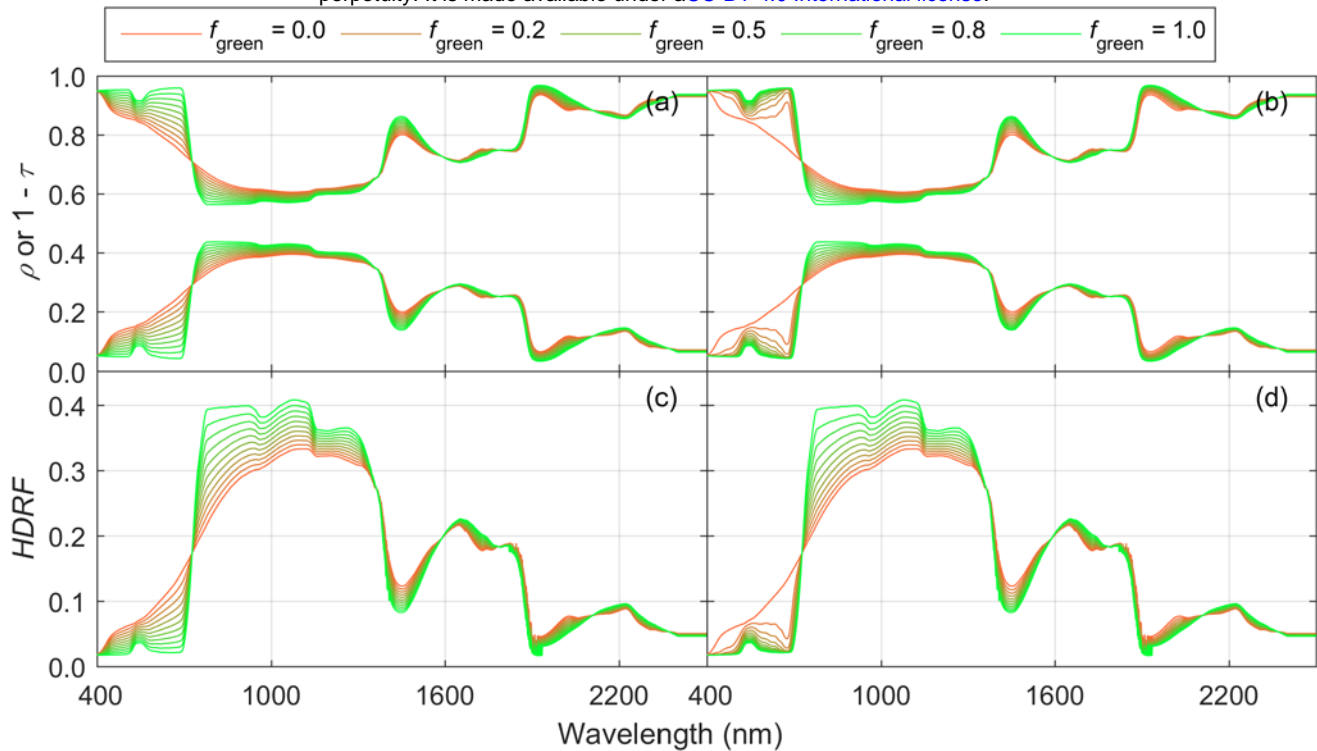
495 modelling it as a function of the averaged leaf parameters X using a Neural Network (NN). The NN was
496 trained from a look up table of individual X_{green} and X_{senes} parameters averaged as a function of f_{green} ; no
497 assumptions on N , C_w and C_{dm} were made (Appendix A). As a result, the same parameters were
498 estimated in the inversion of SCOPE and senSCOPE.

499 As in Pacheco-Labrador et al. (2019), we used pattern-oriented model evaluation approach to assess the
500 retrieval of functional parameters, which cannot be determined from individual leaf measurements in
501 the highly biodiverse grassland under study. To do so, we assessed the relationship of V_{cmax} and C_{ab}
502 against N_{mass} in the green fraction of the canopy ($N_{\text{mass,green}}$), and in the case of V_{cmax} it was compared
503 with the relationship published by Feng and Dietze (2013) for grasslands. We also evaluated model
504 performance and structure using not directly predicted fluxes, but variables derived from them such as
505 EF , which describes energy partitioning (Eq. 19). In addition, a more traditional evaluation was also
506 done assessing the goodness of the fit or prediction of model constraints (R , L_t , F_{760} , and/or GPP) and
507 observed parameters (LAI , f_{green}).

508 **4. Results**

509 **4.1 Comparison of results and performance with SCOPE model: Sensitivity analysis.**

510 For the F_{meteo} runs, green and senescent leaf properties were kept constant for the different combinations
511 of f_{green} . Fig. 3a,b show the leaf optical properties simulated with senSCOPE and SCOPE, respectively.
512 Accordingly Fig. 3c,d shows the TOC Hemispherical-Directional Reflectance Factors ($HDRF$)
513 simulated with each model at midday of DoY 139, the timestamp used for F_{veg} runs. As can be seen,
514 senSCOPE predicts spectroradiometric variables that vary more proportionally to f_{green} , whereas SCOPE
515 simulates stronger absorptions, especially in the visible region. This results from allocating all the
516 absorptive substances to a single leaf type. The largest differences between models are found in the red
517 and blue regions, where senescent leaves in senSCOPE increase scattering. We also verified that when
518 f_{green} equals 1 or 0, the output of both models is the same.

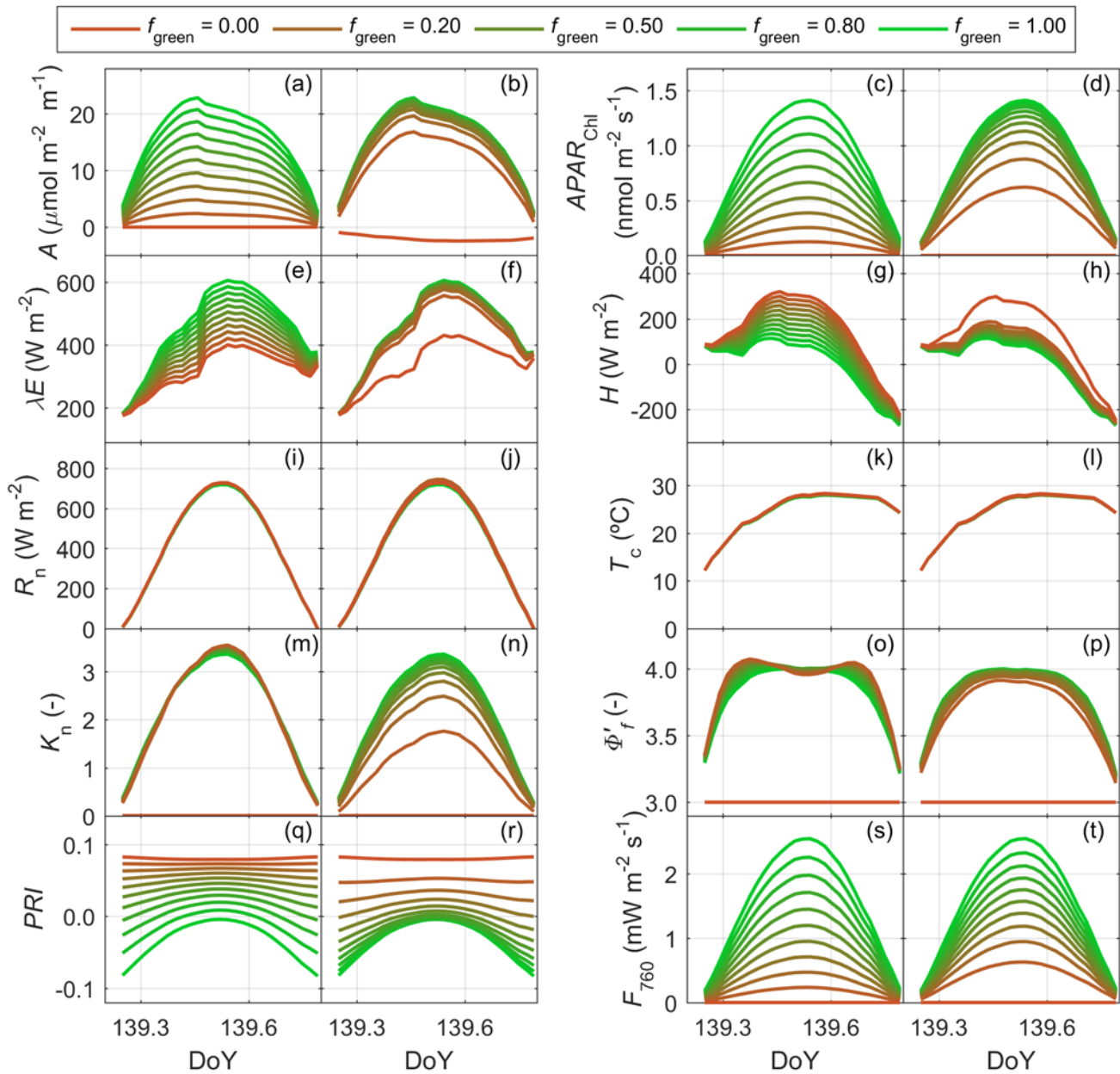


519

520 **Figure 3. Leaf reflectance and transmittance factors predicted by senSCOPE (a) and SCOPE (b); and top**
 521 **of the canopy Hemispherical Directional Reflectance Factors predicted by senSCOPE (c) and SCOPE (d)**
 522 **for different fractions of green and senescent leaves.**

523 Fig. 4 compares some of the spectroradiometric variables and fluxes predicted by senSCOPE (left semi-
 524 columns) and SCOPE (right semi-columns) during DoY 139 in the F_{meteo} runs. As can be seen, those
 525 variables that are strongly controlled by radiative transfer in the optical domain ($APAR_{\text{chl}}$ (Fig. 4c,d),
 526 the Photochemical Reflectance Index (PRI , Gamon et al, (1992)), sensitive to activation of the
 527 xanthophyll cycle (Fig. 4q,r) and F_{760} (Fig. 4s,t)) present a stronger and more linear sensitivity to f_{green} .
 528 The same is observed for the water and energy fluxes (λE (Fig. 4e,f) and H (Fig. 4g,h)). Differences for
 529 variables related with the radiative transfer of thermal radiance seem to be lower (R_n (Fig. 4i,j) and T_c
 530 (Fig. 4k,l)). senSCOPE leaves feature a higher absorption of PAR per unit green leaf area, which
 531 produces a stronger NPQ activation (K_n (Fig. 4m,n)), and a depletion of photosynthetic efficiency
 532 around midday (Φ'_f (Fig. 4o,p)) for low f_{green} (unlike the other parameters, these are only representative
 533 of green leaves). Notice that the example shown is only representative of the meteorological and

534 vegetation properties represented during DoY 139, and the differences shown should not be taken
 535 generally.

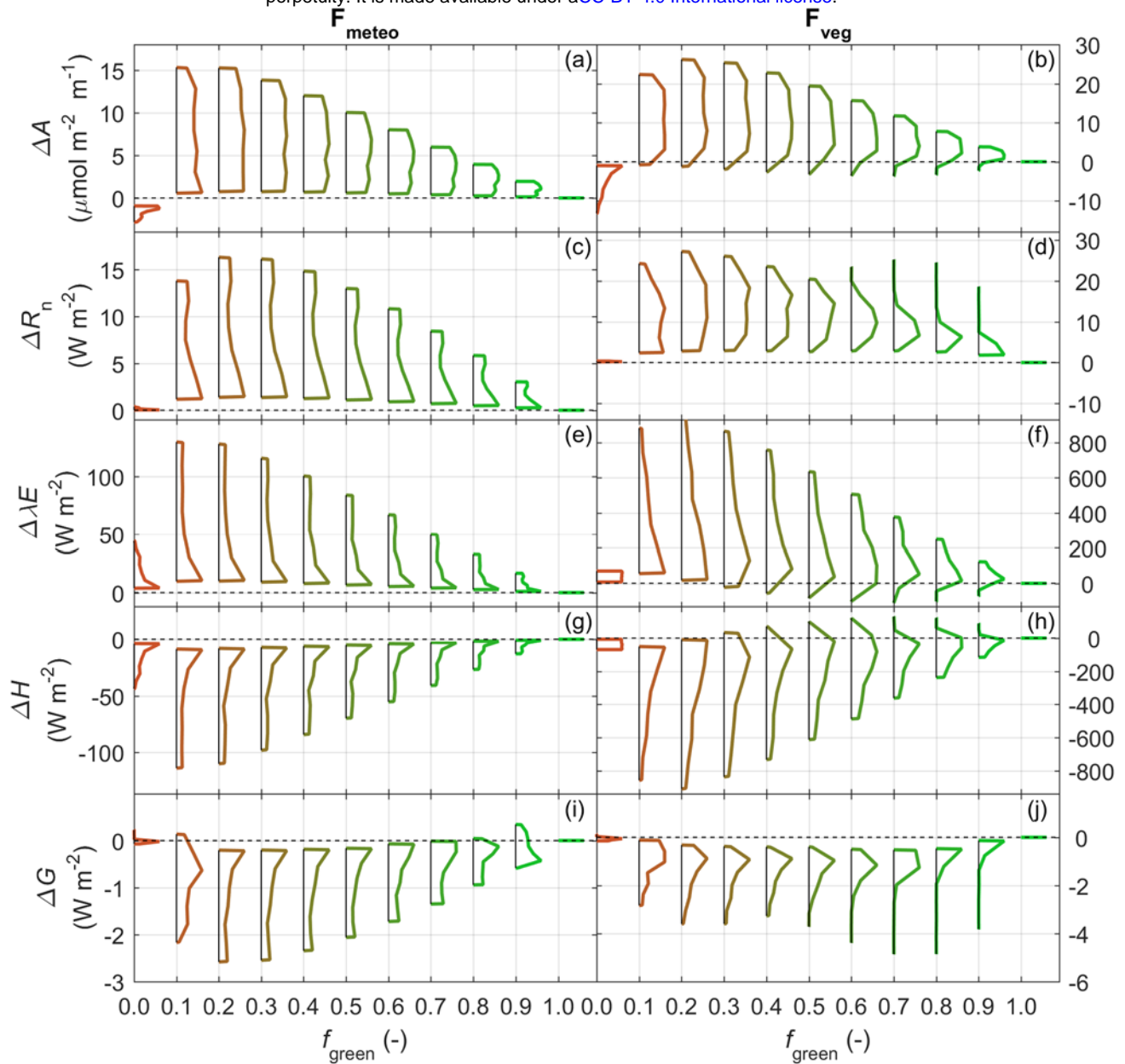


536

537 **Figure 4. Diel cycles of senSCOPE (left semi-column) and SCOPE (right semi-column) predicted variables**
 538 **on DoY 136: Assimilation (a,b), photosynthetically active radiation absorbed by chlorophylls (c,d), latent**
 539 **heat fluxes (d,e) and sensible heat fluxes (g,h), net radiation (i,j), canopy temperature (k,l), rate coefficient for non-**

540 **photochemical quenching (m,n), fluorescence efficiency (o,p), photochemical reflectance index (q,r) and**
541 **TOC fluorescence radiance at 760 nm (s,t).**

542 Fig. 5 shows the distributions of the difference between fluxes predicted by SCOPE and (minus)
543 senSCOPE for each f_{green} level. Results of the F_{meteo} and the F_{veg} simulations are shown in the left and
544 the right columns, respectively. As can be seen, both under varying meteorological conditions and
545 varying plant properties, the two models predict the same fluxes when $f_{\text{green}} = 1$, but not always when
546 $f_{\text{green}} = 0$. For $f_{\text{green}} < 1$ SCOPE predicts higher assimilation (A , Fig. 5a,b); but in the case of $f_{\text{green}} = 0$,
547 where SCOPE predicts negative A due to photorespiration, and senSCOPE represents no photosynthetic
548 leaf area. SCOPE also predicts in most of the cases higher R_n (Fig. 5c,d) and λE (Fig. 5e,f), and lower H
549 (Fig. 5g,h) and G (Fig. 5i,j).



550

551 **Figure 5. Distributions of the difference between the fluxes simulated with SCOPE and (minus) senSCOPE**
552 **in the F_{meteo} run (left column) and the F_{veg} run (right column) for different fractions of green leaf area:**
553 **assimilation (a,b), net radiation (c,d), latent heat flux (e,f), sensible heat flux (g,h) and soil heat flux (i,j).**

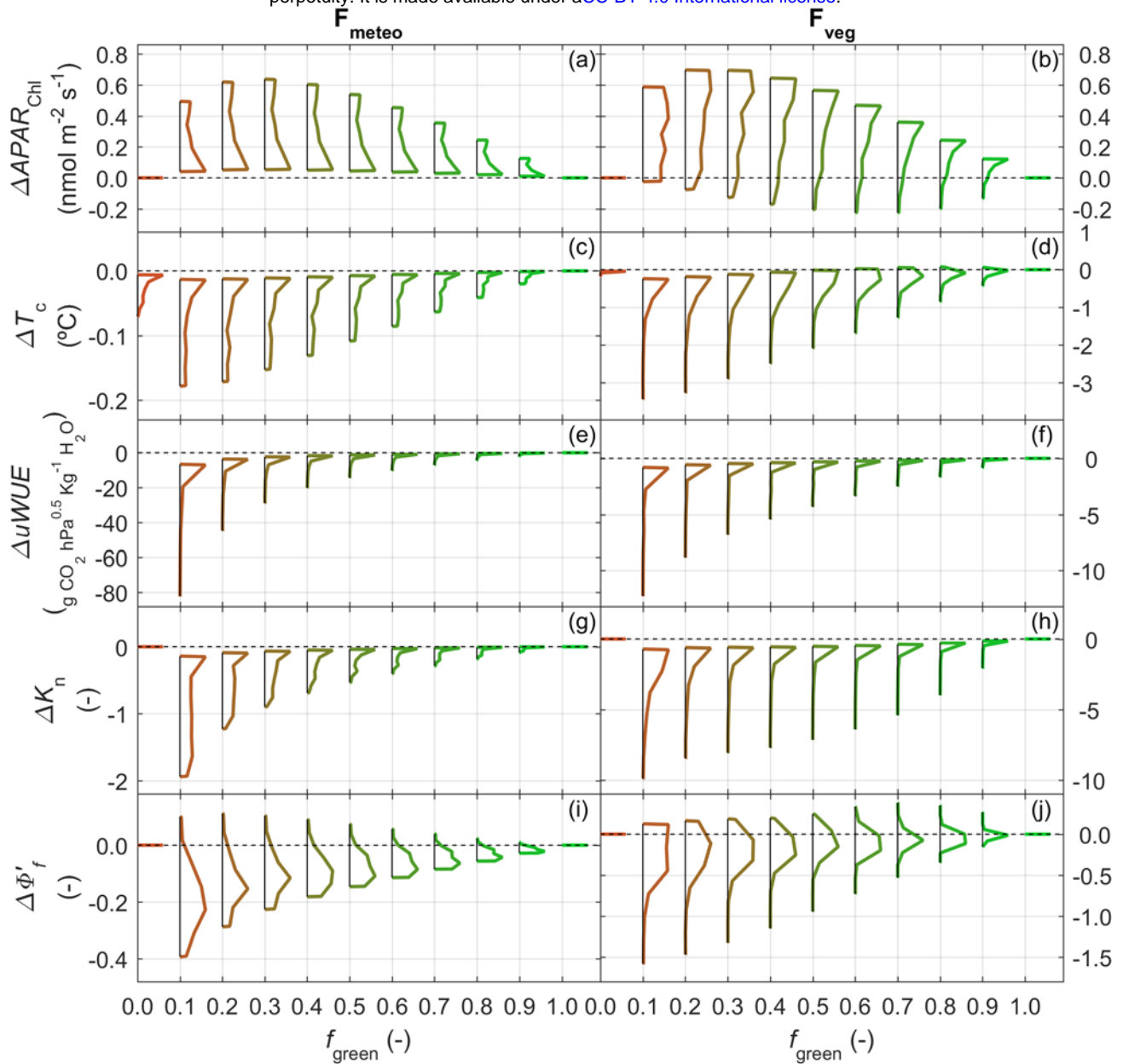
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555

556 Differences between predicted fluxes usually maximize when C_{ab} and LAI increase (Fig. S1a-e and S2
557 a-e, respectively). G (and R_n) also present large differences for low values of these parameters and mid
558 f_{green} . In the analysis of the forward runs, the differences observed from F_{veg} simulations are often larger
559 than those F_{meteo} simulations since the variability in the meteorological variables is -in relative terms-
560 lower than the variability simulated for the vegetation properties.

561 For each f_{green} level, Fig. 6 presents the distribution of the difference between variables related to leaf
562 function, as predicted by SCOPE and (minus) senSCOPE. Results of F_{meteo} and F_{veg} are shown on the
563 left and the right columns, respectively. Similar to the fluxes, these variables are integrated according to
564 LAI and the probability of each sunlit and shaded leaf angle. $APAR_{Chl}$ (Fig. 6a,b) is equal for both
565 models when the canopy is totally green or senescent. For the rest of the cases SCOPE predicts higher
566 $APAR_{Chl}$, except some cases when $C_{ab} < 10 \mu g cm^{-2}$ (not shown). senSCOPE predicts higher canopy
567 temperature (T_c , Fig. 6c,d) than SCOPE; the largest differences are found when C_{ab} is high (Fig. S1g),
568 or when LAI is low (Fig. S2g). Similarly, $uWUE$ (Fig. 6e,f) is higher for senSCOPE, but unlike T_c and
569 most of the variables compared, differences in $uWUE$ are more strongly controlled by meteorological
570 conditions than by vegetation parameters. The largest differences in $uWUE$ are found under cold
571 conditions with $VPD < 5$ hPa (not shown). senSCOPE presents also higher K_n (Fig. 6g,h). Differences
572 between models predictions increase with LAI (Fig. S2i), and decrease with C_{ab} (Fig. S1i). Φ'_f (Fig. 5i,j)
573 is most often higher for senSCOPE than for SCOPE, especially if LAI is high and C_{ab} is low (not
574 shown). On the other hand, SCOPE predicts higher Φ'_f when LAI is low (Fig. S2j) or when C_{ab} is low
575 and LAI is moderate (Fig. S1j). As expected, both models predict the same values for these variables
576 when $f_{green} = 1$.

577

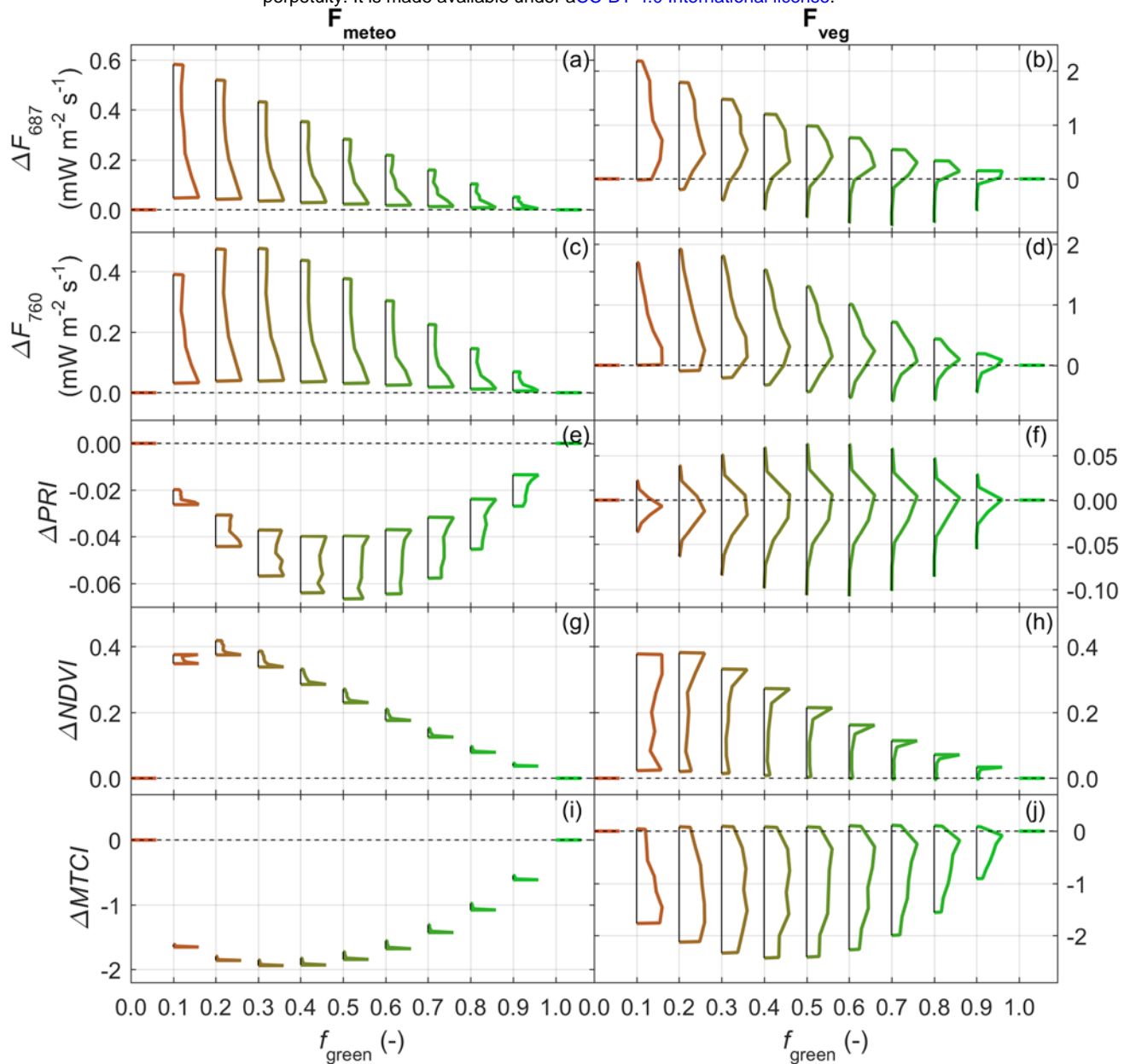


578

579 **Figure 6. Distributions of the difference between variables indicative of plant physiology simulated with**
 580 **SCOPE and (minus) senSCOPE in the F_{meteo} run (left column) and the F_{veg} run (right column) for different**
 581 **fractions of green leaf area: photosynthetically active radiation absorbed by chlorophylls (a,b), canopy**
 582 **temperature (c,d), underlying water use efficiency (e,f), rate coefficient for non-photochemical quenching**
 583 **(g,h) and fluorescence efficiency (i,j).**

584 Fig. 7 shows the distribution of some TOC spectroradiometric variables predicted by SCOPE and
585 (minus) senSCOPE for each f_{green} level. Results of the F_{meteo} and the F_{veg} simulations are presented in the
586 left and the right columns, respectively. F_{687} (Fig. 7a,b) and F_{760} (Fig. 7c,d) are larger for SCOPE in
587 most of the cases; the largest differences are found for low f_{green} and large C_{ab} (Fig. S1k,l) and
588 LAI (Fig. S2k,l). Differences in PRI are negative for F_{meteo} , but of both signs for F_{veg} (Fig. 7e,f). In
589 this case, the influence of vegetation parameters is more complex and less linear than in other variables;
590 since it depends on the combination of C_{ab} and C_{ca} , their ratio and LAI (not shown). A similar analysis
591 carried out on the PRI computed from reflectance factors where the effect of the xanthophyll cycle is
592 not simulated reveals that differences between models rather respond to biophysical properties than to
593 differences in function (not shown). Two more spectral indices responsive to pigments content and
594 canopy structure are also analysed. Fig. 7g,h presents the differences for the Normalized Difference
595 Vegetation Index ($NDVI$, Rouse et al, (1974)); Fig. 7i,j present differences for the MERIS Terrestrial
596 Chlorophyll Index ($MTCI$, Dash and Curran (2007)); senSCOPE predicts lower and higher values,
597 respectively. For these indices, the absolute difference between models increase as f_{green} decreases, and
598 as C_{ab} and LAI increase (Fig. S1n,o and S2n,o, respectively).

599

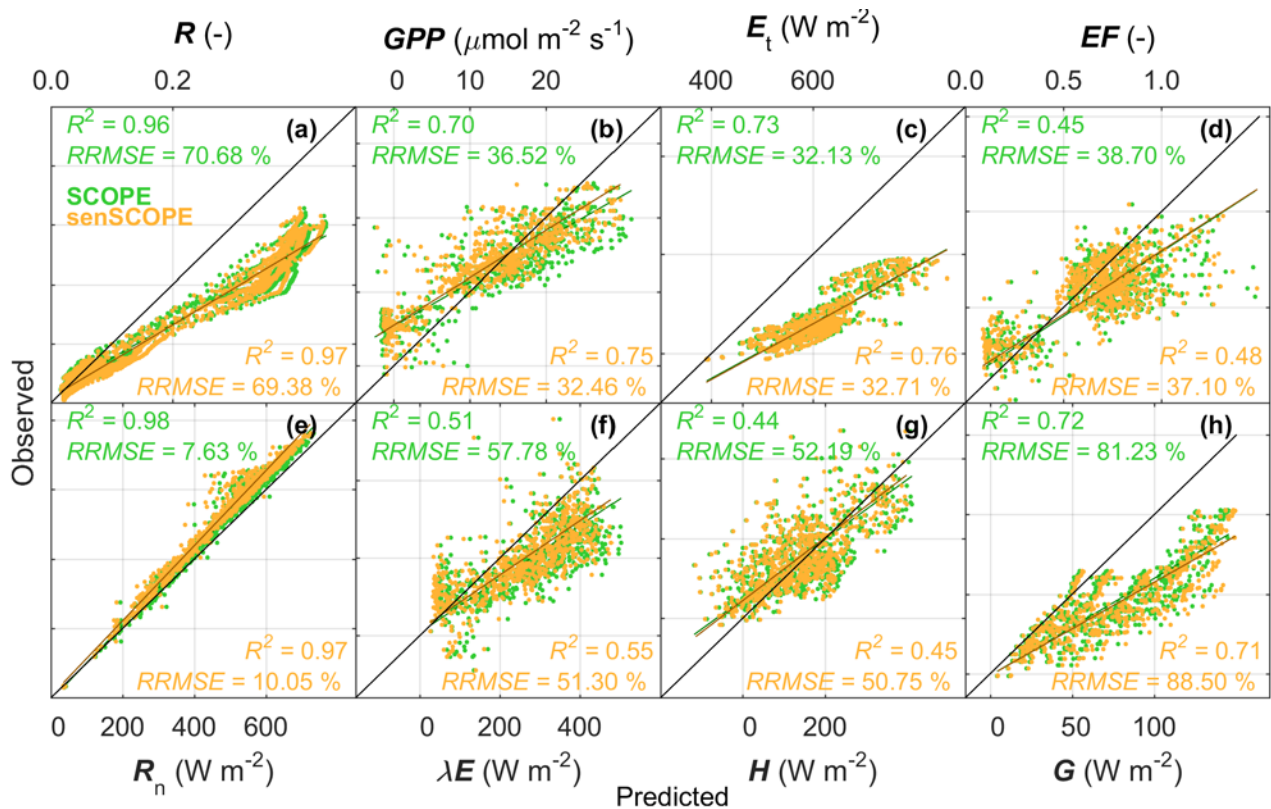


600

601 **Figure 7. Distributions of the difference between spectral variables indicative of plant physiology,**
 602 **structure and biochemical composition simulated with SCOPE and senSCOPE in the F_{meteo} run (left**
 603 **column) and the F_{veg} run (right column) for different fractions of green leaf area: TOC fluorescence**
 604 **radiance at 687 nm (a,b), TOC fluorescence radiance at 760 nm (c,d), photochemical reflectance index**
 605 **including effects of xanthophyll cycle (e,f), normalized difference vegetation index (g,h) MERIS terrestrial**
 606 **chlorophyll index (i,j).**

607 4.2 Comparison with SCOPE model. Forward simulation with observational datasets

608 Fig. 8 compares the different variables predicted by SCOPE and senSCOPE vs. the fluxes measured by
 609 the EC towers and R acquired by the airborne hyperspectral imager in the site of Majadas de Tiétar. The
 610 comparison is done using Total Least Squares (Golub and Loan 1980). In general, senSCOPE achieves
 611 higher coefficients of determination (R^2) and lower relative root mean squared errors ($RRMSE$). Both
 612 models overestimate high R (Fig. 8a), and GPP (Fig. 8b); but senSCOPE is less deviated. SCOPE
 613 overestimates λE and EF , and underestimates H more than senSCOPE. Both models predict R_n quite
 614 accurately and precisely; but senSCOPE predicts R_n , E_t and G with slightly larger errors and in some
 615 cases lower R^2 than SCOPE.

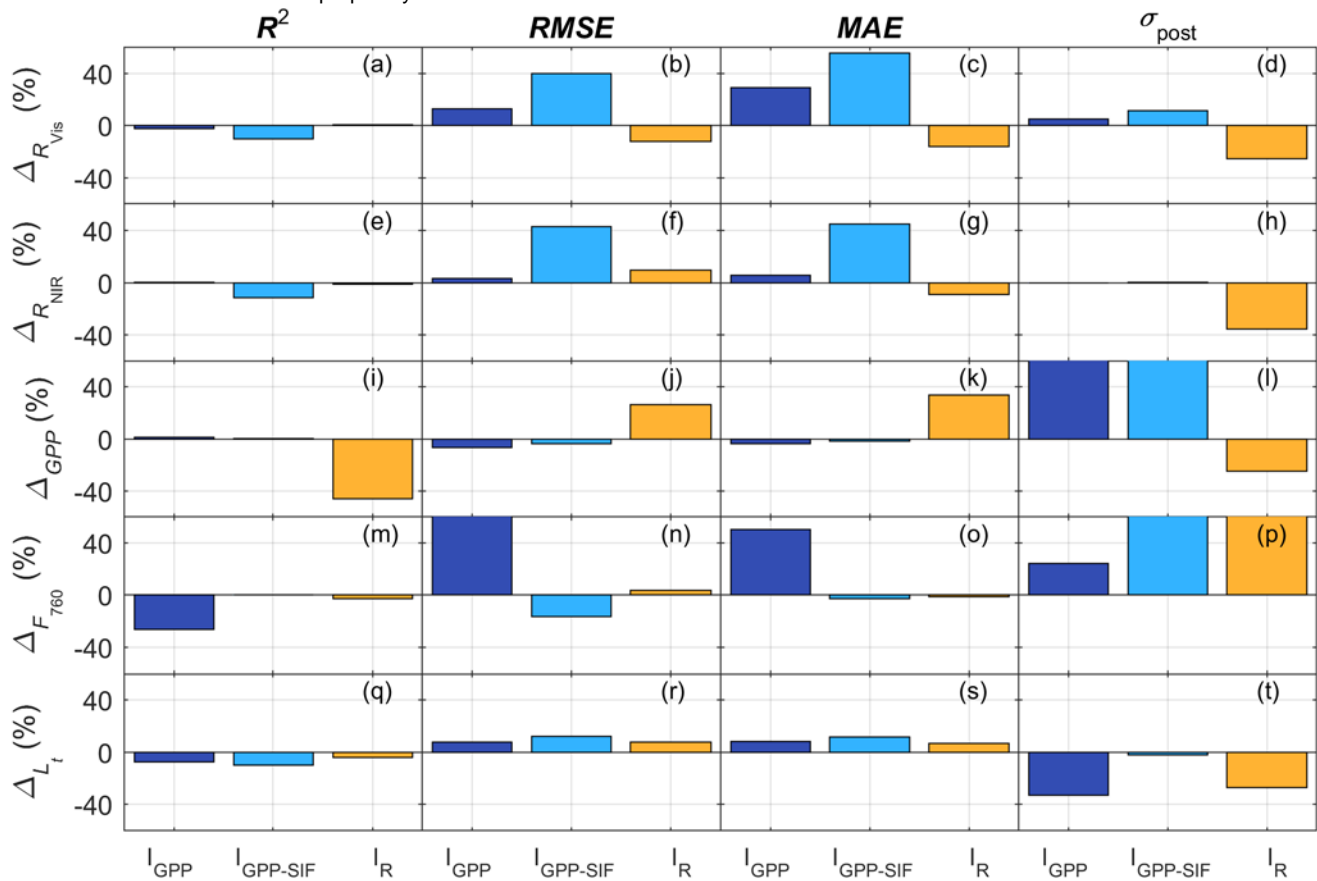


616

617 **Figure 8. Comparison of observed and predicted fluxes and reflectance factors at ecosystem scale.**
 618 **Predictions are done by SCOPE (green) and senSCOPE (orange) using field observations or estimates of**
 619 **vegetation properties, as well as forcing variables measured at the research station of Majadas de Tiétar**
 620 **± 1 day around different airborne campaigns.**

621 **4.3 Comparison with SCOPE model. Inversion on observational datasets**

622 Fig. 9 summarizes the capability of SCOPE and senSCOPE to fit/predict the variables used as inversion
623 constraints in the different schemes tested; notice that not all the constraints are used to optimize
624 parameters in all the schemes. The relative differences between the statistics of the fit are calculated as
625 $(100 \cdot (x_{\text{senSCOPE}} - x_{\text{SCOPE}}) / x_{\text{SCOPE}})$; where x is the statistic and the respective model is presented in the
626 subscript. R^2 is estimated using Total Least Squares (Golub and Loan 1980), and the relative root mean
627 squared error ($RRMSE$) and mean average error (MAE) result of the comparison of the
628 observed/predicted values. Posterior uncertainty (σ_{post}) is estimated according to Omlin and Reichter
629 (1999). The relative differences of R in the visible spectral region (R_{vis} , Fig. 9a-d) and the near infrared
630 (R_{NIR} , Fig. 9e-h), GPP (Fig. 9i-l), F_{760} (Fig. 9m-p) and L_t (Fig. 9q-t) are presented for the three different
631 inversion schemes tested. R is used in all the inversion schemes. senSCOPE fits R_{vis} and R_{NIR} more
632 poorly than SCOPE in the schemes I_{GPP} and $I_{\text{GPP-SIF}}$; whereas in the case of I_{R} senSCOPE these are
633 better fit and posterior uncertainties are lower than for SCOPE. senSCOPE slightly improves the fit of
634 GPP when this is a constraint of the inversion; however, σ_{post} almost duplicate (values ~80%, out of the
635 plot scale). As in Pacheco-Labrador et al., (2019) I_{R} fails to accurately fit GPP , but σ_{post} is lower for
636 senSCOPE. senSCOPE fit of F_{760} improves respect to SCOPE when this is a constraint of the inversion
637 ($I_{\text{GPP-SIF}}$), but σ_{post} increase in all the cases. senSCOPE fits L_t more poorly than SCOPE, but σ_{post}
638 decrease in all the cases.

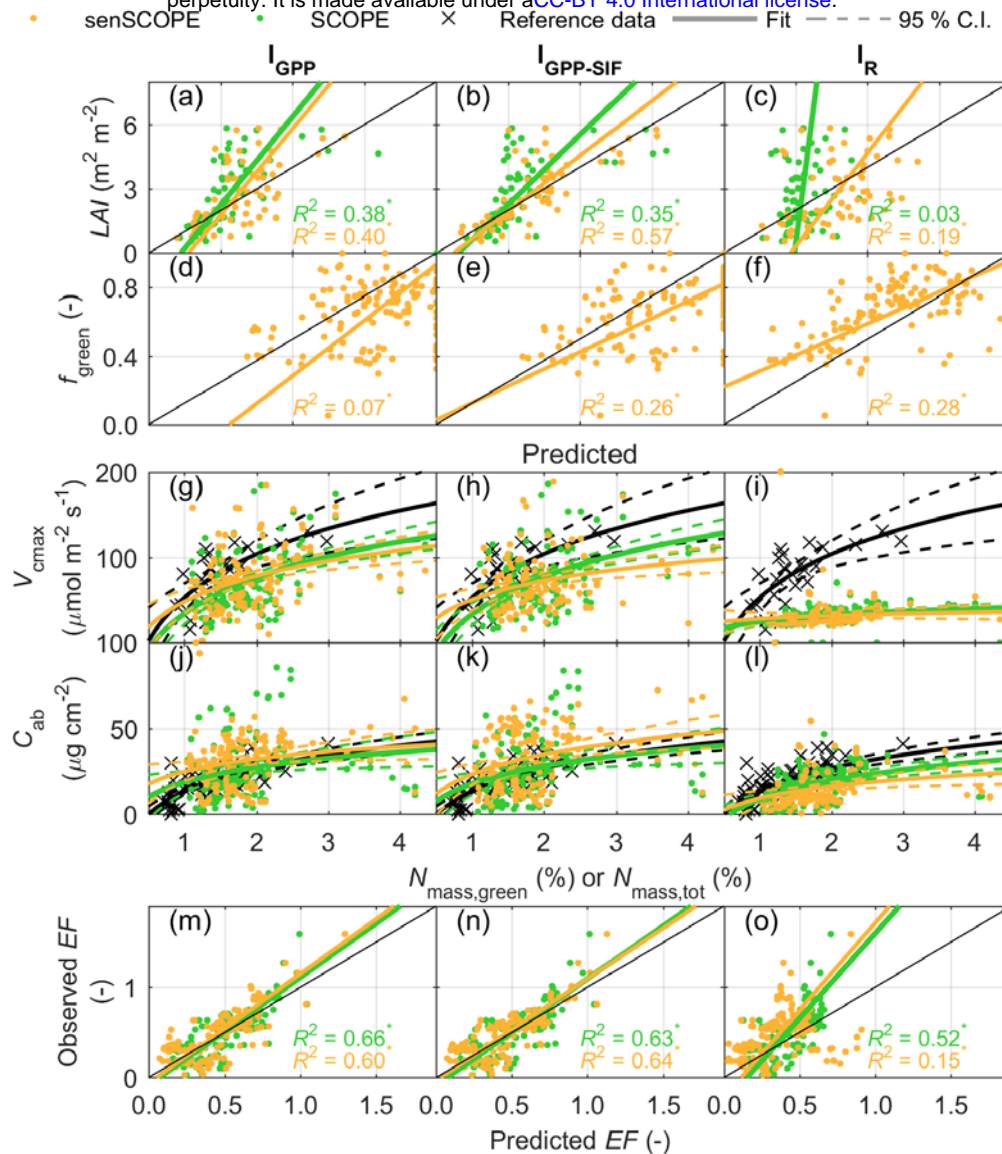


639

640 **Figure 9. Relative difference between the fit/prediction statistics of the inversion constraints obtained by**
 641 **senSCOPE and SCOPE for the different inversion schemes.**

642 Fig. 10 compares the most relevant model parameters estimated by SCOPE and senSCOPE for the
 643 different inversion schemes tested (presented by columns, from left to right: I_{GPP} , $I_{GPP-SIF}$, I_R).
 644 Parameters are evaluated both using field observations and pattern-oriented model evaluation approach.
 645 LAI (Fig. 10a-c) and f_{green} (Fig. 10d-f) are compared against observations using Total Least Squares
 646 (Golub and Loan 1980). As can be seen, senSCOPE predicts similar LAI values but show higher R^2 and
 647 significance. senSCOPE is also capable of providing reasonable estimates of f_{green} , these are often
 648 overestimated but still within the bounds of the relationship $C_{ab} \cdot f_{green}$ observed in the site (Fig. S3).
 649 $N_{mass,green}$ is used to evaluate V_{cmax} (Fig. 10g-i) and to compare the relationship between both variables
 650 with the one reported in the literature for grasslands (Feng and Dietze 2013). Notice that senSCOPE

651 V_{cmax} is provided per unit green leaf area and is thus comparable with SCOPE estimates and the
652 literature data. Results are coherent with those presented in Pacheco-Labrador et al., (2019), I_{R} fails to
653 constrain V_{cmax} , whereas the schemes using GPP provide relationships with $N_{\text{mass,green}}$ which are closer
654 to those in the literature. V_{cmax} estimates are very similar for both models in I_{GPP} ; however, the use of
655 F_{760} in $I_{\text{GPP-SIF}}$ seems to slightly deviate the adjusted logarithmic model from the one fit to the data in
656 Feng and Dietze (2013). Similarly, C_{ab} (per total leaf area) is evaluated against N_{mass} of the whole
657 canopy (Fig. 10j-l), and their relationship is compared with field observations of both variables in the
658 site of Majadas de Tiétar. When GPP constrains the inversion senSCOPE and SCOPE estimates are
659 similar and follow the relationship observed in the field. However, as in Pacheco-Labrador et al.,
660 (2019), SCOPE I_{GPP} and $I_{\text{GPP-SIF}}$ estimates present high values during the dry period, which stand out of
661 the relationship with N_{mass} between 0.5-1.3 %. senSCOPE corrects most of these values, especially in
662 the scheme I_{GPP} ; while the scheme $I_{\text{GPP-SIF}}$ still preserves some of these high values. Fig. 10m-o
663 compares predicted and observed EF using Total Least Squares (Golub and Loan 1980). In general,
664 both models achieve similar results when GPP constrains the inversion; however, senSCOPE R^2 are
665 lower than in SCOPE. As in Pacheco-Labrador et al., (2019), I_{R} fails to constrain functional parameters.



666

667 **Figure 10. Summary of the parameters' evaluation using observations and pattern-oriented model**
 668 **evaluation for the four inversion schemes tested. Leaf area index, (a-c) and green fraction of leaf surface**
 669 **(d-f), and evaporative fraction (q-t) are compared with field observation using Total Least Squares (Golub**
 670 **and Loan 1980). Significance is described with the symbols ' for p -values $0.05 \leq p < 0.10$; and * for $p < 0.05$.**
 671 **The 1:1 line is shown in black. Maximum carboxylation rate (g-i) and chlorophyll concentration (j-p) are**
 672 **evaluated against nitrogen content in green leaves and total nitrogen content, respectively and compared**
 673 **with data from the literature (Feng and Dietze 2013) the first, and relationships observed in the field, the**
 674 **second A logarithmic relationship is fit in both cases, the 95 % confidence interval is show with dashed**
 675 **lines.**

676 5. Discussion

677 This manuscript describes and evaluates senSCOPE, a version of the model SCOPE representing
678 separately radiative transfer and physiological processes of green and senescent leaves; which is
679 relevant in canopies featuring important senescent leaf area fractions. senSCOPE is evaluated against
680 SCOPE 1) by direct comparison of forward synthetic simulations, 2) by comparison of simulated and
681 observed ecosystem-scale fluxes and reflectance factors, and 3) by evaluation of parameter estimates
682 and predicted variables via inversion of the models against a comprehensive dataset including
683 hyperspectral optical R , as well as GPP , SIF and TIR radiance. These data were collected in a
684 fertilization experiment with varying nitrogen and phosphorous additions and degrees of water stress.
685 Results show that in senescent canopies senSCOPE improves the forward modelling of radiative
686 transfer, photosynthesis and fluxes; and that in inversion -if suitably constrained-, it improves the
687 estimation of C_{ab} . At the same time, the performance of both models is comparable when green leaves
688 dominate.

689 senSCOPE distributes senescent and remaining pigments in two conceptual leaves (green and
690 senescent) and predicts separately their respective optical properties, which are later combined. This
691 approach was already proposed by Bach et al., (2001) and used in later works (Bach and Verhoef 2003;
692 Houborg et al. 2009; Houborg et al. 2015; Houborg and McCabe 2016; Verhoef and Bach 2003). This
693 dual-leaf approach generates averaged “brighter” leaves since not all the absorbent species are located
694 in the same leaf (Fig. 3). This has relevant consequences for the canopy-RTM, especially in those
695 spectral regions where senescent and the rest of the pigments overlap, and therefore for $APAR_{Chl}$.
696 senSCOPE produces reflectance factors and $APAR_{Chl}$ that close-to-linearly vary with f_{green} ; whereas in
697 the case of SCOPE, these variables vary logarithmically with f_{green} since leaves absorptivity saturate due
698 to the large presence of pigments. This saturation, combined with the fact that R_{NIR} was overestimated
699 during senescence, led to unrealistically high C_{ab} estimates during the dry period when a strong
700 functional constraint $-GPP-$ was used (Pacheco-Labrador et al. 2019). Notice that only the constraint
701 GPP provided robust estimates of functional parameters. In the present work, we repeated the inversion
702 of SCOPE allowing higher C_s than in Pacheco-Labrador (2019) since this allowed predicting low R_{NIR}

703 values observed in the site (Martín et al. 2019). This approach improved the fit of R_{NIR} for all inversion
704 schemes during SCOPE inversion (not shown), but did not solve the overestimation of C_{ab} in the most
705 strongly constrained schemes (I_{GPP} and $I_{\text{GPP-SIF}}$, Fig. 10a,b). senSCOPE fitted less precisely the
706 inversion constraints, and in some cases posterior uncertainties increased due to the strong control that
707 f_{green} has on most of the model outputs (Fig. 9). For I_{R} senSCOPE improved the fit of R , but the opposite
708 occurred when $a\text{PAR}$ was constrained by GPP , suggesting that the model might not still represent
709 accurately the observed grassland. However, senSCOPE led to C_{ab} values more soundly related with
710 N_{mass} than SCOPE during the dry season (schemes I_{GPP} and $I_{\text{GPP-SIF}}$, Fig. 10j,k).

711 The fact that senSCOPE limits photosynthesis and transpiration to the green fraction results in a close-
712 to-linear relation between f_{green} on the one hand, and A and λE on the other hand (Fig. 4 and 5). SCOPE
713 predicts higher assimilation and transpiration unless f_{green} is very low (~ 0); in that case A is negative
714 while λE is still high. Contrarily, R_{n} and G predictions are similar for both models; also, differences in H
715 are lower than for λE , but still in senSCOPE H varies more linearly with f_{green} than in SCOPE (notice
716 that f_{green} is not a SCOPE parameter, but is used to average leaf parameters). In the forward simulation at
717 ecosystem scale senSCOPE predicted most of the ecosystem fluxes better than SCOPE (Fig. 8). In this
718 case we assumed a fixed value for m , which might be not completely realistic; however additional
719 works at ecosystem scale have shown that senSCOPE can more robustly represent water use efficiency
720 than SCOPE (not shown). In the inversion at plot level, senSCOPE predicted GPP better than SCOPE
721 when used as constraint (Fig. 9k-o). In contrast, EF was predicted more poorly in all the schemes.
722 senSCOPE assumes no transpiration from senescent leaves; however evaporation from their surface
723 might be relevant when these are moisturized by dew or rainfall. Neither SCOPE nor senSCOPE
724 represent that process and their use after such situations might result uncertain.

725 In inversion, both SCOPE and senSCOPE underestimated LAI , while senSCOPE overestimated f_{green}
726 (Fig. 10a-h). As discussed in Pacheco-Labrador et al, (2019) and Melendo-Vega (2018), the optical
727 properties of dry standing material might not be accurately described by RTM, leading to an
728 overestimation of R_{NIR} , which seems to be counter-weighted in inversion by reducing LAI . In fact,
729 inversion schemes using GPP (I_{GPP} and $I_{\text{GPP-SIF}}$) improved the estimation of LAI since GPP demands

730 higher $APAR_{Chl}$ in exchange for increasing the fitting error of R_{NIR} (Pacheco-Labrador et al., (2019), this
731 work). In senSCOPE, underestimation of LAI was also compensated also by overestimating f_{green} . These
732 facts suggest that the optical properties of the senescent material and/or the death standing material of
733 this grassland (and likely other ecosystems) are not accurately represented, leading to biased estimates
734 of some of the parameters. In fact, it was necessary increasing the upper bound of C_s to be able to
735 predict low R_{NIR} in the dry season. We allowed C_s up to 7.5; whereas values up to 5.0 are reported in
736 literature (Houborg and Anderson 2009). Too high C_s might have led to unrealistic representation of ρ
737 and τ of senescent leaves, very dark in the visible region but also with low R_{NIR} . In some cases SCOPE
738 estimated $C_s = 7.5$, whereas senSCOPE predicted $C_s < 5$ in most of the cases (Fig. S4c). Apart from
739 LAI , C_{dm} and C_w , -which are weakly constrained because the spectroradiometric measurements did not
740 include the short wave infrared range (SWIR)-, might have been affected by this problem. SCOPE and
741 senSCOPE estimates of C_{dm} often hit the upper bound established from observations in the field. High
742 C_{dm} also serves to reduce R_{NIR} . In contrast, senSCOPE C_w estimates are less often saturated; C_w has
743 little effect below 970 nm, but influences leaf optical properties in the SWIR. The relationship between
744 N , C_{dm} and C_w of green and senescent leaves assumed during inversion might have contributed to
745 increase the uncertainty of the parameter estimates; for example, it has been observed that leaf thickness
746 decreases during senescence (Castro and Sanchez-Azofeifa 2008); whereas other works assign high N
747 values to senescent leaves (Houborg et al. 2009). However, a balance between model error and
748 equifinality must be also observed. Site-specific relationships between the parameters of each leaf type
749 or relationships found in global databases could be used in the future to improve the representation of
750 semi-arid canopies. senSCOPE does not include improved calibrated absorption coefficients or
751 refractive indices to more realistically represent senescent leaves and death standing material, but it
752 offers a formally more correct representation of mixed canopies. The model improves the representation
753 of these canopies, which could be used in the future to calibrate or validate specific absorption spectra
754 of senescent material. senSCOPE can also be applied to other canopies, such as crops and forests, which
755 are characterized a senescent stage. Moreover, the approach adopted in senSCOPE could be similarly
756 used to represent other mixed canopies combining plants with different biophysical properties and
757 function, such as C3 and C4 species. An additional problem for the representation of mixed canopies

758 would be the vertical distribution of the senescent material. The impact on the observed R and fluxes is
759 unclear, and further research is needed in this direction. In such studies, senSCOPE could also be
760 extended to other versions of SCOPE, such as mSCOPE (Yang et al. 2017) to describe the vertical
761 distribution of senescent matter.

762 f_{green} is a critical parameter in senSCOPE, it strongly controls RTM and fluxes and increases equifinality
763 of the inverse problem. Thus, the use of prior information about this variable is strongly
764 recommended during inversion. For this reason, in this work f_{green} was indirectly predicted from leaf
765 parameter estimates using a NN while the model was inverted. The design of this model was critical to
766 achieve acceptable results, and during training C_{ab} (and C_{ca}) had to be limited to the ranges observed in
767 the study site (up to $\sim 40 \mu\text{g cm}^{-2}$). During inversion higher C_{ab} values were allowed, but still, $C_{\text{ab}} \cdot f_{\text{green}}$
768 estimates stood within or very close to the bounds observed and used to train the NN (Fig. S3)

769 As a result of the combination of changes in RTM and photosynthesis, not only carbon and water
770 fluxes, but also photosynthetic efficiency and downregulation resulted modified (Fig. 6). On one side,
771 senSCOPE tends to predict higher canopy temperatures than SCOPE, especially when f_{green} decreases.
772 Senescent leaves are warmer than green leaves, but senSCOPE green leaves are not necessarily cooler
773 than SCOPE leaves (not shown). Leaf temperature strongly influences photosynthetic efficiency and
774 together with $APAR_{\text{Chl}}$ on photosynthesis down-regulation. Fig. 4m,h show how senSCOPE diel cycles
775 of K_n reach higher midday values than SCOPE. SCOPE predicts larger variability of K_n as a function of
776 f_{green} under conditions of low illumination, whereas senSCOPE K_n varies more strongly with f_{green} under
777 high temperature and irradiance conditions (not shown). Non-photochemical quenching has also
778 different effects on the predicted Φ'_f . For example, Fig. 4o,p show how senSCOPE predicts a decrease
779 of this efficiency at midday whereas this is hardly noticeable for SCOPE. K_n and Φ'_f are fundamental
780 variables to mechanistically interpret SIF signals to determine functional status of vegetation and stress
781 (Frankenberg and Berry 2018; Porcar-Castell et al. 2014). Thus considering the differences shown, both
782 models can lead to very different interpretations. Adequate representation of physiological processes
783 and their drivers is fundamental to mechanistically interpret these signals; but also the representation of
784 the spectral variables used to obtain information about these processes, such as fluorescence radiance or

785 *PRI*. Similarly as *R*, spectral indices vary more linearly with f_{green} in senSCOPE than in SCOPE (e.g.,
786 Fig. 4q,r). Unlike other spectroradiometric variables, *PRI* show no clear differences between models
787 (e.g. distributions of the difference centre around 0). *PRI* is known to result sensitive to pigments pool,
788 ratio and to *LAI* (Gamon and Berry 2012; Garbulsy et al. 2011); results of this work also show that this
789 index is also strongly sensitive to the presence of senescent material. The magnitude of SIF emissions is
790 also modified by senSCOPE, which tends to predict less SIF when f_{green} decreases, (Fig. 7a-d).

791 In this study we compare the inversion of SCOPE and senSCOPE using the data and approaches of in
792 Pacheco-Labrador et al, (2019), but allowing for higher values for C_s (as well as C_{dm} and C_w). The
793 wider parameter bounds did not change significantly the results obtained with SCOPE, and differences
794 were mainly related to the use of senSCOPE; which improved the estimation of C_{ab} in the dry season.
795 As with SCOPE, SIF (not shown) and *R* failed to constrain functional parameters (e.g., V_{cmax}) and *LAI*;
796 and only inversion schemes relying on *GPP* provided robust estimates. However with senSCOPE, the
797 schemes relying on SIF reduced their performance respect to SCOPE. $I_{\text{GPP-SIF}}$ fitted the inversion
798 constraints more poorly, and could not correct high C_{ab} estimates during senescence as much as I_{GPP} .
799 This might be result from the use of large C_s , which suggests further work is needed to more accurately
800 characterize the optical properties of death standing and senescent material. Also for senSCOPE,
801 functional parameters resulted insensitive to I_R constraints (partly due to inversion method, see
802 Pacheco-Labrador et al, (2019)). Bayat et al., (2018) inverted SCOPE using *R* and found troubles to
803 predict low *GPP* and λE in a grassland during senescence, which was corrected constraining the model
804 with *R* and TIR radiance to reduce V_{cmax} during this period. Fig. 10i-l compares V_{cmax} estimates of both
805 models; for senSCOPE V_{cmax} is presented respect to green leaf area, whereas in SCOPE, it is presented
806 respect to total leaf area (all considered “green”). As can be seen, when adequately constrained
807 estimates of both models are comparable. In senSCOPE *GPP* scales with f_{green} , and V_{cmax} (in the green
808 leaves) does not need to decrease to predict low assimilation.

809 senSCOPE is computationally more demanding (around 10% slower) than SCOPE since more
810 processes and calculations are needed, and more iterations are required to close the energy balance
811 (Table S5). However, senSCOPE seems more robust and provides lower energy balance closure error.

812 Since performance of both models is similar for large f_{green} , both models can be alternately used through
813 the season according the presence of senescent material.

814 **6. Conclusions**

815 The combination of advanced radiative transfer models with models representing exchanges of matter
816 and energy between vegetation, soil and atmosphere is bringing new opportunities to improve our
817 understanding of ecosystem function from remote observations. For example, the model SCOPE is
818 being used in the last years with this purpose. However, the accuracy with which these models represent
819 reality limits their application; and ecosystem-specific features can bias results and their interpretation.
820 In this context, we present the model senSCOPE; which adapts SCOPE radiative transfer, energy
821 balance, photosynthesis and transpiration in homogeneous canopies with mixed green and dry leaves.
822 The separated representation of green and senescent leaves significantly modifies the simulation of
823 fluxes and spectra signals respect to a model featuring a single leaf with “averaged” properties.
824 senSCOPE reflectance factors, carbon assimilation and water and energy fluxes linearly scale with f_{green} ;
825 it also improves the prediction of these variables in forward simulations as well as the estimation of
826 vegetation parameters, notably C_{ab} , during the dry season. This is significant for the remote sensing of
827 vegetation function of semi-arid ecosystems, and potentially for phenology monitoring. Despite the
828 improvements, results suggest that not only model structure needs to be corrected; a more accurate
829 characterization of the optical properties of senescent material in grasslands is still needed. The use of
830 SCOPE and derived models is growing in the remote sensing community; however, further assessment
831 of their performance to inform about plant function should be tested in different ecosystems. For
832 example, the role of vertical and horizontal heterogeneity is still unclear. Robust evaluation, e.g.
833 pattern-oriented model evaluation approach, would contribute to identify caveats and ecosystem-
834 specific features that prevent accurate monitoring of their function; and that therefore, should be also
835 represented.

836 **Appendix A: Green fraction Neural Network predictor**

837 In senSCOPE inversion, the fraction of green leaf area in the canopy (f_{green}) is estimated as a function of
838 the canopy averaged leaf RTM parameters using a NN model trained from simulated data. Latin
839 Hypercube Sampling was used to generate a look-up table (LUT) with 5000 samples of different leaf
840 constituents (C_{ab} , C_{ant} , C_{dm} , C_{w} , C_{s}), N and f_{green} . C_{ca} was included in the LUT as a function of C_{ab}
841 according to the relationship reported in Sims and Gamon (2002), and an uncertainty estimated in the
842 relationship of $\sim 4.5 \mu\text{g cm}^{-2}$ according to field measurements was used to add Gaussian noise. The same
843 bounds that were applied in inversion (Section 3.3.2) were used to design the LUTs; however C_{ab} and
844 C_{ca} of green leaves were limited to 40 and $10 \mu\text{g cm}^{-2}$, respectively; according to field observations.
845 LUT values were assumed to belong to pure green and senescent leaves, and averaged leaf parameters
846 were mixed according with Eq. 21, assuming that in green leaves $C_{\text{s}} = 0$, and that in senescent leaves
847 $C_{\text{ab}} = 0$, $C_{\text{ca}} = 0$, $C_{\text{ant}} = 0$. No additional assumptions about the values of the parameters of each leaf type
848 and therefore the N , C_{dm} , C_{w} were taken directly from the LUT.

849 A NN was trained using SimpleR (Camps-Valls et al. 2012) to predict f_{green} as function of the canopy
850 averaged leaf RTM parameters. During the training, 60 % of the dataset was used for fitting and 40 %
851 for testing. Performance statistics are presented in Table A1.

852 Table A1. Statistics of the fraction green leaf area (f_{green}) Neural Network (NN) model.

Dataset	R^2	RMSE	ME	MAE
Training	0.818	0.123	0.005	0.093
Validation	0.718	0.230	0.158	0.180

853 **Code availability**

854 senSCOPE code and further developments, as well as the code for the multiple constraint inversion of
855 the model are publicly available at <https://github.com/JavierPachecoLabrador/senSCOPE>.

856 **Author contributions**

857 JPL, TSEM, MM and CvdT designed the model. JPL and MM designed model evaluation. TSEM, AC,
858 OPP, JG, PM, RGC, GM, MR and MM provided measurements of fluxes, plant parameters and spectral
859 variables. JPL, CvdT, MM, OPP, JG, PM and RGC wrote the paper.

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874 **References**

875 Anderson, R.C. (2006). Evolution and origin of the Central Grassland of North America: climate, fire,
876 and mammalian grazers. *The Journal of the Torrey Botanical Society*, 133, 626-647, 622

877 Bach, H., Schneider, K., Verhoef, W., Stolz, R., Mauser, W., Van Leeuwen, H., Schouten, L., &
878 Borgeaud, M. (2001). *Retrieval of geo-and biophysical information from remote sensing through*
879 *advanced combination of a land surface process model with inversion techniques in the optical and*
880 *microwave spectral range.*

- 881 Bach, H., & Verhoef, W. (2003). Sensitivity studies on the effect of surface soil moisture on canopy
882 reflectance using the radiative transfer model GeoSAIL. In, *IGARSS 2003. 2003 IEEE International*
883 *Geoscience and Remote Sensing Symposium. Proceedings (IEEE Cat. No.03CH37477)* (pp. 1679-1681)
- 884 Bacour, C., Jacquemoud, S., Leroy, M., Hauteœur, O., Weiss, M., Prévot, L., Bruguier, N., & Chauki,
885 H. (2002). Reliability of the estimation of vegetation characteristics by inversion of three canopy
886 reflectance models on airborne POLDER data. *Agronomie*, 22, 555-565
- 887 Bayat, B., van der Tol, C., & Verhoef, W. (2018). Integrating satellite optical and thermal infrared
888 observations for improving daily ecosystem functioning estimations during a drought episode. *Remote*
889 *Sensing of Environment*, 209, 375-394
- 890 Braswell, B.H., Schimel, D.S., Privette, J.L., Moore Iii, B., Emery, W.J., Sulzman, E.W., & Hudak,
891 A.T. (1996). Extracting ecological and biophysical information from AVHRR optical data: An
892 integrated algorithm based on inverse modeling. *Journal of Geophysical Research: Atmospheres*, 101,
893 23335-23348
- 894 Camino, C., Gonzalez-Dugo, V., Hernandez, P., & Zarco-Tejada, P.J. (2019). Radiative transfer Vcmax
895 estimation from hyperspectral imagery and SIF retrievals to assess photosynthetic performance in
896 rainfed and irrigated plant phenotyping trials. *Remote Sensing of Environment*, 111186
- 897 Camps-Valls, G., Munoz-Mari, J., Gomez-Chova, L., Guanter, L., & Calbet, X. (2012). Nonlinear
898 Statistical Retrieval of Atmospheric Profiles From MetOp-IASI and MTG-IRS Infrared Sounding Data.
899 *IEEE Transactions on Geoscience and Remote Sensing*, 50, 1759-1769
- 900 Castro, K.L., & Sanchez-Azofeifa, G.A. (2008). Changes in Spectral Properties, Chlorophyll Content
901 and Internal Mesophyll Structure of Senescing Populus balsamifera and Populus tremuloides Leaves.
902 *Sensors (Basel, Switzerland)*, 8, 51-69
- 903 Cleland, E.E., Chiariello, N.R., Loarie, S.R., Mooney, H.A., & Field, C.B. (2006). Diverse responses of
904 phenology to global changes in a grassland ecosystem. *Proceedings of the National Academy of*
905 *Sciences*, 103, 13740
- 906 Croft, H., Chen, J.M., Luo, X., Bartlett, P., Chen, B., & Staebler, R.M. (2017). Leaf chlorophyll content
907 as a proxy for leaf photosynthetic capacity. *Global Change Biology*, 23, 3513-3524
- 908 Dash, J., & Curran, P.J. (2007). Evaluation of the MERIS terrestrial chlorophyll index (MTCI).
909 *Advances in Space Research*, 39, 100-104
- 910 Dutta, D., Schimel, D.S., Sun, Y., van der Tol, C., & Frankenberg, C. (2019). Optimal inverse
911 estimation of ecosystem parameters from observations of carbon and energy fluxes. *Biogeosciences*, 16,
912 77-103
- 913 El-Madany, T.S., Reichstein, M., Perez-Priego, O., Carrara, A., Moreno, G., Pilar Martín, M., Pacheco-
914 Labrador, J., Wohlfahrt, G., Nieto, H., Weber, U., Kolle, O., Luo, Y.-P., Carvalhais, N., & Migliavacca,
915 M. (2018). Drivers of spatio-temporal variability of carbon dioxide and energy fluxes in a
916 Mediterranean savanna ecosystem. *Agricultural and Forest Meteorology*, 262, 258-278

- 917 Feng, X., & Dietze, M. (2013). Scale dependence in the effects of leaf ecophysiological traits on
918 photosynthesis: Bayesian parameterization of photosynthesis models. *New Phytologist*, *200*, 1132-1144
- 919 Feret, J.-B., François, C., Asner, G.P., Gitelson, A.A., Martin, R.E., Bidel, L.P.R., Ustin, S.L., le Maire,
920 G., & Jacquemoud, S. (2008). PROSPECT-4 and 5: Advances in the leaf optical properties model
921 separating photosynthetic pigments. *Remote Sensing of Environment*, *112*, 3030-3043
- 922 Féret, J.B. (2009). Apport de la modélisation pour l'estimation de la teneur en pigments foliaires par
923 télédétection. In (p. 214): Université Pierre et Marie Curie
- 924 Féret, J.B., Gitelson, A.A., Noble, S.D., & Jacquemoud, S. (2017). PROSPECT-D: Towards modeling
925 leaf optical properties through a complete lifecycle. *Remote Sensing of Environment*, *193*, 204-215
- 926 Figueroa, M.E., & Davy, A.J. (1991). Response of Mediterranean Grassland Species to Changing
927 Rainfall. *Journal of Ecology*, *79*, 925-941
- 928 Frankenberg, C., & Berry, J. (2018). 3.10 - Solar Induced Chlorophyll Fluorescence: Origins, Relation
929 to Photosynthesis and Retrieval A2 - Liang, Shunlin. *Comprehensive Remote Sensing* (pp. 143-162).
930 Oxford: Elsevier
- 931 Friedlingstein, P., Meinshausen, M., Arora, V.K., Jones, C.D., Anav, A., Liddicoat, S.K., & Knutti, R.
932 (2014). Uncertainties in CMIP5 Climate Projections due to Carbon Cycle Feedbacks. *Journal of*
933 *Climate*, *27*, 511-526
- 934 Gamon, J.A., & Berry, J.A. (2012). Facultative and constitutive pigment effects on the Photochemical
935 Reflectance Index (PRI) in sun and shade conifer needles. *Israel Journal of Plant Sciences*, *60*, 85-95
- 936 Gamon, J.A., Peñuelas, J., & Field, C.B. (1992). A narrow-waveband spectral index that tracks diurnal
937 changes in photosynthetic efficiency. *Remote Sensing of Environment*, *41*, 35-44
- 938 Garbulsky, M.F., Peñuelas, J., Gamon, J., Inoue, Y., & Filella, I. (2011). The photochemical reflectance
939 index (PRI) and the remote sensing of leaf, canopy and ecosystem radiation use efficiencies: A review
940 and meta-analysis. *Remote Sensing of Environment*, *115*, 281-297
- 941 Golub, G.H., & Loan, C.F.v. (1980). An Analysis of the Total Least Squares Problem. *SIAM Journal on*
942 *Numerical Analysis*, *17*, 883-893
- 943 Gonzalez-Cascon, R., Jiménez-Fenoy, L., Verdú-Fillola, I., & Martín, M.P. (2017). Short
944 communication: Aqueous-acetone extraction improves the drawbacks of using dimethylsulfoxide as
945 solvent for photometric pigment quantification in *Quercus ilex* leaves. *2017*, *26*
- 946 Gonzalez-Cascon, R., & Martin, M.P. (2018). Protocol for pigment content quantification in herbaceous
947 covers: sampling and analysis, *October 2019*
- 948 Guyot, S., Vercauteren, J., & Cheynier, V. (1996). Structural determination of colourless and yellow
949 dimers resulting from (+)-catechin coupling catalysed by grape polyphenoloxidase. *Phytochemistry*, *42*,
950 1279-1288

- 951 He, Y., & Mui, A. (2010). Scaling up Semi-Arid Grassland Biochemical Content from the Leaf to the
952 Canopy Level: Challenges and Opportunities. *Sensors*, *10*, 11072-11087
- 953 Henry, H.A.L., Brizgys, K., & Field, C.B. (2008). Litter Decomposition in a California Annual
954 Grassland: Interactions Between Photodegradation and Litter Layer Thickness. *Ecosystems*, *11*, 545-554
- 955 Hörtensteiner, S. (2006). CHLOROPHYLL DEGRADATION DURING SENESCENCE. *Annual*
956 *Review of Plant Biology*, *57*, 55-77
- 957 Houborg, R., & Anderson, M. (2009). Utility of an image-based canopy reflectance modeling tool for
958 remote estimation of LAI and leaf chlorophyll content at regional scales. In (p. 29): SPIE
- 959 Houborg, R., Anderson, M., & Daughtry, C. (2009). Utility of an image-based canopy reflectance
960 modeling tool for remote estimation of LAI and leaf chlorophyll content at the field scale. *Remote*
961 *Sensing of Environment*, *113*, 259-274
- 962 Houborg, R., & Boegh, E. (2008). Mapping leaf chlorophyll and leaf area index using inverse and
963 forward canopy reflectance modeling and SPOT reflectance data. *Remote Sensing of Environment*, *112*,
964 186-202
- 965 Houborg, R., McCabe, M., Cescatti, A., Gao, F., Schull, M., & Gitelson, A. (2015). Joint leaf
966 chlorophyll content and leaf area index retrieval from Landsat data using a regularized model inversion
967 system (REGFLEC). *Remote Sensing of Environment*, *159*, 203-221
- 968 Houborg, R., & McCabe, M.F. (2016). Adapting a regularized canopy reflectance model (REGFLEC)
969 for the retrieval challenges of dryland agricultural systems. *Remote Sensing of Environment*, *186*, 105-
970 120
- 971 IPCC (2014). Climate Change 2014: Synthesis Report. Contribution of Working Groups I, II and III to
972 the Fifth Assessment Report of the Intergovernmental Panel on Climate Change. In R.K.P.a.L.A. Meyer
973 (Ed.) (p. 151). Geneva, Switzerland: IPCC
- 974 Jacquemoud, S. (1988). Modélisation des propriétés optiques des feuilles. In: USTL / ENSA
975 Montpellier / INRA
- 976 Jacquemoud, S., & Baret, F. (1990). PROSPECT: A model of leaf optical properties spectra. *Remote*
977 *Sensing of Environment*, *34*, 75-91
- 978 Jacquemoud, S., Verhoef, W., Baret, F., Bacour, C., Zarco-Tejada, P.J., Asner, G.P., François, C., &
979 Ustin, S.L. (2009). PROSPECT+SAIL models: A review of use for vegetation characterization. *Remote*
980 *Sensing of Environment*, *113*, S56-S66
- 981 Kidnie, S., Cruz, M.G., Gould, J., Nichols, D., Anderson, W., & Bessell, R. (2015). Effects of curing on
982 grassfires: I. Fuel dynamics in a senescing grassland. *International Journal of Wildland Fire*, *24*, 828-
983 837
- 984 Koukoura, Z., Mamolos, A.P., & Kalburtji, K.L. (2003). Decomposition of dominant plant species litter
985 in a semi-arid grassland. *Applied Soil Ecology*, *23*, 13-23

- 986 Luo, Y., El-Madany, T., Filippa, G., Ma, X., Ahrens, B., Carrara, A., Gonzalez-Cascon, R., Cremonese,
987 E., Galvagno, M., Hammer, T., Pacheco-Labrador, J., Martín, M., Moreno, G., Perez-Priego, O.,
988 Reichstein, M., Richardson, A., Römermann, C., & Migliavacca, M. (2018). Using Near-Infrared-
989 Enabled Digital Repeat Photography to Track Structural and Physiological Phenology in Mediterranean
990 Tree–Grass Ecosystems. *Remote Sensing*, *10*, 1293
- 991 Martín, M.P., Pacheco-Labrador, J., Gonzalez-Cascon, R., Moreno, G., Migliavacca, M., García, M.,
992 Yebra, M., & Riaño, D. (2019). Estimación de variables esenciales de la vegetación en un ecosistema de
993 dehesa utilizando factores de reflectividad simulados con PROSAIL + FLIGHT. In A.E.d.
994 Teledetección (Ed.), *XVIII Congreso Nacional de Teledetección*. Valladolid, Spain, 24-27 September
995 2019
- 996 Martini, D., Pacheco-Labrador, J., Perez-Priego, O., van der Tol, C., El-Madany, S.T., Julitta, T.,
997 Rossini, M., Reichstein, M., Christiansen, R., Rascher, U., Moreno, G., Martín, P.M., Yang, P., Carrara,
998 A., Guan, J., González-Cascón, R., & Migliavacca, M. (2019). Nitrogen and Phosphorus Effect on Sun-
999 Induced Fluorescence and Gross Primary Productivity in Mediterranean Grassland. *Remote Sensing*, *11*
- 1000 McKay, M.D., Beckman, R.J., & Conover, W.J. (1979). A Comparison of Three Methods for Selecting
1001 Values of Input Variables in the Analysis of Output from a Computer Code. *Technometrics*, *21*, 239-
1002 245
- 1003 Melendo-Vega, J., Martín, M., Pacheco-Labrador, J., González-Cascón, R., Moreno, G., Pérez, F.,
1004 Migliavacca, M., García, M., North, P., & Riaño, D. (2018). Improving the Performance of 3-D
1005 Radiative Transfer Model FLIGHT to Simulate Optical Properties of a Tree-Grass Ecosystem. *Remote*
1006 *Sensing*, *10*, 2061
- 1007 Migliavacca, M., Galvagno, M., Cremonese, E., Rossini, M., Meroni, M., Sonnentag, O., Cogliati, S.,
1008 Manca, G., Diotri, F., Busetto, L., Cescatti, A., Colombo, R., Fava, F., Morra di Cella, U., Pari, E.,
1009 Siniscalco, C., & Richardson, A.D. (2011). Using digital repeat photography and eddy covariance data
1010 to model grassland phenology and photosynthetic CO₂ uptake. *Agricultural and Forest Meteorology*,
1011 *151*, 1325-1337
- 1012 Migliavacca, M., Perez-Priego, O., Rossini, M., El-Madany, T.S., Moreno, G., van der Tol, C., Rascher,
1013 U., Berninger, A., Bessenbacher, V., Burkart, A., Carrara, A., Fava, F., Guan, J.-H., Hammer, T.W.,
1014 Henkel, K., Juarez-Alcalde, E., Julitta, T., Kolle, O., Martín, M.P., Musavi, T., Pacheco-Labrador, J.,
1015 Pérez-Burgueño, A., Wutzler, T., Zaehle, S., & Reichstein, M. (2017). Plant functional traits and
1016 canopy structure control the relationship between photosynthetic CO₂ uptake and far-red sun-induced
1017 fluorescence in a Mediterranean grassland under different nutrient availability. *New Phytologist*, *214*,
1018 1078-1091
- 1019 Omlin, M., & Reichert, P. (1999). A comparison of techniques for the estimation of model prediction
1020 uncertainty. *Ecological Modelling*, *115*, 45-59
- 1021 Pacheco-Labrador, J., El-Madany, T., Martín, M., Migliavacca, M., Rossini, M., Carrara, A., & Zarco-
1022 Tejada, P.J. (2017). Spatio-Temporal Relationships between Optical Information and Carbon Fluxes in
1023 a Mediterranean Tree-Grass Ecosystem. *Remote Sensing*, *9*, 608

- 1024 Pacheco-Labrador, J., Perez-Priego, O., El-Madany, T.S., Julitta, T., Rossini, M., Guan, J., Moreno, G.,
1025 Carvalhais, N., Martín, M.P., Gonzalez-Cascon, R., Kolle, O., Reischtein, M., van der Tol, C., Carrara,
1026 A., Martini, D., Hammer, T.W., Moossen, H., & Migliavacca, M. (2019). Multiple-constraint inversion
1027 of SCOPE. Evaluating the potential of GPP and SIF for the retrieval of plant functional traits. *Remote*
1028 *Sensing of Environment*, 234, 111362
- 1029 Perez-Priego, O., El-Madany, T.S., Migliavacca, M., Kowalski, A.S., Jung, M., Carrara, A., Kolle, O.,
1030 Martín, M.P., Pacheco-Labrador, J., Moreno, G., & Reichstein, M. (2017). Evaluation of eddy
1031 covariance latent heat fluxes with independent lysimeter and sapflow estimates in a Mediterranean
1032 savannah ecosystem. *Agricultural and Forest Meteorology*, 236, 87-99
- 1033 Perez-Priego, O., Guan, J., Rossini, M., Fava, F., Wutzler, T., Moreno, G., Carvalhais, N., Carrara, A.,
1034 Kolle, O., Julitta, T., Schrupf, M., Reichstein, M., & Migliavacca, M. (2015). Sun-induced
1035 chlorophyll fluorescence and photochemical reflectance index improve remote-sensing gross primary
1036 production estimates under varying nutrient availability in a typical Mediterranean savanna ecosystem.
1037 *Biogeosciences*, 12, 6351-6367
- 1038 Porcar-Castell, A., Tyystjärvi, E., Atherton, J., van der Tol, C., Flexas, J., Pfündel, E.E., Moreno, J.,
1039 Frankenberg, C., & Berry, J.A. (2014). Linking chlorophyll a fluorescence to photosynthesis for remote
1040 sensing applications: mechanisms and challenges. *Journal of Experimental Botany*, 65, 4065-4095
- 1041 Pourcel, L., Routaboul, J.-M., Cheynier, V., Lepiniec, L., & Debeaujon, I. (2007). Flavonoid oxidation
1042 in plants: from biochemical properties to physiological functions. *Trends in Plant Science*, 12, 29-36
- 1043 Ren, H., & Zhang, B. (2018). Spatiotemporal variations in litter mass and their relationships with
1044 climate in temperate grassland: A case study from Xilingol grassland, Inner Mongolia (China).
1045 *Advances in Space Research*, 61, 1055-1065
- 1046 Richardson, A.D., Keenan, T.F., Migliavacca, M., Ryu, Y., Sonnentag, O., & Toomey, M. (2013).
1047 Climate change, phenology, and phenological control of vegetation feedbacks to the climate system.
1048 *Agricultural and Forest Meteorology*, 169, 156-173
- 1049 Rogers, A. (2014). The use and misuse of $V_{c,max}$ in Earth System Models. *Photosynthesis Research*,
1050 119, 15-29
- 1051 Rogers, A., Medlyn Belinda, E., Dukes Jeffrey, S., Bonan, G., Caemmerer, S., Dietze Michael, C.,
1052 Kattge, J., Leakey Andrew, D.B., Mercado Lina, M., Niinemets, Ü., Prentice, I.C., Serbin Shawn, P.,
1053 Sitch, S., Way Danielle, A., & Zaehle, S. (2016). A roadmap for improving the representation of
1054 photosynthesis in Earth system models. *New Phytologist*, 213, 22-42
- 1055 Rouse, J.W., Haas, R.H., Schell, J.A., & Deering, D.W. (1974). Monitoring vegetation systems in the
1056 Great Plains with ERTS. In S.C. Freden, E.P. Mercanti, & M.A. Becker (Eds.), *Third Earth Resources*
1057 *Technology Satellite- 1 Symposium* (pp. 301–317). Greenbelt, MD, USA: NASA
- 1058 Sanaullah, M., Chabbi, A., Lemaire, G., Charrier, X., & Rumpel, C. (2010). How does plant leaf
1059 senescence of grassland species influence decomposition kinetics and litter compounds dynamics?
1060 *Nutrient Cycling in Agroecosystems*, 88, 159-171

- 1061 Schaefer, K., Schwalm Christopher, R., Williams, C., Arain, M.A., Barr, A., Chen Jing, M., Davis
1062 Kenneth, J., Dimitrov, D., Hilton Timothy, W., Hollinger David, Y., Humphreys, E., Poulter, B.,
1063 Raczka Brett, M., Richardson Andrew, D., Sahoo, A., Thornton, P., Vargas, R., Verbeeck, H.,
1064 Anderson, R., Baker, I., Black, T.A., Bolstad, P., Chen, J., Curtis Peter, S., Desai Ankur, R., Dietze, M.,
1065 Dragoni, D., Gough, C., Grant Robert, F., Gu, L., Jain, A., Kucharik, C., Law, B., Liu, S., Lokipitiya,
1066 E., Margolis Hank, A., Matamala, R., McCaughey, J.H., Monson, R., Munger, J.W., Oechel, W., Peng,
1067 C., Price David, T., Ricciuto, D., Riley William, J., Roulet, N., Tian, H., Tonitto, C., Torn, M., Weng,
1068 E., & Zhou, X. (2012). A model-data comparison of gross primary productivity: Results from the North
1069 American Carbon Program site synthesis. *Journal of Geophysical Research: Biogeosciences*, 117
- 1070 Serbin, S.P., Singh, A., Desai, A.R., Dubois, S.G., Jablonski, A.D., Kingdon, C.C., Kruger, E.L., &
1071 Townsend, P.A. (2015). Remotely estimating photosynthetic capacity, and its response to temperature,
1072 in vegetation canopies using imaging spectroscopy. *Remote Sensing of Environment*, 167, 78-87
- 1073 Silva-Perez, V., Molero, G., Serbin, S.P., Condon, A.G., Reynolds, M.P., Furbank, R.T., & Evans, J.R.
1074 (2018). Hyperspectral reflectance as a tool to measure biochemical and physiological traits in wheat.
1075 *Journal of Experimental Botany*, 69, 483-496
- 1076 Sims, D.A., & Gamon, J.A. (2002). Relationships between leaf pigment content and spectral reflectance
1077 across a wide range of species, leaf structures and developmental stages. *Remote Sensing of*
1078 *Environment*, 81, 337-354
- 1079 Taranto, F., Pasqualone, A., Mangini, G., Tripodi, P., Miazzi, M.M., Pavan, S., & Montemurro, C.
1080 (2017). Polyphenol Oxidases in Crops: Biochemical, Physiological and Genetic Aspects. *International*
1081 *Journal of Molecular Sciences*, 18, 377
- 1082 van der Tol, C., Rossini, M., Cogliati, S., Verhoef, W., Colombo, R., Rascher, U., & Mohammed, G.
1083 (2016). A model and measurement comparison of diurnal cycles of sun-induced chlorophyll
1084 fluorescence of crops. *Remote Sensing of Environment*, 186, 663-677
- 1085 van der Tol, C., Verhoef, W., Timmermans, J., Verhoef, A., & Su, Z. (2009). An integrated model of
1086 soil-canopy spectral radiances, photosynthesis, fluorescence, temperature and energy balance.
1087 *Biogeosciences*, 6, 3109-3129
- 1088 Verhoef, W. (1984). Light scattering by leaf layers with application to canopy reflectance modeling:
1089 The SAIL model. *Remote Sensing of Environment*, 16, 125-141
- 1090 Verhoef, W., & Bach, H. (2003). Remote sensing data assimilation using coupled radiative transfer
1091 models. *Physics and Chemistry of the Earth, Parts A/B/C*, 28, 3-13
- 1092 Verhoef, W., van der Tol, C., & Middleton, E.M. (2018). Hyperspectral radiative transfer modeling to
1093 explore the combined retrieval of biophysical parameters and canopy fluorescence from FLEX –
1094 Sentinel-3 tandem mission multi-sensor data. *Remote Sensing of Environment*, 204, 942-963
- 1095 Vilfan, N., van der Tol, C., Muller, O., Rascher, U., & Verhoef, W. (2016). Fluspect-B: A model for
1096 leaf fluorescence, reflectance and transmittance spectra. *Remote Sensing of Environment*, 186, 596-615

- 1097 Vilfan, N., Van der Tol, C., Yang, P., Wyber, R., Malenovský, Z., Robinson, S.A., & Verhoef, W.
1098 (2018). Extending Fluspect to simulate xanthophyll driven leaf reflectance dynamics. *Remote Sensing of*
1099 *Environment*, 211, 345-356
- 1100 Wang, Q., Tenhunen, J., Dinh, N.Q., Reichstein, M., Otieno, D., Granier, A., & Pilegarrrd, K. (2005).
1101 Evaluation of seasonal variation of MODIS derived leaf area index at two European deciduous
1102 broadleaf forest sites. *Remote Sensing of Environment*, 96, 475-484
- 1103 Wenhan, Q. (1993). Modeling bidirectional reflectance of multicomponent vegetation canopies. *Remote*
1104 *Sensing of Environment*, 46, 235-245
- 1105 Whitfield, D.M., & Rowan, K.S. (1974). Changes in the chlorophylls and carotenoids of leaves of
1106 *Nicotiana tabacum* during senescence. *Phytochemistry*, 13, 77-83
- 1107 Yang, P., Verhoef, W., & van der Tol, C. (2017). The mSCOPE model: A simple adaptation to the
1108 SCOPE model to describe reflectance, fluorescence and photosynthesis of vertically
1109 heterogeneous canopies. *Remote Sensing of Environment*, 201, 1-11
- 1110 Yuan, Z., & Chen, H.Y.H. (2009). Global trends in senesced-leaf nitrogen and phosphorus. *Global*
1111 *Ecology and Biogeography*, 18, 532-542
- 1112 Zhang, Y., Guanter, L., Berry Joseph, A., Joiner, J., Tol, C., Huete, A., Gitelson, A., Voigt, M., &
1113 Köhler, P. (2014). Estimation of vegetation photosynthetic capacity from space-based measurements of
1114 chlorophyll fluorescence for terrestrial biosphere models. *Global Change Biology*, 20, 3727-3742
- 1115 Zhang, Y., Guanter, L., Joiner, J., Song, L., & Guan, K. (2018). Spatially-explicit monitoring of crop
1116 photosynthetic capacity through the use of space-based chlorophyll fluorescence data. *Remote Sensing*
1117 *of Environment*, 210, 362-374
- 1118