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# 1    **Downscaling of solar-induced chlorophyll fluorescence from** 2    **canopy level to photosystem level using a random forest** 3    **model**

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23

## 24    **Abstract**

25    Solar-induced chlorophyll fluorescence (SIF), an electromagnetic signal that can potentially indicate  
26    vegetation photosynthetic activity, can be retrieved from ground-based, airborne and satellite  
27    measurements. However, due to the scattering and re-absorption effects inside the leaves and canopy,  
28    SIF measured at the canopy level is only a small part of the total SIF emission at the photosystem

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29 level. Therefore, a downscaling mechanism of SIF from the canopy level to the photosystem level is  
30 important for better understanding the relationship between SIF and the vegetation gross primary  
31 production (GPP). In this study, firstly, we analyzed the canopy scattering effects using a simple  
32 parameterization model based on the spectral invariant theory. The probability for SIF photons to  
33 escape from the canopy was found to be related to the anisotropic spectral reflectance, canopy  
34 interception of the upward solar radiation, and leaf absorption. An empirical approach based on a  
35 Random Forest (RF) regression algorithm was applied to downscale SIF constrained by the red,  
36 red-edge and far-red anisotropic reflectance. The RF was trained using simulations conducted with  
37 the Soil Canopy Observation, Photochemistry and Energy fluxes (SCOPE) model. The performance of  
38 the SIF downscaling method was evaluated with SCOPE and Discrete Anisotropic Radiative Transfer  
39 (DART) model simulations, ground measurements and airborne data. Results show that estimated  
40 SIF at the photosystem level matches well with simulated reference data, and the relationship  
41 between SIF and photosynthetically active radiation absorbed by chlorophyll is improved by SIF  
42 downscaling. This finding in combination with other evaluation criteria suggests the downscaling of  
43 canopy SIF as an efficient strategy to normalize species dependent effects of canopy structure and  
44 varying solar-view geometries. Based on our results for the SIF-APAR relationship, we expect that  
45 such normalization approaches can be helpful to improve estimates of photosynthesis using remote  
46 sensing measurements of SIF.

47 **Keywords:** Solar-induced chlorophyll fluorescence; Downscaling; Canopy level; Photosystem level;  
48 Spectral invariant theory; Random Forest regression

## 49 1. Introduction

50 Solar-induced chlorophyll fluorescence (SIF) has been proved to be an efficient tool for  
51 monitoring of gross primary production (GPP), showing large advantages compared with other  
52 remote sensing indicators based on reflectance-data (Guanter et al. 2014; Migliavacca et al. 2017;  
53 Porcar-Castell et al. 2014; Sun et al. 2017; Zhang et al. 2016). The photosynthetically active energy  
54 absorbed by leaf pigments can be: i) used in photochemical reactions, ii) dissipated as heat, or iii)  
55 re-emitted as fluorescence (Porcar-Castell et al. 2014). Unlike the reflectance based parameters, SIF is,  
56 as a by-product of photosynthesis, more directly related to GPP (Berry et al. 2012; Coops et al. 2010;  
57 Damm et al. 2015a; Zarco-Tejada et al. 2013).

58 Validity of the resource balancing paradigm (Field et al. 1998) in combination with the Monteith  
59 light use efficiency (LUE) model (Monteith 1972; Monteith and Moss 1977) is the foundation of most  
60 of the approaches for the estimation of GPP from remote sensing data. The LUE model can be  
61 expressed as:

$$62 \quad \text{GPP} = \text{PAR} \times \text{fAPAR} \times \text{LUE} \quad (1)$$

63 where PAR stands for the photosynthetically active radiation, fAPAR is the fraction of PAR absorbed  
64 by vegetation, and LUE is the light use efficiency, defined as the number of  $\mu\text{mol}$  of  $\text{CO}_2$  absorbed per  
65  $\mu\text{mol}$  of photons.

66 Similarly, the total SIF emission at the photosystem (PS) level (the total SIF emission inside the  
67 leaves without any scattering or re-absorption) can be expressed as (Berry et al. 2012; Liu et al.  
68 2017a; Moya and Cerovic 2004; Porcar-Castell et al. 2014; Wieneke et al. 2016):

$$69 \quad \text{SIF}_{\text{PS}}(\lambda) = \text{PAR} \times \text{fAPAR} \times F_{\text{yield}}(\lambda) \quad (2)$$

70 where  $\lambda$  is the wavelength, and  $F_{\text{yield}}$  is the quantum yield for chlorophyll fluorescence. If  $F_{\text{yield}}$  is  
71 constant, then  $\text{SIF}_{\text{PS}}$  is linearly related to the PAR absorbed by vegetation.

72 In recent years, we have been experiencing a rapid development of methods for SIF retrieval  
73 from spectral remote sensing data (Malenovský et al. 2009). The SIF signal can be detected by  
74 ground-based (Grossmann 2014; Liu et al. 2017a; Liu et al. 2015; Liu et al. 2005; Wyber et al. 2017;  
75 Yang et al. 2015; Cogliati et al. 2015; Burkart et al. 2015), airborne (Damm et al. 2014, Rascher et al.  
76 2015; Wieneke et al. 2016), and space-borne sensors (Frankenberg et al. 2011; Guanter et al. 2012;  
77 Joiner et al. 2013; Joiner et al. 2011; Köhler et al. 2015). However, SIF is emitted by chlorophyll *a*  
78 molecules, which are contained inside chloroplasts at different leaf mesophyll layers. Reabsorption  
79 and scattering of SIF are both taking place inside leaves as well as within the canopy. Using remote  
80 sensing approaches at large scales, it is only possible to measure SIF at the canopy level ( $\text{SIF}_{\text{Canopy}}$ ,  
81 defined as SIF escaping from the canopy in a specific viewing direction).

82 The SIF spectrum extends over the wavelength range from about 640 to 850 nm, with two peaks  
83 centered at 685 nm and 740 nm. Ramos and Lagorio (2004) pointed out that the spectral shape of  
84 fluorescence measured at leaf level was influenced by the leaf re-absorption, and developed a model  
85 to correct the spectral shape using leaf reflectance. Van Wittenberghe et al. (2015) studied the  
86 upward and downward SIF emission at the leaf level separately using a special leaf probe called  
87 FluoWat, and found that the partitioning of the upward and downward SIF components is influenced  
88 by scattering and absorption processes related to the leaf structure and the pigment content. This  
89 indicates that the red SIF at 685 nm is strongly influenced by chlorophyll absorption within the leaves,  
90 while far-red SIF is mainly influenced by scattering effect of leaf tissue structures. Several studies  
91 have reported a decrease in the red/far-red SIF ratio from leaf level to canopy level (Fournier et al.

92 2012; Moya et al. 2006; Romero et al. 2018), which can be, besides the environmental stress exposure  
93 (Ač et al. 2015), explained by the strong re-absorption of SIF by chlorophyll at the red band  
94 (Daumard et al. 2012; Fournier et al. 2012; Agati et al. 1993; Cordon et al. 2006; Porcar-Castell et al.  
95 2014; Romero et al. 2018). Liu et al. (2016) observed similar anisotropic characteristics for SIF and  
96 reflectance at the canopy level, and claimed that the phenomenon can be attributed to re-absorption  
97 by canopy components and the bidirectional canopy gap fraction. Other studies also reported a  
98 similar anisotropic effect for SIF retrieved from space (e.g. Guanter et al. 2012, Joiner et al. 2012),  
99 while He et al. (2017) proved that an angular normalization of SIF strengthens SIF-GPP relationships.  
100 Further, Du et al. (2017) reported a species-dependent relationship between  $SIF_{\text{canopy}}$  and PAR  
101 absorbed by chlorophyll ( $APAR_{\text{chl}}$ ), and pointed out that the uncertainty in the SIF escape probability  
102 weakens the relationship between SIF and  $APAR_{\text{chl}}$  or GPP, especially at the red band. Therefore,  
103 downscaling of SIF from canopy level to PS level is important to better constrain estimates of GPP  
104 using remote sensing observations of SIF.

105 There are two very recent studies focusing on the problem of SIF downscaling. Romero et al.  
106 (2018) developed a physical model based on the canopy reflectance, canopy transmittance and soil  
107 reflectance to correct the spectral shape of fluorescence emission from canopy level to leaf level.  
108 Together with the study by Ramos and Lagorio (2004), the fluorescence spectral shape at PS level  
109 could also be retrieved. However, the absolute SIF intensity was not available. Yang and Van der Tol  
110 (2018) linked the canopy scattering of far-red SIF to the canopy reflectance, canopy interceptance  
111 and leaf albedo based on canopy radiative transfer analysis, but the model was not valid for the red  
112 band and the input parameters were not easy to be accurately measured or estimated. Moreover, the  
113 SIF downscaling from leaf level to PS level was not included.

114 Given the fact that the radiative transfer of emitted SIF within a canopy is similar to that for  
115 scattered solar radiation, it can be assumed that the modelling of top-of-canopy (TOC) spectral  
116 reflectance can approximate the canopy effects on SIF, which is needed for the estimation of SIF  
117 escape probability from PS level to canopy level ( $\epsilon_{CP}$ ) (Van der Tol et al. 2009; Liu et al. 2016). To  
118 express the radiative transfer equation within the canopy together with the leaf scattering coefficient,  
119 Knyazikhin et al. (1998) introduced a spectral invariant  $p$ , which was defined by Smolander and  
120 Stenberg (2005) as photon recollision probability. Another spectral invariant, bi-directional gap  
121 fraction, was introduced to quantify the probability of scattered photons to escape the canopy via  
122 gaps in the direction of viewing (Huang et al. 2007; Knyazikhin et al. 2011). The so-called ‘spectral  
123 invariant theory’ has been successfully used to better understand the absorption and scattering  
124 effects within the canopy and also to link the reflectance at the canopy level and leaf level (Huang et  
125 al. 2007; Knyazikhin et al. 2013; Smolander and Stenberg 2005; Stenberg et al. 2016; Wang et al.  
126 2003). Similarly, the spectral invariant theory can be applied to model the escape probability for SIF  
127 with a number of parameters describing the leaf optical properties, canopy structure, and  
128 background reflectance. However, these parameters are usually difficult to accurately measure or  
129 estimate. Moreover, spectral invariant theory can only model the radiative transfer process from leaf  
130 level to canopy level, while SIF is emitted from inside the leaves, which means that the re-absorption  
131 of SIF photons within the leaves (leaf internal absorption) is not accounted for. Although the canopy  
132 reflectance also contains information about the leaf absorption, it is difficult to directly link this to the  
133 SIF absorption inside the leaves.

134 Supervised machine learning approaches trained on appropriate training dataset are capable of  
135 building accurate prediction models (Ma, 2014) that can empirically overcome the difficulties in the

136 physical modelling described above (the unavailable input parameters for the physical model can be  
137 estimated by machine learning approaches using available information). The physically based  
138 analysis of the radiative transfer process is, in turn, able to point out the appropriate input  
139 parameters used in the machine learning methods.

140 This study aims to define and evaluate a practical solution for the downscaling of SIF from the  
141 canopy level to the PS level. The SIF radiative transfer within canopy and inside leaves is analyzed  
142 based on the spectral invariant theory and leaf-level simulations to define the key parameters driving  
143 the SIF downscaling from canopy level to leaf and PS levels. We then employ an empirical approach  
144 based on random forest (RF) regression (Breiman 2001) to predict the SIF escape probability from  
145 leaf level to canopy level ( $\epsilon_{CL}$ ) and from PS level to canopy level ( $\epsilon_{CP}$ ) using reflectance information.  
146 The Soil Canopy Observation, Photochemistry and Energy fluxes (SCOPE) model (Van der Tol et al.  
147 2009) was then used for the simulation of the training dataset. Finally, we evaluate the performance  
148 of the SIF downscaling using SCOPE and Discrete Anisotropic Radiative Transfer (DART) model  
149 simulations, ground and airborne data. The presented approach facilitates the normalization of SIF  
150 observations across canopy types observed under varying sun-view geometries, and eventually  
151 improves our understanding on the relationship between SIF emission and photosynthetic activity.

## 152 **2. Materials and methods**

### 153 **2.1 Simulated datasets**

#### 154 **2.1.1 SCOPE simulation**

155 The SCOPE model (Van der Tol et al. 2009) is a vertical (1-D) integrated radiative transfer and



156 energy balance model, which is able to simulate leaf and canopy spectral reflectance and SIF as well  
 157 as photosynthesis and water and heat flux by linking the radiative transfer with micro-meteorological  
 158 processes. SCOPE has been widely used in the field of SIF research (e.g. Verrelst et al. 2015; Zhang et  
 159 al. 2016; Yang and Van der Tol. 2018). The latest version of SCOPE (v1.7) provides users with SIF at  
 160 canopy level, leaf level (SIF emitted by all leaves, excluding the re-absorption and scattering within  
 161 the canopy) and at PS level (SIF emitted by all photosystems, excluding the re-absorption within the  
 162 leaves). Therefore, we used SCOPE v1.7 for the simulation of SIF at the canopy, leaf and PS levels,  
 163 along with that of the canopy directional reflectance, leaf reflectance and transmittance.

164 In the SIF emission spectral range ( $\sim 640 - 850$  nm), the amount of absorption by leaves is  
 165 mainly related to chlorophyll content (Jacquemoud and Baret 1990). The canopy scattering is mainly  
 166 related to the canopy structure parameters (leaf area index (LAI), leaf inclination distribution, etc.)  
 167 and solar-view geometries (solar zenith angle (SZA), view zenith angle (VZA) and relative azimuth  
 168 angle (RAA)) (Verhoef 1984). We parameterized SCOPE for sets of different leaf chlorophyll contents  
 169 ( $C_{ab}$ ), LAI levels and six typical leaf inclination distributions to cover most common vegetation  
 170 conditions. Additionally, different SZAs and VZAs in the solar principal plane were also defined. The  
 171 full-width-at-half-maximum spectral response (FWHM) and spectral sampling interval (SSI) for the  
 172 SCOPE simulations are 1 nm. Details about the SCOPE input parameters are listed in Table 1. As a  
 173 result, 6240 different samples were generated.

174 Table 1. Main input parameters for the SCOPE simulations.

Parameter	Values	Unit	Description
$C_{ab}$	20, 40, 60, 80	$\mu\text{g}/\text{cm}^2$	Leaf chlorophyll a + b content
$C_{dm}$	0.012	$\text{g}/\text{cm}^2$	Dry matter content
$C_w$	0.009	cm	Leaf water equivalent layer
N	1.4	-	Leaf mesophyll scattering parameter
LAI	1, 2, 3, 4	$\text{m}^2/\text{m}^2$	Leaf area index
$LIDF_a$	1, -1, 0, 0, -0.35, 0	-	Leaf inclination parameter

LIDF <sub>b</sub>	0, 0, -1, 1, -0.15, 0	-	Bimodality parameter
FQE	0.01	-	Fluorescence quantum yield efficiency
SZA	20, 30, 40, 50, 60	degree	Solar zenith angle
VZA	0, 10, 20, 30, 40, 50, 60	degree	View zenith angle
RAA	0, 180	degree	Relative azimuth angle

## 175 2.1.2 DART simulation

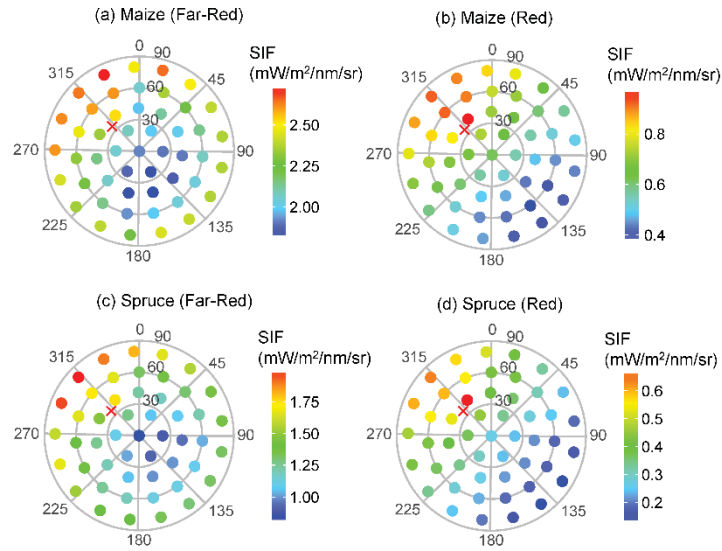
176 DART is a three-dimensional (3-D) radiative transfer model that allows simulating the radiation  
177 budget as well as remotely sensed images of natural and urban surfaces covering the range from the  
178 ultraviolet to the thermal infrared band (Gastellu-Etcheberry et al. 2015). Recently, a SIF module that  
179 allows simulations of SIF radiative transfer within 3-D canopies has been added to DART  
180 (Gastellu-Etcheberry et al. 2017). Similar to SCOPE, DART uses the Fluspect model (Vilfan et al. 2016)  
181 to simulate the reflectance, transmittance and SIF emission at the leaf level. In this study, the DART  
182 model (v5.6.6) was employed to simulate SIF at both the canopy and leaf levels, together with the  
183 directional reflectance of 50 different viewing angles for two geometrically explicit and  
184 architecturally different canopies of maize (*Zea mays L.*) and Norway spruce (*Picea abies /L./ H.*  
185 *Karst.*). The DART parameterization details are listed in Table 2. Figure 1 shows the simulated  
186 multi-angular SIF at canopy level for maize and spruce at the far-red (740 nm) and red bands (687  
187 nm).

188 Table 2. Major input parameters for the DART simulations of maize and spruce canopies.

Parameter	Values	Unit	Description
$C_{ab}$	58	$\mu\text{g}/\text{cm}^2$	Leaf chlorophyll a + b content
$C_{dm}$	0.0037	$\text{g}/\text{cm}^2$	Dry matter content
$C_w$	0.0131	cm	Leaf water equivalent layer
N	1.518	-	Leaf mesophyll scattering parameter
LAI	4 (maize), 7 (spruce)	$\text{m}^2/\text{m}^2$	Leaf area index
Canopy Height	2.25 (maize), 10 (spruce)	m	Canopy Height
FQE (PSI)	0.002	-	Fluorescence quantum yield efficiency for photosystem I
FQE (PSII)	0.008	-	Fluorescence quantum yield

			efficiency for photosystem II
SZA	37.94	degree	Solar zenith angle
VZA	15 – 65	degree	View zenith angle
SAA	311.89	degree	Solar azimuth angle
VAA	0 – 180	degree	View azimuth angle

189



190

191 Figure 1. Multi-angular SIF at canopy level for maize and spruce at the far-red (740 nm) and red (687

192 nm) bands, as simulated by DART. The labels are the view azimuth ( $0^\circ - 360^\circ$ ,  $0^\circ$  for the north) and

193 zenith ( $0^\circ - 90^\circ$ ) angles. The red cross indicates the solar position (zenith angle:  $37.94^\circ$ ; azimuth

194 angle:  $311.89^\circ$ ). The incident PAR is  $1185.76 \text{ W/m}^2$ , and the temperature is 300 K.

195

## 196 2.2 Ground measurements

### 197 2.2.1 Multi-species experiments

198 A dataset comprising ground spectral measurements of different species, acquired at three sites,

199 following three specific experimental settings was used to evaluate the performance of SIF

200 downscaling for different canopy structures.

201 Spectral measurements of winter wheat (*Triticum*) were carried out on five days at the National  
202 Precision Agriculture Demonstration Base located at Xiao Tangshan Farm (XTS, 40°11'N, 116°27'E),  
203 north of Beijing, China. Diurnal cycles of radiance measurements (nadir view) were conducted on  
204 April 8 - 9 and 18, 2016, when the growth stages of the winter wheat were jointing and booting, and  
205 on November 7 and December 8, 2016 when the growth stages were emergence and tillering,  
206 respectively. The leaf inclination distribution function (LIDF) of winter wheat was assumed to be  
207 spherical based on a visual inspection.

208 Measurements of cotton (*Gossypium*) and different kinds of vegetables (i.e. sweet potato  
209 (*Ipomoea batatas*), Chinese cabbage (*Brassica rapa pekinensis*), thyme (*Thymus*), pumpkin (*Cucurbita*  
210 *Cucurbita*)) were carried out on December 18, 2016 at Nanbin Farm (NBF, 18°22'N, 109°10'E) in  
211 Hainan Province, China. The LIDF types of the vegetables and cotton are mostly close to planophile  
212 based on visual assessment. For convenience, the term 'vegetables' is used to represent all the species  
213 on this site (including cotton).

214 Diurnal measurements of gold coin grass (*Lysimachiae Herba*) were also carried out on  
215 December 18, 2016 at the Sanya Remote Sensing Satellite Data Receiving Station (SYS, 18°18'N,  
216 109°18'E) in Hainan Province, China. The LIDF of this grass was assessed to be close to planophile by  
217 visual inspection.

218 Details of the multi-species measurements described above are summarized in Table 3. All the  
219 spectral measurements were conducted using a customized Ocean Optics QE Pro spectrometer  
220 (Ocean Optics, Dunedin, FL, USA), characterized by a FWHM of 0.31 nm, a SSI of 0.155 nm, and a peak  
221 signal-to-noise ratio (SNR) higher than 1000. For more details of the experiments, please refer to [Du](#)  
222 [et al. \(2017\)](#).

223 Table 3. Parameters of multi-species measurements. Cab stands for leaf chlorophyll a+b content, LIDF  
 224 is the leaf inclination distribution function, and Fc is the fraction of vegetation coverage.

Site	Location	Date	Species	Cab ( $\mu\text{g}/\text{cm}^2$ )	LIDF	Fc
Xiao Tangshan (XTS)	40°11'N 116°27'E	Apr. 8, 9 & 18, Nov. 7, Dec. 8, 2016	Winter wheat	21.22 – 55.29	Spherical	0.15 – 0.79
Nanbin Farm (NBF)	18°22'N 109°10'E	Dec. 18, 2016	Vegetables and cotton	15.22 – 56.68	Planophile	0.28 – 0.91
Sanya Station (SYS)	18°18'N 109°18'E	Dec. 18, 2016	Gold coin grass	40.83	Planophile	0.67

225

### 226 2.2.2 Multi-angular experiments

227 Due to the influence of the canopy structure (i.e. variable gap fraction and LIDF), SIF at the  
 228 canopy level is anisotropic. To test the performance of the SIF downscaling algorithm, we carried out  
 229 a series of multi-angular measurements on a winter wheat canopy during the springs of 2015 and  
 230 2016 at the Xiao Tangshan Farm, Beijing, China, using a multi-angular observation system (MAOS)  
 231 (Yan et al. 2012). The MAOS consists of a two-dimensional automatic goniometer, a spectrometer (QE  
 232 Pro) and a laptop for control. It automatically collects the canopy radiance at different viewing angles,  
 233 together with the downwelling solar irradiance reflected from a reference panel. In this study, the  
 234 multi-angular spectral measurements were taken in the solar principal planes with the view zenith  
 235 angles ranging from  $-60^\circ$  to  $60^\circ$  with an interval of  $10^\circ$  (a smaller interval of  $2^\circ$  was set around the  
 236 hotspot position). The multi-angular measurements of canopy reflectance and SIF were carried out  
 237 under stable sunny weather conditions from 8:00 to 16:30 (local time) during eight days of different  
 238 winter wheat growth stages in 2015 and 2016 (as listed in Table 4). It takes about 7 minutes for each  
 239 set of multi-angular measurements. In total, 32 sets of valid measurements were acquired.

240 Table 4. Parameters of multi-angular measurements on winter wheat at Xiao Tangshan Farm, Beijing,  
 241 China during the springs of 2015 and 2016.

Date	LAI	Cab ( $\mu\text{g}/\text{cm}^2$ )	SZA ( $^\circ$ )
Apr. 3, 2015	1.46	47.9	43.6 – 54.5
Apr. 13, 2015	1.94	51.5	38.4 – 57.8
Apr. 24, 2015	2.40	50.0	32.3 – 47.4
Apr. 25, 2015	2.40	50.0	31.1 – 62.4
Apr. 18, 2016	2.92	47.5	36.4 – 61.5
May 3, 2016	1.93	49.3	29.3 – 50.5
May 4, 2016	1.93	49.3	32.8 – 60.5
May 17, 2016	1.43	45.6	27.4 – 47.6

### 242 2.2.3 SIF retrieval

243 At the canopy level, measured radiance signals comprise the sum of emitted SIF and reflected solar  
 244 radiation. Disentangling both components is frequently based on the Fraunhofer Line Discrimination  
 245 (FLD) principle (Plascyk 1975). Frequently used algorithms include the 3-band FLD (3FLD) (Maier et  
 246 al. 2003), the improved FLD (iFLD) (Alonso et al. 2008) and the spectral fitting methods (SFM)  
 247 (Meroni et al. 2010). According to the analysis by Damm et al (2011) and Liu et al. (2015), the 3FLD  
 248 algorithm is relatively simple and robust for the spectral resolution and SNR of the spectral data  
 249 acquired by our QE Pro spectrometer. Therefore, we estimated SIF at the canopy level with the 3FLD  
 250 algorithm. The selected wavelengths are 757.92 nm, 760.72 nm and 768.87 nm for the O2-A band,  
 251 and 686.44 nm, 687.09 nm and 688.23 nm for O2-B band (Du et al. 2017).

### 252 2.2.4 Estimation of APAR<sub>chl</sub>

253 According to Eq. (2), SIF emission at photosystem level is closely related to APAR (more  
 254 specifically, PAR absorbed by chlorophyll (APAR<sub>chl</sub>)). APAR<sub>chl</sub> is difficult to measure directly, but is  
 255 closely related to the photosynthetically active radiation absorbed by green leaves (APAR<sub>green</sub>) (Du et

256 al. 2017; Porcar-Castell et al. 2014). Liu et al. (2013) proposed an efficient method for making *in-situ*  
 257 measurements of the fraction of  $APAR_{green}$  ( $fAPAR_{green}$ ) for a low vegetation canopy using a digital  
 258 camera and a reference panel. A color image of the canopy with the reference panel is first taken by a  
 259 digital camera at nadir position. Pixels in the image are then classified into green leaves, ground litter,  
 260 sunlit soil, shaded soil, and reference panel. Consequently, the  $fAPAR_{green}$  could be calculated as:

$$261 \quad fAPAR_{green} = \frac{PAR_i - PAR_r - (APAR_{EB} + APAR_{CB})}{PAR_i} \quad (3)$$

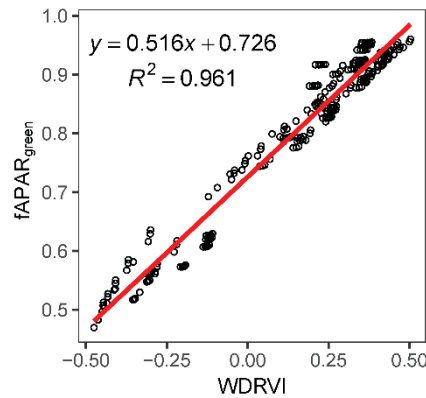
262 where  $PAR_i$  and  $PAR_r$  are, respectively, the incident and reflected (including all exposed components)  
 263 PAR derived from the DN values of the digital image.  $APAR_{EB}$  and  $APAR_{CB}$  are the PAR absorbed by the  
 264 exposed background (EB, including the non-photosynthetic components) and the vegetation-covered  
 265 background (CB) respectively.

266 In the multi-species experiments described in Section 2.2.1,  $fAPAR_{green}$  was measured with the  
 267 digital camera based approach as described above. Unfortunately,  $fAPAR_{green}$  was not measured in the  
 268 multi-angular experiments (Section 2.2.2). To eliminate the saturation effect of the normalized  
 269 difference vegetation index (NDVI), Gitelson (2004) proposed a wide dynamic range vegetation index  
 270 (WDRVI), which has been proved to be well linearly correlated with  $fAPAR_{green}$  (Viña and Gitelson  
 271 2005). The WDRVI is defined as:

$$272 \quad WDRVI = (\alpha R_{NIR} - R_{Red}) / (\alpha R_{NIR} + R_{Red}) \quad (4)$$

273 where  $R_{NIR}$  and  $R_{Red}$  are the reflectances at the near infrared and red band, respectively, and  $\alpha$  is a  
 274 weighting coefficient with a value of 0.1 – 0.2 (Gitelson 2004). Figure 2 shows the relationship  
 275 between WDRVI ( $\alpha = 0.1$ ) and  $fAPAR_{green}$  for SCOPE simulations with different values of the LAI (1 –  
 276 4), leaf chlorophyll content (20 – 80  $\mu\text{g}/\text{cm}^2$ ), SZA (20 – 60 °) and three typical leaf inclination  
 277 distribution functions (planophile, plagiophile and spherical). Therefore, in the multi-angular

278 experiments  $fAPAR_{green}$  was estimated using the linear model based on the WDRVI.



279

280 Figure 2. Linear regression of the fraction of photosynthetically active radiation absorbed by green

281 leaves ( $fAPAR_{green}$ ) on the wide dynamic range vegetation index (WDRVI) computed from SCOPE

282 simulations for canopies with different leaf area indices, leaf chlorophyll contents and leaf inclination

283 distributions.

284 Chlorophyll is the main absorbing compound for PAR in green leaves (Jacquemoud and Baret

285 1990; Porcar-Castell et al. 2014). According to Du et al. (2017),  $fAPAR_{chl}$  can be approximated from

286  $fAPAR_{green}$  with a linear function:

$$287 \quad fAPAR_{chl} = k \times fAPAR_{green} \quad (5)$$

288 where the coefficient  $k$  is related to the leaf chlorophyll content. Analysis of SCOPE simulations

289 conducted by Du et al. (2017) revealed that the value of  $k$  varies from 0.78 to 0.80 for the leaf

290 chlorophyll content from 20 to 60  $\mu\text{g}/\text{cm}^2$ . Since the leaf chlorophyll content of most of the samples

291 was within the range 20 – 60  $\mu\text{g}/\text{cm}^2$  (except for one sample for which the value was 15.22  $\mu\text{g}/\text{cm}^2$ ),

292 we estimated  $fAPAR_{chl}$  using  $k$  equal to 0.79 in this study.

293 The incident photosynthetically active radiation (PAR) was calculated using the radiance

294 reflected from a white reference panel measured by a spectrometer. Consequently, the  $APAR_{chl}$  can be

295 calculated as:



296 
$$\text{APAR}_{\text{chl}} = \text{PAR} \times f\text{APAR}_{\text{chl}} \quad (6)$$

297 **2.3 Airborne measurements**

298 The airborne image, used to evaluate the method introduced in this study, was acquired using  
299 the imaging spectrometer *HyPlant* (Specim, Oulo, Finland). As an airborne demonstrator for the ESA's  
300 Fluorescence Explorer (FLEX) mission, *HyPlant* was specifically designed for the monitoring of  
301 vegetation canopy spectral characteristic parameters, including SIF. There are two modules in  
302 *HyPlant*: the first is the FLUO module, which is used for the SIF measurements and which covers the  
303 range from 670 nm to 780 nm with a high spectral resolution (FWHM = 0.25 nm); the other module is  
304 the DUAL module, which covers a broader spectral range (380 – 2500 nm) with a FWHM of ~ 4 nm  
305 for bands from 380 nm to 970 nm, and of ~ 13.3 nm for bands from 970 nm to 2500 nm. More  
306 technical details about the *HyPlant* configurations and the data processing are available in [Rascher et](#)  
307 [al. \(2015\)](#).

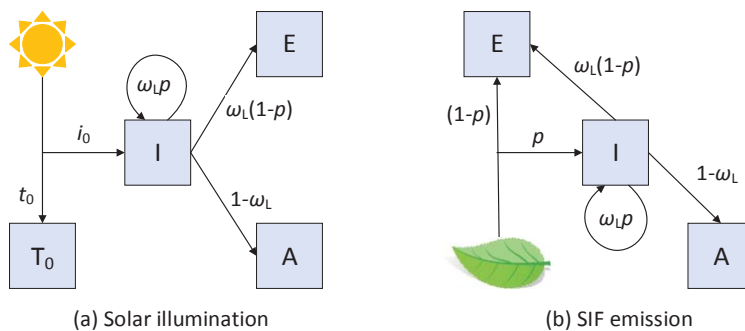
308 In this study, we used a *HyPlant* image acquired at 14:58 (local time) on June 30 2015 over the  
309 study area located in the Ruhr catchment in the central western part of North Rhine-Westphalia,  
310 Germany (50.864° N, 6.452° E). The flight height of 600 m above ground and the swath wide of ~ 400  
311 m resulted in a spatial resolution of 1 m and view zenith angles from 0° to about 16.7° from the  
312 center to the edges of the swath. The flight heading direction was 345.89°, under the solar zenith  
313 angle of 31.89°, and the solar azimuth angle of 217.52°.

314 The far-red (760 nm) and red (687 nm) SIF at canopy level were retrieved using the iFLD  
315 method ([Alonso et al. 2008](#)). A semi-empirical technique that made use of SIF-free reference pixels  
316 (e.g., bare soil) was used to empirically account for uncertainties in estimated upward transmittance

317 of the atmosphere (Damm et al. 2014). For further technical details of SIF retrieval from the *HyPlant*  
 318 image, please refer to Damm et al. (2014) and Wieneke et al. (2016).  $fAPAR_{green}$  was estimated using  
 319 the WDRVI-based linear model that was introduced in Section 2.2.4. As explained in Section 2.2.4, the  
 320 linear relationship between  $fAPAR_{chl}$  and  $fAPAR_{green}$  was assumed also for the *HyPlant* image. The  
 321 missing of information about chlorophyll content made it difficult to decide a proper coefficient for  
 322 the  $fAPAR_{chl}$  -  $fAPAR_{green}$  relationship, so we did not calculate the  $fAPAR_{chl}$  for the *HyPlant* image, but  
 323 used the  $fAPAR_{green}$  directly to evaluate the results of SIF downscaling.

## 324 2.4 Physical analysis of SIF radiation transfer within the canopy

325 The absorption and scattering of SIF photons within the canopy is ruled by the same physical  
 326 interactions as in the case of the reflected radiation. The difference is only the location of the photons'  
 327 source. SIF photons are emitted inside the leaves while, photons of reflected radiation originate from  
 328 the solar illumination at the top of canopy (Figure 3).



329 Figure 3. An illustration of the canopy absorption and scattering model for solar illumination (a) and  
 330 SIF emission (b) assuming with non-reflecting soil background. State  $T_0$  represents photons that go  
 331 through the canopy without interacting with the canopy or being absorbed by the soil; state I  
 332 represents photons that interact with the canopy; state A represents photons absorbed by the canopy;  
 333 and state E represents photons that escape from the canopy.  $p$  is the recollision probability,  $\omega_L$  is

335 the leaf scattering coefficient (single scattering albedo),  $i_0$  is the canopy interception of the  
 336 incoming radiation, which means the probability of an incident photon that will be intercepted by the  
 337 canopy, and  $t_0$  is the probability that a photon can pass through the canopy without any  
 338 interactions ( $t_0 = 1 - i_0$ ).

339

340 Using the concept of recollision probability (so-called 'p-theory') (Stenberg et al. 2016) and  
 341 assuming that the canopy is bounded underneath by a non-reflecting surface (the 'black-soil'  
 342 condition), the four probable states of photons originating from solar illumination are as illustrated  
 343 in Figure 3(a) (Smolander and Stenberg 2005). The canopy absorptance can be expressed as:

$$344 \quad a_i(\lambda) = i_0 \left[ (1 - \omega_L(\lambda)) + \omega_L(\lambda)p(1 - \omega_L(\lambda)) + \omega_L(\lambda)^2 p^2(1 - \omega_L(\lambda)) + \dots \right] = i_0 \frac{1 - \omega_L(\lambda)}{1 - p\omega_L(\lambda)} \quad (7)$$

345 where  $p$  is the recollision probability,  $\omega_L$  is the leaf scattering coefficient (single scattering albedo),  
 346 and  $i_0$  is the canopy interception of the incoming radiation. The canopy scattering can then be  
 347 expressed as:

$$348 \quad s_i(\lambda) = i_0 - a_i(\lambda) = \frac{1-p}{1-p\omega_L(\lambda)} i_0 \omega_L(\lambda) \quad (8)$$

349 The recollision probability describes the multiple scattering process within the canopy. To  
 350 describe the anisotropic escape probability of photons to leave the canopy, the bi-directional gap  
 351 fraction, another spectral invariant, is needed. The term  $(1 - p)$  can be expressed as the integrated  
 352 canopy density over all directions in the unit sphere (Knyazikhin et al. 2013):

$$353 \quad 1 - p = \frac{1}{\pi} \int_{4\pi} \rho(\Omega) |\mu| d\Omega \quad (9)$$

354 where  $\rho(\Omega)$  is the gap fraction for direction  $\Omega$ ,  $4\pi$  denotes the unit sphere, and  $\mu$  is the cosine of  
 355 the polar angle of  $\Omega$ . The canopy structure is the main factor influencing its reflectance anisotropy.

356 According to Knyazikhin et al. (2011 & 2013), the bi-directional reflectance factor (BRF),

357 representing the canopy scattering in a specific observing direction, can be approximately expressed  
 358 as:

$$359 \quad \text{BRF}(\lambda, \Omega_s, \Omega_v) = \frac{\rho(\Omega_s, \Omega_v)}{1 - p\omega_L(\lambda)} i_0 \omega_L(\lambda) \quad (10)$$

360 where  $\rho(\Omega_s, \Omega_v)$  is the bi-directional gap fraction which contains the information of canopy  
 361 structure and the fraction of sunlit and shaded leaves.  $\Omega_s$  and  $\Omega_v$  are the solar and view directions,  
 362 respectively.

363 Similarly, for SIF emission, the probable states of the SIF photons emitted from leaves are as  
 364 illustrated in Figure 3(b). It needs to be noted that, there is also probability for SIF photons to be  
 365 absorbed by the soil without any interactions in the canopy (similar as the state of  $T_0$  in Figure 3(a)).  
 366 However, such probability is considered to be very low, because the SIF photons absorbed by soil  
 367 directly are most likely from the bottom leaves, while the illumination on leaves at the bottom of  
 368 canopy is usually very low for dense canopy. Additionally, for the red-band, the downward SIF at leaf  
 369 level has been proved to be much weaker than the upward SIF (Van Wittenberghe et al. 2015).  
 370 Therefore, the portion of SIF photons directly absorbed by the soil is neglected in this study.  
 371 Accordingly, the canopy absorptance of SIF photons can be expressed as:

$$372 \quad a_f(\lambda) = p(1 - \omega_L(\lambda)) + \omega_L(\lambda)p^2(1 - \omega_L(\lambda)) + \omega_L(\lambda)^2p^3(1 - \omega_L(\lambda)) + \dots = p \frac{1 - \omega_L(\lambda)}{1 - p\omega_L(\lambda)} \quad (11)$$

373 and the canopy scattering of SIF photons as:

$$374 \quad s_f(\lambda) = 1 - a_f(\lambda) = \frac{1 - p}{1 - p\omega_L(\lambda)} \quad (12)$$

375 The scattering processes for SIF photons and for reflected photons by canopy elements are similar.  
 376 Consequently, the SIF escape probability from leaf level to canopy level ( $\varepsilon_{CL} = \text{SIF}_{\text{Canopy}} / \text{SIF}_{\text{Leaves}}$ ) in  
 377 observing direction  $\Omega$  can be expressed as:

$$378 \quad \varepsilon_{CL}(\lambda, \Omega) = \frac{\rho(\Omega)}{1 - p\omega_L(\lambda)} \quad (13)$$

379 If we substitute Eq. (10) into Eq. (13), then we have,

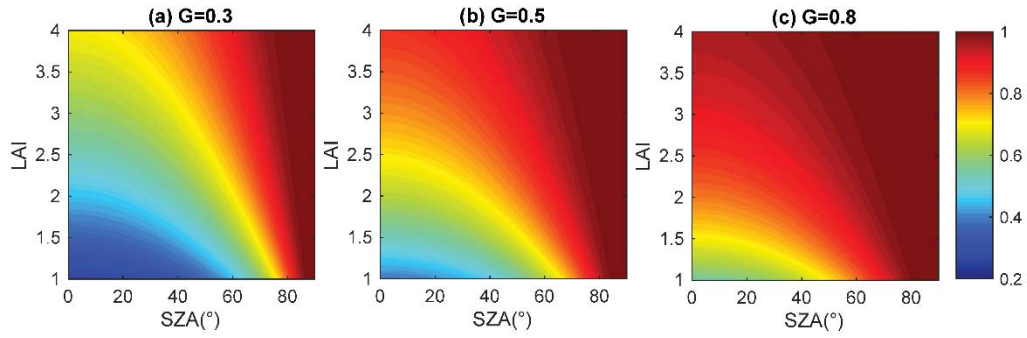
$$380 \quad \varepsilon_{CL}(\lambda, \Omega) = \frac{\text{BRF}(\lambda, \Omega)}{i_0 \omega_L(\lambda)} \quad (14)$$

381 According to the analysis above, under the 'black-soil' condition, the SIF escape probability from  
382 leaf to canopy level is related to the directional reflectance, the canopy interception and the leaf  
383 scattering coefficient. In practice, the directional reflectance can be acquired concurrently with the  
384 SIF measurements, but canopy interception and leaf scattering coefficients can not, in general, be  
385 accurately estimated. The canopy interception is driven by the canopy structure and the actual solar  
386 position. If the clumping effect is assumed to be of minor impact, the canopy interception can be  
387 expressed as (Chen and Black 1992; Ross 2012):

$$388 \quad i_0 = 1 - \exp\left(\frac{-G(\theta) \cdot LAI}{\cos(\theta)}\right) \quad (15)$$

389 where  $\theta$  is the SZA and  $G(\theta)$  is the mean projection coefficient for foliages on a plane  
390 perpendicular to  $\theta$ . The function,  $G$ , is determined by the LIDF. For the spherical leaf inclination  
391 distribution type with an LIDF that is a sine function, the value of  $G$  is 0.5 and is independent of  $\theta$ .  
392 For other values of the LIDF, the value of  $G$  ranges from 0 to 1 when  $\theta$  varies from  $0^\circ$  to  $90^\circ$ , and  
393 generally converges to 0.5 when  $\theta$  is approximately  $57.3^\circ$  for all LIDF types (Nilson 1971; Ross 2012;  
394 Ryu et al. 2010).  $G(\theta) \cdot LAI$  represents the projected LAI in the solar direction.

395 Figure 4 shows the values of  $i_0$  for different values of  $G$ , LAI and SZA. For a dense canopy with  
396 large values of LAI and  $G$ , the value of  $i_0$  is close to 1, while for sparse canopies, the value of  $i_0$  shows a  
397 large degree of variability.



398

399

Figure 4. Values of the canopy interception of the incoming radiation ( $i_0$ ) for different  $G$  function

400

values, leaf area index (LAI) and solar zenith angle (SZA) combinations, calculated using Eq. (15).  $G$

401

function is the mean projection coefficient for foliages on a plane perpendicular to the solar zenith

402

direction.

403

Since absorption by chlorophyll  $a$  molecules is very weak at the far-red band, leaf single

404

scattering albedo ( $\omega_L$ ) is strongly influenced by chlorophyll content only in the red wavelengths of

405

SIF emission.  $\omega_L$  at the far-red band is, therefore, almost independent of chlorophyll content and it is

406

driven by a minor absorptance of leaf tissue biochemical compounds. Figure 5 shows the variations

407

of  $\omega_L$  at the far-red (760 nm) and red (687 nm) bands simulated by the Fluspect model for leaf

408

chlorophyll content from 10 to 80  $\mu\text{g}/\text{cm}^2$ . As expected, the value of  $\omega_L$  at the far-red band is almost

409

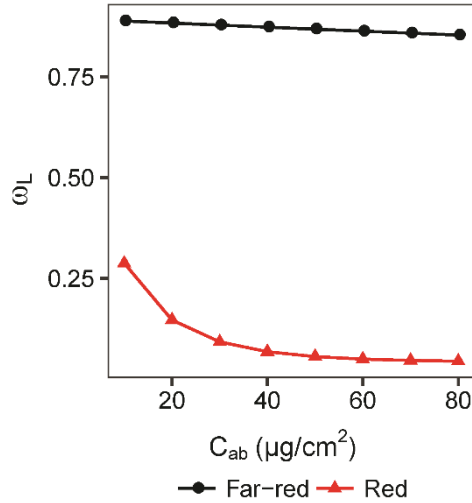
invariant, reaching values between 0.853 and 0.888, while it varies from 0.044 to 0.287 for the red

410

band, where the absorption by chlorophyll is strong. It exhibits a large variation in the value of  $\omega_L$ ,

411

especially for the chlorophyll content lower than 40  $\mu\text{g}/\text{cm}^2$ .



412

413 Figure 5. Values of  $\omega_L$  at the far-red (760 nm) and red (687 nm) bands simulated by the Fluspect  
 414 model for different values of the leaf chlorophyll content. The values for other input parameters for  
 415 the Fluspect model were set as default (same as in Table 1).

416 Another fact needs to be noted is, the spectral invariant theory ignores the difference between  
 417 the leaf reflectance and leaf transmittance (combined as  $\omega_L$ ). Therefore, the spectral invariant theory  
 418 performs well at the far-red band, where multi-scattering dominates, but not so well at the red band,  
 419 where single scattering dominates. Nevertheless, the  $\varepsilon_{CL}$  and  $\frac{\text{BRF}}{i_0 \omega_L}$  are still proportional at the red  
 420 band (Yang and Van der Tol. 2018). This problem is discussed in Section 4.4.

421 The escape probability for SIF from the PS level to the leaf level ( $\varepsilon_{LP} = \text{SIF}_{\text{Leaves}}/\text{SIF}_{\text{PS}}$ ) is related  
 422 to the leaf internal absorptance (from the photosystems to the leaf surface). The leaf internal  
 423 absorptance at the spectral range of the SIF emission is caused mainly by the leaf chlorophyll content,  
 424 but the relationship is non-linear, because the increment in radiation absorption per unit of  
 425 chlorophyll decreases at high chlorophyll content (Adams et al. 1990; Gitelson et al. 1998;  
 426 Porcar-Castell et al. 2014). Besides, chlorophyll molecules are distributed in different cell layers of  
 427 leaf mesophyll tissues. Although the radiative transfer processes at the molecular-level are complex

428 for accurate modelling,  $\varepsilon_{LP}$  can be expressed as a non-linear function of the chlorophyll content (Cab)  
429 and wavelength as:

$$430 \quad \varepsilon_{LP}(\lambda) \approx f(\text{Cab}, \lambda) \quad (16)$$

431 Consequently, the SIF escape probability from the PS level to the canopy level ( $\varepsilon_{CP}$ ) can be  
432 expressed as:

$$433 \quad \varepsilon_{CP}(\lambda, \Omega) = \varepsilon_{LP}(\lambda) \cdot \varepsilon_{CL}(\lambda) \approx f(\text{Cab}, \lambda) \cdot \frac{\text{BRF}(\lambda, \Omega)}{i_0 \omega_L(\lambda)} \quad (17)$$

434 To summarize, the SIF escape probability from the PS level to the canopy level can be  
435 approximately modeled using the canopy BRF, canopy interceptance and Cab, under the assumption  
436 of 'black-soil' condition. For remote sensing observations, the directional reflectance is available.  
437 However, the  $i_0$  and  $\omega_L$  is not easy to be accurately measured or estimated. According to Eq. (15) and  
438 Figure (4),  $i_0$  is related to canopy structure, which is not easy to be accurately retrieved with optical  
439 remote sensing approaches. It is not possible to observe leaf reflectance and transmittance directly at  
440 canopy level, and  $\omega_L$  varies among different leaves. So  $\omega_L$  is also difficult to be estimated from  
441 remote sensing observations at canopy level. But for a dense canopy and for leaves with a relatively  
442 high value of Cab,  $i_0$  and  $\omega_L$  are relatively stable, and the directional reflectance is the main factor  
443 that influences  $\varepsilon_{CP}$ , especially at the far-red band.

## 444 **2.5 Estimation of $\varepsilon_{CP}$ and $\varepsilon_{CL}$ using the random forest approach**

445 Given the difficulties involved in acquiring the parameters required for physical modelling of the  
446 SIF downscaling, a statistical model based on the Random Forest (RF) regression, which is one of the  
447 most effective machine learning models for predictive analytical approaches (Breiman 2011), was  
448 trained on the dataset simulated in SCOPE to estimate  $\varepsilon_{CP}$ .



449 As shown in [Section 2.4](#), the BRF has significant impact on  $\varepsilon_{CP}$ . Taking all other factors together  
450 as  $f_{CP}$ , Eq. (17) can be modified thus:

$$451 \quad \varepsilon_{CP}(\lambda, \Omega) = f_{CP} \cdot \text{BRF}(\lambda, \Omega) \quad (18)$$

452 where  $f_{CP}$  is the ratio of  $\varepsilon_{CP}$  to BRF. In the SCOPE simulations,  $\varepsilon_{CP}(\lambda, \Omega)$  and  $\text{BRF}(\lambda, \Omega)$  can be  
453 simulated directly, and  $f_{CP}$  later calculated. As  $f_{CP}$  is acquired from SCOPE simulation instead of  
454 physical analysis, the assumption of 'black-soil' condition for Eq. (17) is no longer needed here.  
455 Similarly,  $\varepsilon_{CL}$  can be expressed as,

$$456 \quad \varepsilon_{CL}(\lambda, \Omega) = f_{CL} \cdot \text{BRF}(\lambda, \Omega) \quad (19)$$

457 We only estimated  $f_{CP}$  or  $f_{CL}$  with the random forest approach to increase robustness of estimated  
458  $\varepsilon_{CP}$  and  $\varepsilon_{CL}$ . Directional reflectance was obtained from measurements or simulations.  $f_{CP}$  and  $f_{CL}$  are  
459 mainly related to the leaf scattering coefficient and canopy structure. These kinds of information can  
460 be derived from directional reflectance at different bands and from various vegetation indices.

461 At the near infrared band, the canopy reflectance is dominated by the scattering effect, which  
462 primarily originates from the leaf and canopy structure. At the red band, the canopy reflectance is  
463 dominated by the absorption effect of chlorophyll pigments ([Colwell 1974](#); [Sims and Gamon 2002](#)). It  
464 has been demonstrated that the red-edge band is important for the estimation of  $C_{ab}$  as it is less  
465 impacted by the absorption saturation effect for a high  $C_{ab}$  than the red band ([Clevers and Gitelson](#)  
466 [2013](#); [Dash and Curran 2004](#); [Gitelson et al. 2005](#); [Malenovský et al. 2013](#)). Several vegetation indices  
467 (VIs), based on the reflectance at the red, red-edge and near infrared bands, have been developed for  
468 the retrieval of vegetation parameters. In this study, the NDVI, simple ratio (SR) and the MERIS  
469 terrestrial chlorophyll index (MTCI) were used (formulae and references in Table 5). Considering the  
470 possible available wavelength range of spectral measurements for SIF retrieval, and to avoid the SIF

471 in-filling effect at the oxygen absorption bands at about 687 nm and 760 nm, we selected 685 nm as  
 472 the red band, 710 nm as the red-edge band, and 758 nm as the near infrared band for the calculation  
 473 of the Vis. The NDVI is sensitive to the canopy structural parameters such as LAI (Soudani et al. 2012).  
 474 The SR is sensitive to the chlorophyll absorption at the red band. Finally, MTCI was designed for  
 475 estimation of the chlorophyll content (Dash and Curran 2004). Consequently, NDVI, SR and MTCI,  
 476 together with the canopy directional reflectance at 685 nm, 710 nm and 758 nm, were selected as the  
 477 potential input variables to establish the RF regression. The scatter matrix of the relationships among  
 478 the potential input variables and  $f_{CP}$  is provided in the Supplementary materials (Figure S1). The final  
 479 selection of inputs was decided by testing the performance of RF regression with different  
 480 combinations of the six potential variables, which is shown in Section 3.1.

481 Table 5. Mathematical formulations and references for the Vis ( $R_{758}$ ,  $R_{685}$  and  $R_{710}$  stand for the  
 482 directional reflectance at 758 nm, 685 nm and 710 nm, respectively).

Equation	Reference
$NDVI = (R_{758} - R_{685}) / (R_{758} + R_{685})$	(Rouse et al. 1973)
$SR = R_{758} / R_{685}$	(Jordan 1969)
$MTCI = (R_{758} - R_{710}) / (R_{710} - R_{685})$	(Dash and Curran 2004)

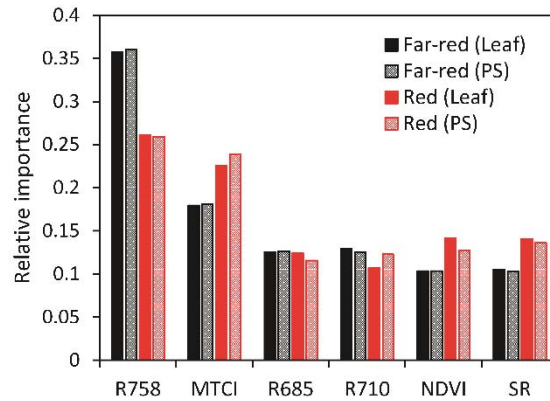
483  
 484 500 decision trees were used to construct the RF model, and the minimum number of terminal  
 485 nodes were set as 5. The SCOPE simulations (cf., Section 2.1.1), which cover most common vegetation  
 486 conditions, were employed for the training of the RF. SIF of the red (687 nm) and far-red (760 nm)  
 487 bands at canopy, leaf, and PS levels were simulated by the SCOPE model, together with the directional  
 488 reflectance at 685 nm, 710 nm and 758 nm. Consequently,  $f_{CP}$  and  $f_{CL}$  could be calculated according to  
 489 Eq. (18) and Eq. (19), respectively.

490

## 491 **3. Results**

### 492 **3.1 Selection of the inputs for the RF regression**

493 To optimize the inputs for the RF regression, we tested the performance of the RF model with  
494 different combinations of the six potential input parameters explained in Section 2.5. Firstly, all the  
495 six potential parameters were used as the inputs for the RF regression to calculate their relative  
496 importance using the mean decrease accuracy (MDA) method based on the concept of out-of-bag  
497 (OOB) error. The OOB error is a parameter that represents the RF prediction error. It is considered as  
498 the mean prediction error on each training sample  $x_i$ , which uses only the trees that did not have  $x_i$  in  
499 their bootstrap sample (Breiman, 2001). To measure the importance of the  $j$ -th feature for training,  
500 the values of the  $j$ -th feature are permuted among the training data and the OOB error is computed  
501 for each perturbed data set. The importance score for the  $j$ -th feature is computed by averaging the  
502 difference in the OOB error before and after the permutation over all trees. Figure 6 shows the  
503 relative importance of the input variables of the RF model for SIF downscaling from canopy level to  
504 leaf level or PS level. These results indicate that the far-red directional reflectance and MTCI were  
505 found as the most important variables for the SIF downscaling model at both the far-red and red  
506 bands, while the importance of the directional reflectance at the red and red-edge bands, the NDVI,  
507 and the SR was on similar, lower level.



508

509 Figure 6. Relative importance of input variables of the RF model for SIF downscaling from canopy

510 level to leaf level or PS level. R<sub>758</sub>, R<sub>685</sub> and R<sub>710</sub> stand for the directional reflectance at 758 nm, 685

511 nm and 710 nm, respectively.

512 Secondly, the performance of the RF model was tested with different combinations of input

513 parameters. 2/3 of the SCOPE simulations were randomly selected to train the RF model, and the

514 remaining 1/3 were used as reference samples to evaluate the performance of the trained model with

515 the relative root-mean-square error with respect to mean value (RRMSE) and the coefficient of

516 determination (R<sup>2</sup>). To reduce the random errors, for each combination of input parameters, 30 RF

517 models were trained and the RRMSE and R<sup>2</sup> were averaged. The results are listed in Table 6. In

518 addition, a significance test was also carried out for further comparing the performance of different

519 combinations of input parameters (shown in Table S1). For the far-red band, when four parameters

520 (R<sub>758</sub>, MTCI, R<sub>685</sub>, R<sub>710</sub>) were used, the RRMSE and R<sup>2</sup> became relatively stable, and the difference

521 comparing with using all six parameters became insignificant (the p-value is 0.273 and 0.335 for leaf

522 level and PS level, respectively). When adding more input parameters (SR and NDVI), the variation of

523 RRMSE was less than 0.5%. For the red band, in contrast, the difference between the performance of

524 using four input parameters (R<sub>758</sub>, MTCI, R<sub>685</sub>, R<sub>710</sub>) and using all six parameters was still significant

525 for both leaf level and PS level (p-value < 10<sup>-9</sup>, see Table S1). When adding SR or NDVI as the input  
 526 parameters, the RRMSE of the RF model was improved clearly (the RRMSE was reduced about 10%  
 527 for the leaf level and about 6% for the PS level). But the performance of the RF model had no  
 528 significant improvement when using both SR and NDVI (p-values > 0.300, see Table S1). The results  
 529 also indicated that, although the vegetation indices can be calculated using the reflectance at the  
 530 three wavelengths, they can still provide important information for the estimation of  $f_{CL}$  and  $f_{CP}$ ,  
 531 because vegetation indices are able to enhance some information by non-linearly combining the  
 532 reflectance at different wavelengths, and the special non-linear relationship may be difficult for the  
 533 RF regression to find out.

534 According to the results,  $R_{758}$ , MTCI,  $R_{685}$ , and  $R_{710}$  were selected as the input parameters of the  
 535 RF model for the estimation of  $f_{CL}$  and  $f_{CP}$  at the far-red band, while  $R_{758}$ , MTCI,  $R_{685}$ ,  $R_{710}$ , and SR were  
 536 selected for the red band.

537 Table 6. The relative root-mean-square error (RRMSE) and the coefficient of determination ( $R^2$ ) of RF  
 538 models for the ratios of SIF escape probability to BRF ( $f_{CL}$  for leaf level to canopy level and  $f_{CP}$  for  
 539 photosystem level to canopy level) at far-red and red bands with different combinations of input  
 540 parameters.

Input parameters	$f_{CL}$ (Far-red)		$f_{CP}$ (Far-red)		$f_{CL}$ (Red)		$f_{CP}$ (Red)	
	RRMSE	$R^2$	RRMSE	$R^2$	RRMSE	$R^2$	RRMSE	$R^2$
$R_{758}$ , $R_{710}$ , $R_{685}$	0.0492	0.871	0.0569	0.901	0.0981	0.960	0.0942	0.954
$R_{758}$ , MTCI, $R_{685}$	0.0463	0.886	0.0502	0.928	0.0990	0.961	0.0969	0.957
$R_{758}$ , MTCI, $R_{685}$ , $R_{710}$	0.0462	0.886	0.0489	0.931	0.0871	0.964	0.0849	0.961
$R_{758}$ , MTCI, $R_{685}$ , $R_{710}$ , SR	0.0461	0.887	0.0487	0.931	0.0804	0.968	0.0797	0.964
$R_{758}$ , MTCI, $R_{685}$ , $R_{710}$ , NDVI	0.0463	0.886	0.0488	0.930	0.0800	0.969	0.0797	0.964
$R_{758}$ , MTCI, $R_{685}$ ,	0.0461	0.887	0.0487	0.931	0.0799	0.969	0.0795	0.966

541

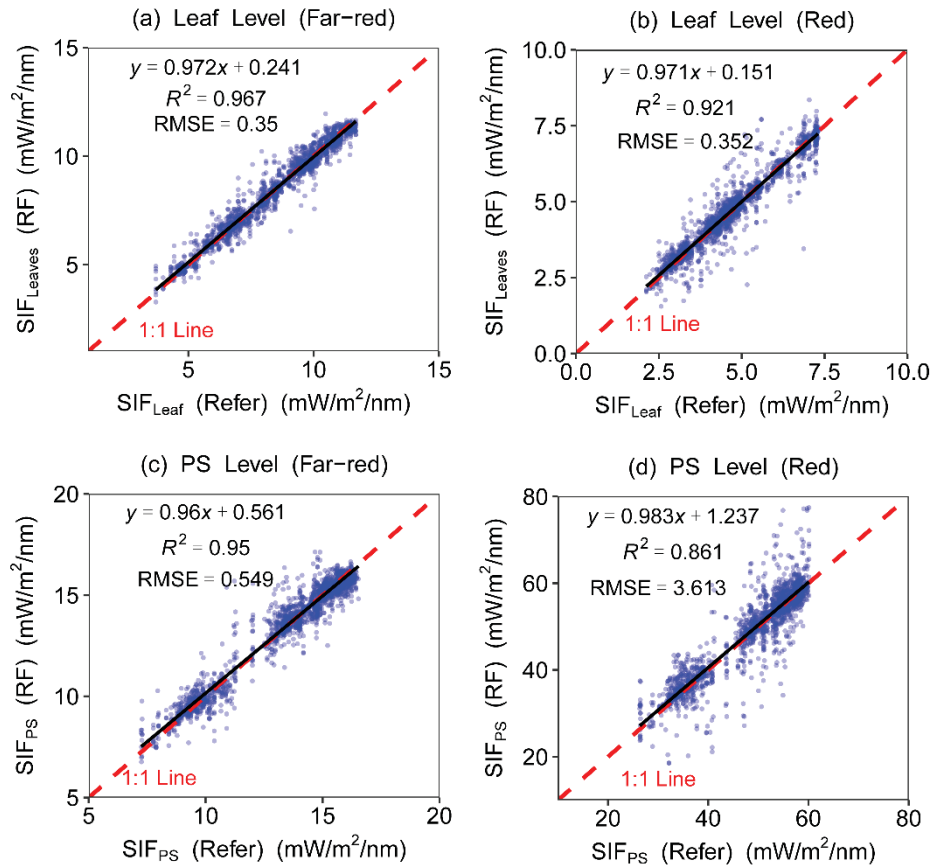
542 **3.2 Evaluation of the SIF downscaling accuracy using SCOPE and DART simulations**

543 SCOPE and DART based simulations were used in the first instance to quantitatively evaluate the  
544 performance of the RF approach for SIF downscaling. SCOPE allows simulating SIF values at the  
545 canopy, leaf, and PS levels, but there is no module for SIF simulation at PS level in DART, so the DART  
546 model is only able to provide the SIF values at the canopy and leaf levels.

547 The SCOPE simulations were first used for accuracy assessments at the leaf and PS levels. 2/3 of  
548 the SCOPE simulations were randomly selected to train the RF model, and the remaining 1/3 was  
549 used for validation. Figure 7 shows a comparison of the far-red and red SIF estimated by the RF  
550 approach with the reference SIF simulated by SCOPE for the leaf and PS levels. In general, the  
551 estimated values of SIF at the leaf and PS levels matched well with the reference values. Most of the  
552 points were located near to the 1:1 line, and the values of the coefficient of determination ( $R^2$ ) were  
553 higher or close to 0.9. The estimation of red SIF at the PS level was not as robust as that of the far-red  
554 SIF, but the root-mean-square error (RMSE) was still as low as 3.613 mW/m<sup>2</sup>/nm, resulting in the  
555 relative root-mean-square error (RRMSE) of 7.299%. The relationship of SIF at canopy level and leaf  
556 level, SIF at leaf level and PS level, SIF at canopy level and PS level from SCOPE simulations are also  
557 provided in the Supplementary materials (Figure S2) for comparisons.

558

559



560

561

562 Figure 7. Comparison of far-red (760 nm) and red (687 nm) SIF estimated by the RF approach with  
 563 reference SIF simulated by SCOPE for leaf and PS levels.  $R^2$  is the coefficient of determination, and  
 564 RMSE is the root-mean-square error.

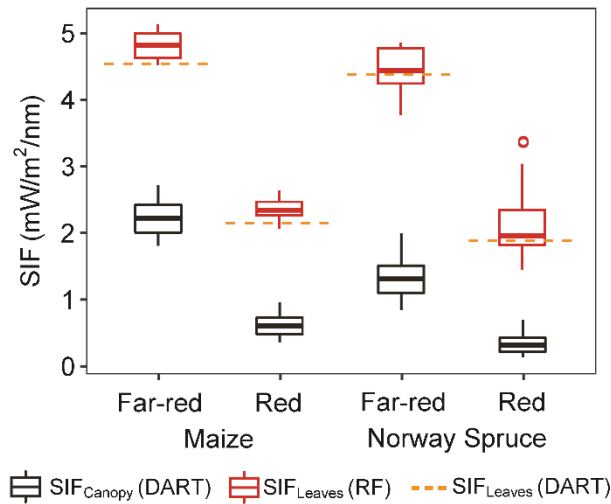
565

566 Simulations performed in the 3-D DART model (cf., [Section 2.1.2](#)) were used for further  
 567 evaluation of the RF model trained by the SCOPE simulations. Since DART produced canopy and leaf  
 568 SIF simulations for two modeled canopies of maize and spruce, only the downscaling of SIF from the  
 569 canopy level to the leaf level could be evaluated. Figure 8 shows SIF simulated by DART at canopy and  
 570 leaf level vs. estimates of downscaled SIF. The leaf SIF estimates for the maize canopy were more  
 571 robust (less variable) for the spruce canopy, but the downscaled estimates matched well the

572 reference values in both cases. The RRMSE between the estimated and reference far-red and red leaf  
 573 SIF was 7.42% and 12.10% for the maize canopy, and 7.57% and 25.92% for the spruce canopy.

574

575



576

577 Figure 8. Boxplot of far-red (740 nm) and red (687 nm) SIF simulated by DART for maize and spruce  
 578 canopies and corresponding downscaled leaf SIF using the Random Forest (RF) model. The orange  
 579 dashed line shows the reference values of SIF at leaf level, as simulated in DART by Fluspect. The  
 580 bottom and top of each box represent the first and third quartiles, respectively, the thick horizontal  
 581 line in the box is the median, the whiskers show the maximum/minimum values within 1.5 times the  
 582 interquartile range (IQR, the difference between the third and the first quartiles), and the circles  
 583 show the outliers out of 1.5IQR. The units of mW/m<sup>2</sup>/nm/sr were applied to SIF at canopy level as  
 584 well as leaf level to make the values comparable.

585

586 The evaluation carried out on datasets simulated by two different radiative transfer models  
 587 using different vegetation representations and solar-viewing geometries revealed accurate and



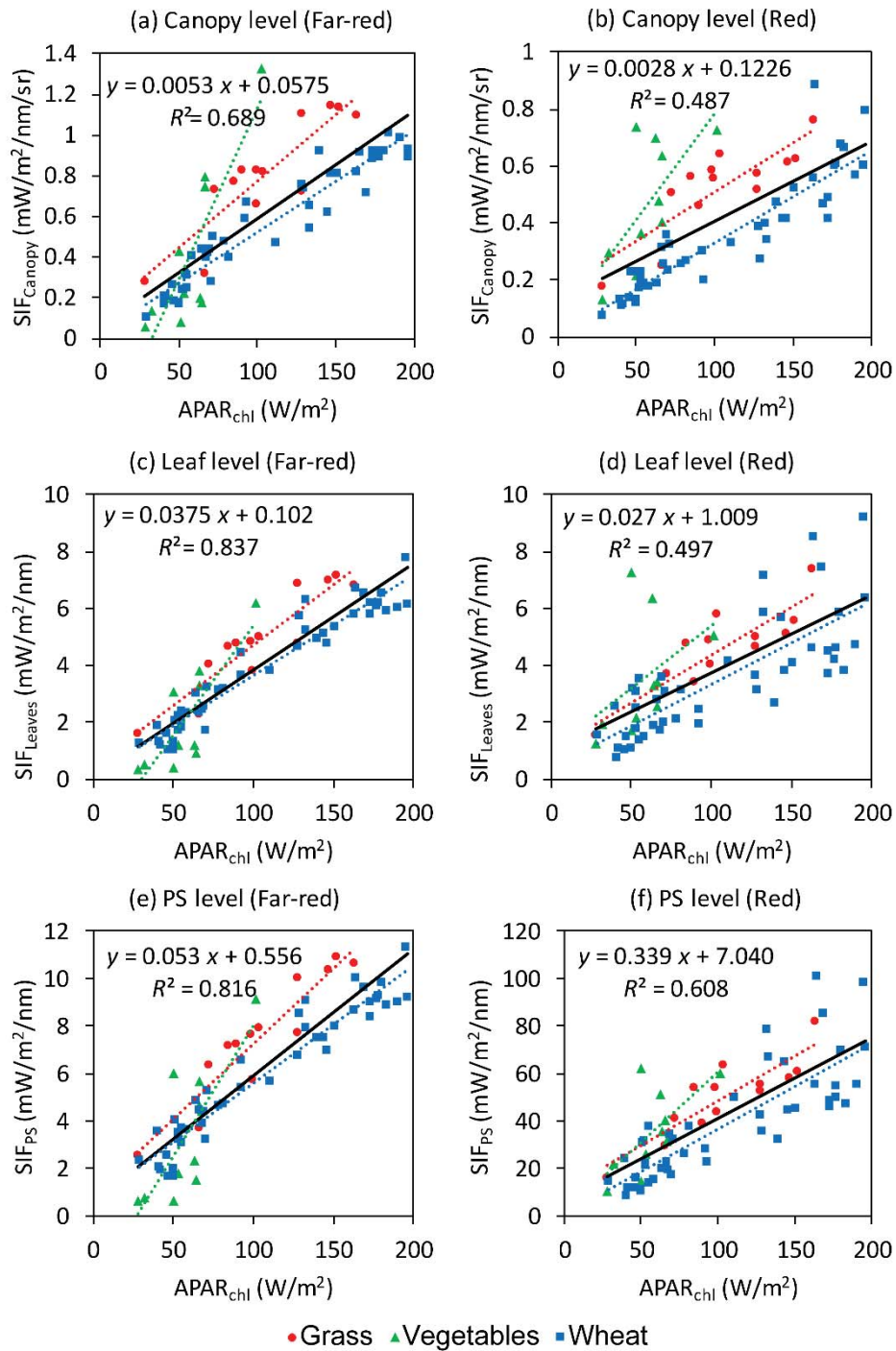
588 robust performance of the RF downscaling approach, especially for the far-red SIF. The lower  
589 accuracy for the red band is discussed in Section 4.4.

### 590 **3.3 Evaluation of SIF downscaling through in-situ multi-species experiments**

591 Under conditions with no stress and with high light, the SIF yield varies little (Van der Tol et al,  
592 2014; Damm et al. 2015), so the total SIF emission of a plant at PS level is strongly related to  $APAR_{chl}$ .  
593 However, SIF at the canopy level is strongly influenced by re-absorption and scattering effects, which  
594 are related to leaf pigments and the canopy structure. Therefore, we compared  $APAR_{chl}$  measured for  
595 multi-species canopies of different structures with SIF downscaled to PS level with the RF approach  
596 (cf., Section 2.2.1).

597 Figure 9 shows the relationship between  $APAR_{chl}$  and nadir-observed canopy SIF, SIF at leaf level  
598 and SIF at PS level estimated by the RF approach. The relationship between  $APAR_{chl}$  and  $SIF_{canopy}$   
599 varied for different species, while the slope of the linear regression lines of the SIF- $APAR_{chl}$  models for  
600 different species became closer to each other when SIF was downscaled from canopy level to PS level,  
601 which indicated that the relationship between  $APAR_{chl}$  and  $SIF_{PS}$  was less species-dependent. At the  
602 far-red band, the values of  $R^2$  increased significantly when SIF was downscaled from canopy level to  
603 leaf level, but did not vary much (decreased a little) when SIF was further downscaled to the PS level.  
604 Differently, at the red band, the  $R^2$  for the PS level was much higher than that for the leaf level.

605



606

607 Figure 9. The relationship between  $APAR_{chl}$  and canopy SIF observed at nadir (a, b), SIF at leaf level (c,

608 d) and PS level (e, f) estimated by the RF approach for several different species (grass, various

609 vegetables and wheat). The colored dash lines are the linear regression lines for specific species. The

610 black solid lines and the equations are the linear regression lines and models for all the samples.

611

612 Table 7. Linear regression models of the SIF-APAR<sub>chl</sub> relationship for different species at canopy, leaf  
 613 and photosystem (PS) levels. The ‘CV of slopes’ are the coefficients of variation of the slopes for  
 614 different species at specific levels.

Band	Level	Grass	Vegetables	Wheat	CV of slopes
Far-red	Canopy	$y = 0.0065x + 0.122$ $R^2 = 0.7873$	$y = 0.017x - 0.5606$ $R^2 = 0.7078$	$y = 0.005x + 0.0213$ $R^2 = 0.9182$	0.688
	Leaf	$y = 0.0423x + 0.468$ $R^2 = 0.8567$	$y = 0.0778x - 2.3764$ $R^2 = 0.6803$	$y = 0.0352x + 0.1319$ $R^2 = 0.9292$	0.441
	PS	$y = 0.0634x + 0.8884$ $R^2 = 0.8786$	$y = 0.1108x - 3.0645$ $R^2 = 0.6122$	$y = 0.0495x + 0.6585$ $R^2 = 0.9227$	0.431
Red	Canopy	$y = 0.0035x + 0.1653$ $R^2 = 0.7068$	$y = 0.0074x + 0.0417$ $R^2 = 0.4672$	$y = 0.0033x + 0.0056$ $R^2 = 0.8232$	0.488
	Leaf	$y = 0.0336x + 0.9976$ $R^2 = 0.7621$	$y = 0.0444x + 0.9485$ $R^2 = 0.1964$	$y = 0.0292x + 0.4097$ $R^2 = 0.6182$	0.219
	PS	$y = 0.3808x + 10.094$ $R^2 = 0.7719$	$y = 0.5914x + 1.3347$ $R^2 = 0.4455$	$y = 0.358x + 1.031$ $R^2 = 0.6831$	0.290

615 The linear regression models of the SIF-APAR<sub>chl</sub> relationship for different species at canopy, leaf  
 616 and PS levels were summarized in Table 7, and the coefficients of variation (CV) of the slopes for  
 617 different species at each level were also calculated. For grass and wheat, the relationships between  
 618 SIF at all levels and APAR were close to linear. But for the vegetation, the relationship was some  
 619 erratic, especially at the red band. The reason may partly due to the measurement errors. For both  
 620 the far-red and red bands, the CV of slopes for different species decreased significantly when SIF was  
 621 downscaled from canopy level to leaf or PS level. At the far-red band, both the CV of slopes and the R<sup>2</sup>  
 622 of each model at the PS level were very close to that at the leaf level. At the red band, the CV of slopes  
 623 at the PS level was some higher than that for the leaf level, but the R<sup>2</sup> of the regression model for all  
 624 the three species were higher than that at the leaf level, especially for the model of the vegetables

625 (increased from 0.1964 to 0.4455 when SIF was downscaled from leaf level to PS level).

626

627 The results shown in Figure 9 and Table 7 confirmed that the species-dependency of the  
628 SIF-APAR<sub>chl</sub> relationship could be reduced by SIF downscaling from canopy level to leaf or PS level.  
629 These results also indicated that the canopy structure is the main factor influencing the far-red SIF  
630 escape probability, while the leaf internal absorption mainly influence the red SIF.

### 631 **3.4 Evaluation of SIF downscaling using multi-angular experiments**

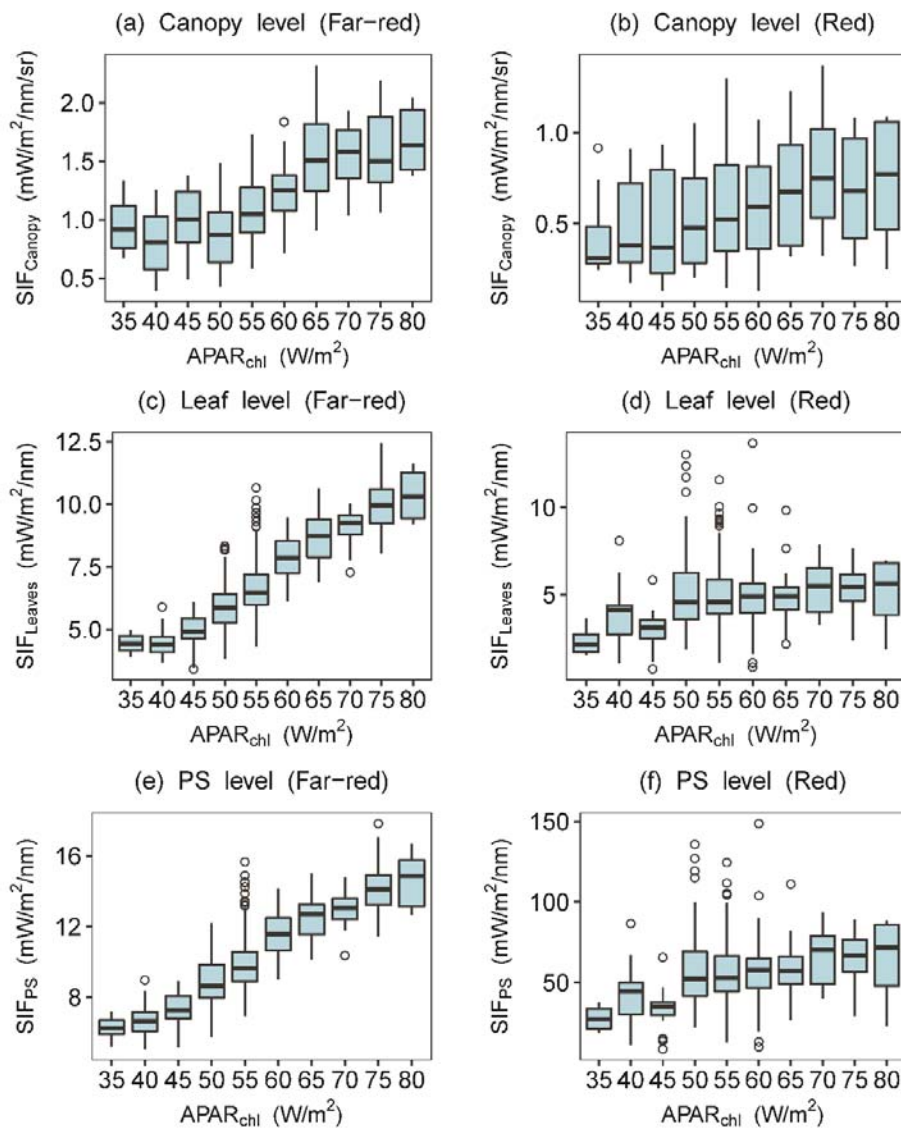
632 The SIF emission at the PS level can be regarded as isotropic whereas, due to re-absorption and  
633 scattering within the canopy, the observed SIF at the canopy level is obviously anisotropic.  
634 Consequently, multi-angular measurements of a winter wheat canopy (cf., [Section 2.2.2](#)) were used  
635 for further evaluation of the SIF downscaling approach, in particular its potential to normalize the  
636 anisotropy in the SIF measurements.

637 Figure 10 shows the relationship between APAR<sub>chl</sub> and values of the multi-angular observed SIF  
638 at canopy level, leaf level or PS level in the form of boxplots. The APAR<sub>chl</sub> values were divided into  
639 groups with an interval of 5W/m<sup>2</sup>. Moreover, for each set of multi-angular observations (with  
640 different VZAs in the solar principal plane), we calculated the coefficients of variation (CV) of SIF at  
641 canopy level, leaf level or PS level, as shown in Figure 11. Lower CV values indicated less anisotropy  
642 of SIF. The results shown in Figure 10 and Figure 11 demonstrate that, for each APAR<sub>chl</sub> level, SIF at  
643 canopy level varied substantially at both the far-red and red bands due to its anisotropic  
644 characteristics caused by the scattering within the canopy. Computed CV values varied from 0.12 to  
645 0.32 for the far-red band, and from 0.33 to 0.61 for the red band. The value of R<sup>2</sup> for the relationship

646 between  $SIF_{Canopy}$  and  $APAR_{chl}$  is 0.43 and 0.09 for the far-red band and the red band, respectively. The  
647 estimated SIF at the leaf level and PS level was much more closely related to  $APAR_{chl}$  and the variation  
648 of SIF in predefined  $APAR_{chl}$  level was visibly reduced. At the far-red band, the value of  $R^2$  for the  
649 relationship between  $SIF_{PS}$  and  $APAR_{chl}$  was 0.76, and the values of CV for  $SIF_{PS}$  varied from 0.04 to  
650 0.18. At the red band, there were some outliers in the boxplot which indicates a less robust  
651 performance of the SIF downscaling. Overall, the value of  $R^2$  for the relationship between  $SIF_{PS}$  and  
652  $APAR_{chl}$  was 0.14, and the values of CV for  $SIF_{PS}$  for most sets of multi-angular observations were also  
653 reduced and lie within the range 0.14 to 0.42. The results for SIF downscaling to leaf level and to PS  
654 level were very similar; because the leaf absorptance did not vary a lot (the chlorophyll contents for  
655 all the samples were very similar as shown in Table 4). The results also confirmed the assumption  
656 that the SIF emission at both leaf level and PS level is isotropic.

657

658



659

660 Figure 10. The relationship between  $APAR_{chl}$  and multi-angular observations of SIF at canopy level (a,

661 b) and estimated SIF at leaf level (c, d) or PS level (e, f) by the RF approach. The bottom and top of the

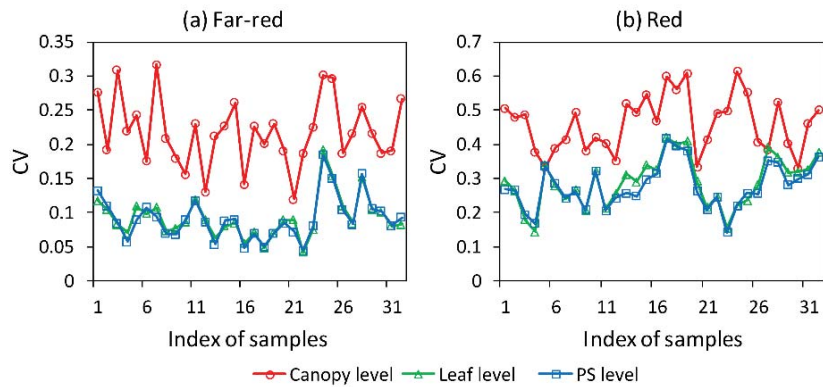
662 boxes correspond to the first and third quartiles, the thick horizontal line in each box is the median,

663 the whiskers show the maximum/minimum values within 1.5 IQR, and the circles show the outliers

664 that lie outside 1.5 IQR. The multi-angular observations were conducted on a wheat canopy. The

665 averaged number of observations per APAR interval is 49.

666



667

668 Figure 11. The coefficients of variation (CV) of the observed canopy SIF and leaf or PS SIF estimated  
 669 by the RF approach for each set of multi-angular observations in the solar principal plane. Each  
 670 sample was calculated using a set of multi-angular observations taken within 7 minutes and the SIF  
 671 at PS level was expected to be constant.

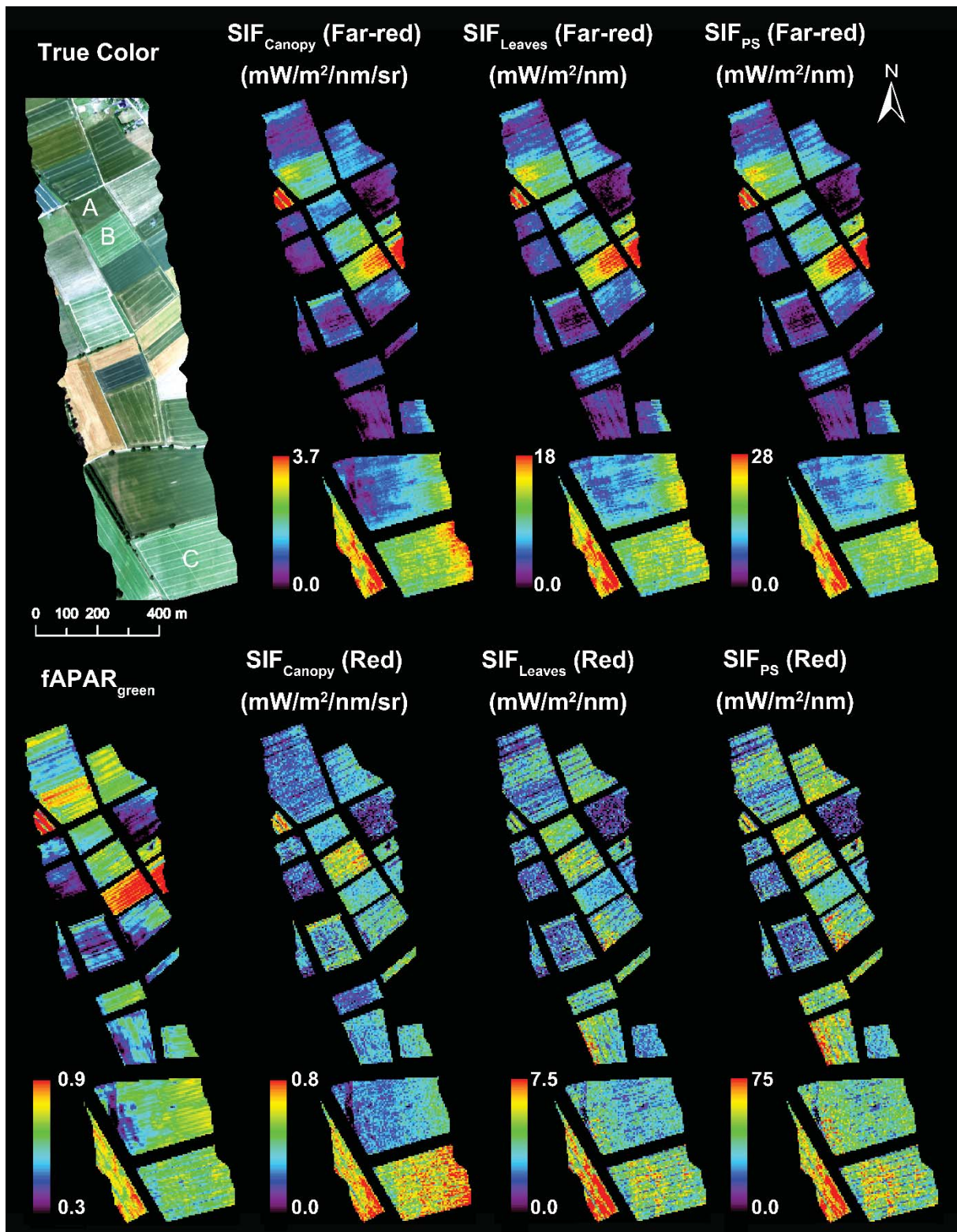
672

673

### 674 3.5 Downscaling of canopy SIF retrieved from *HyPlant* image

675 Besides the ground-based measurements, in this study, a *HyPlant* image was also employed for  
 676 the evaluation of the SIF downscaling results. Before application of SIF downscaling, the original pixel  
 677 size of the *HyPlant* was reduced from 1 m × 1 m to 5 m × 5 m in order to reduce the influence of  
 678 sensor noise.

679



680

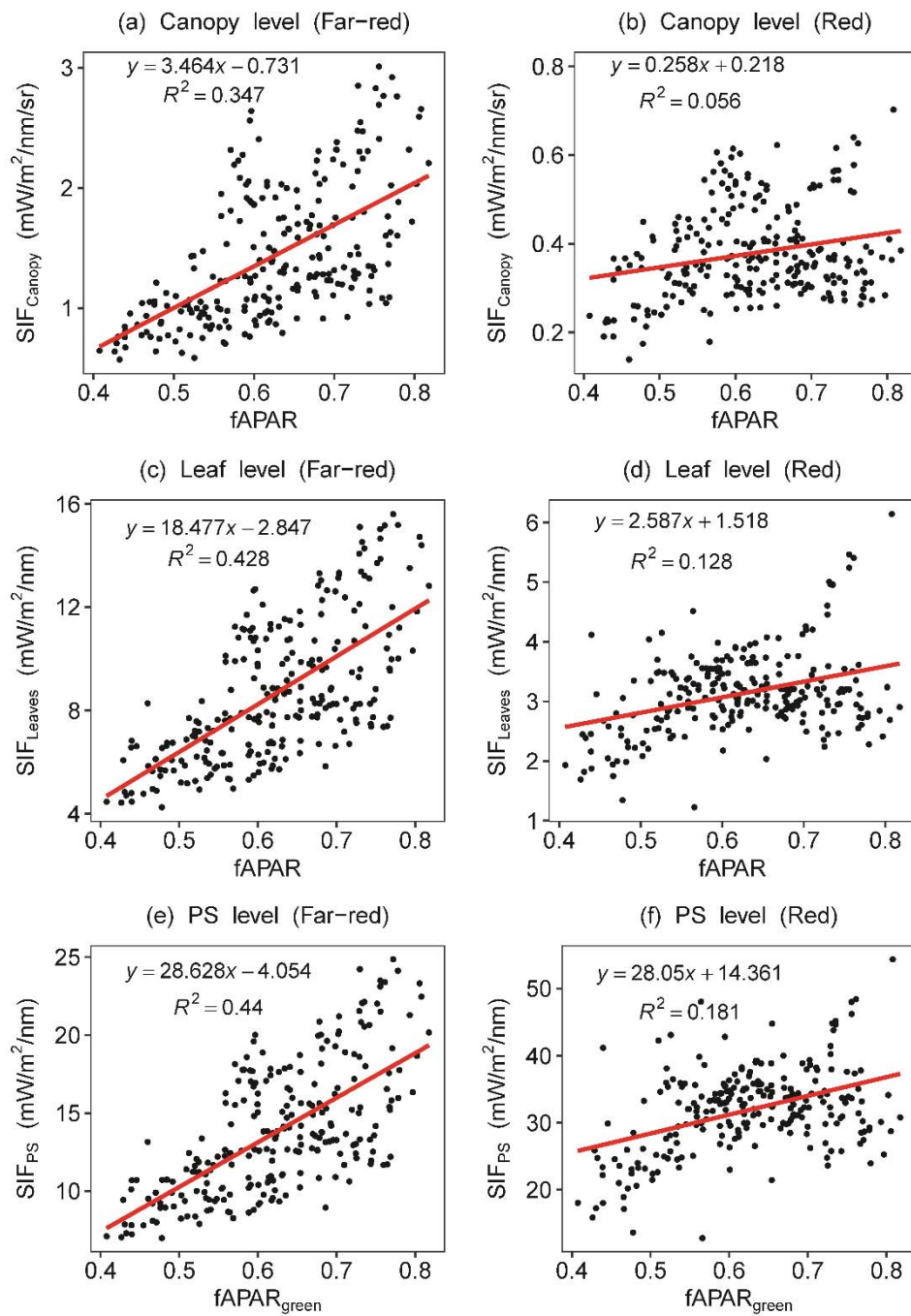
681 Figure 12. True color composed *HyPlant* image and values of  $fAPAR_{green}$ , SIF at canopy level

682 (retrieved using the iFLD method), SIF at leaf level and PS level (estimated using the RF approach) at

683 both the far-red (760 nm) and red (687 nm) bands. The image was acquired at 14:58 (local time) on



684 June 30 2015 over the study area located in the Ruhr catchment in the central western part of North  
685 Rhine-Westphalia, Germany (50.864° N, 6.452° E). The flight height was 600 m above ground. The  
686 species in the fields labeled as “A”, “B” and “C” in the true color image are winter wheat, potato and  
687 sugar beet, respectively. The three fields are selected as examples for further analysis.  
688



689

690 Figure 13. Relationship between  $fAPAR_{green}$  and SIF at canopy level, leaf level and PS level retrieved

691 from the HyPlant image. Non-vegetation pixels were excluded. In order to reduce the propagation of

692 noise, each point represents the averaged pixel value in a  $50\text{ m} \times 50\text{ m}$  window.

693

694 Next to the true color composite of the *HyPlant* image, Figure 13 shows  $fAPAR_{green}$ , canopy SIF  
695 retrieved by the iFLD method, and SIF at leaf and PS levels as estimated by the RF approach for both  
696 far-red and red bands. In Figure 12, an obvious variation in the value of  $\epsilon_{CP}$  for the different fields  
697 can be seen. As an example, *Field A* (winter wheat) and *Field B* (potato) feature similar levels of  
698  $fAPAR_{green}$  and  $SIF_{PS}$  but their  $SIF_{canopy}$  were quite different, which indicated significant differences in  
699 their canopy structure (see the color of *Field A* and *Field B* in the true color image in Figure 12). Their  
700 different relationships between  $fAPAR_{green}$  and  $SIF_{canopy}$  could be attributed to the differences in  $\epsilon_{CP}$ .  
701 Moreover, the *HyPlant* results also demonstrated that the SIF anisotropy at canopy level was  
702 efficiently corrected after the downscaling. For example, as shown in the image, despite a relative  
703 spatial visual homogeneity of *Field C* (see the true color image in Figure 12), the map of  $SIF_{canopy}$   
704 showed a systematically increasing trend from west to east. The view zenith angle for *HyPlant* varied  
705 from  $-16.7^\circ$  to  $\sim 16.7^\circ$  for pixels from the left to the right of the swath and so this variation in  $SIF_{canopy}$   
706 within a homogeneous field may be related to SIF anisotropy. In contrast, the value of  $SIF_{PS}$  in this  
707 field was much more homogeneous.

708 Relationship between  $fAPAR_{green}$  and SIF at canopy, leaf or PS level extracted from the *HyPlant*  
709 image vegetation pixels were presented in Figure 13. Although the spatial resolution of the *HyPlant*  
710 image was reduced from 1 m to 5 m, the SIF images still appear noisy, especially for the red band. To  
711 further reduce the noise influence, we aggregated image pixels into  $50\text{ m} \times 50\text{ m}$  bins, in which the  
712  $fAPAR_{green}$  and SIF values were averaged (the scatter plots for the  $5\text{ m} \times 5\text{ m}$  images are available in  
713 the Supplementary materials (Figure S3)). Since the *HyPlant* image used in this study was acquired  
714 within one minute and the study area was flat, the PAR was expected to be constant for all pixels. The  
715 graphs showed a stronger and more linear relationship between  $SIF_{PS}$  and  $fAPAR_{green}$  than between

716 SIF<sub>Canopy</sub> and fAPAR<sub>green</sub> for both the far-red band and the red band. The downscaling of SIF from  
717 canopy to PS level using the RF approach has increased the value of R<sup>2</sup> for the linear relationship  
718 between SIF and fAPAR<sub>green</sub> from 0.347 to 0.440 at the far-red band, and from 0.056 to 0.181 at the  
719 red band. For the far-red band, values of R<sup>2</sup> for the leaf level and PS level were very similar, while for  
720 the red band, the value of R<sup>2</sup> for the PS level was higher than that for the leaf level.

## 721 **4. Discussion**

### 722 **4.1 Downscaling of SIF for the correction of SIF anisotropy**

723 The observed SIF anisotropy at the canopy level is due to the re-absorption and scattering effects  
724 within the canopy. [Guanter et al. \(2012\)](#) and [Joiner et al. \(2012\)](#) reported the influence of the  
725 sun-view geometry on satellite remotely sensed SIF. Since the upwelling radiative transfer process  
726 from leaf level to canopy level for SIF emission is similar to that of reflected radiation, one can assume  
727 that SIF anisotropy is similar to that of reflectance ([Liu et al. 2016](#)).

728 According to the physical analysis of the SIF radiative transfer within the canopy conducted in  
729 this study, which was neglecting the influence of soil reflectance (is applicable for dense canopies),  
730 the SIF anisotropy at canopy level can be normalized by the BRF as expressed by Eq. (14), which is  
731 consistent with [Liu et al. \(2016\)](#). Multi-angular measurements of a winter wheat canopy were used in  
732 the evaluation of the SIF downscaling (Figure 11 and Figure 12). The results showed that, after the  
733 downscaling process, the difference in the values of SIF observed at different VZAs was reduced  
734 effectively. Similarly, in the *HyPlant* image, due to the variation of view zenith angle, SIF at canopy  
735 level showed obvious differences between the center and edges of the swath, while SIF at PS level was

736 more homogeneous within each field.

737 [Pinto et al. \(2017\)](#) showed the angular distribution of SIF emission of a sugar beet canopy which  
738 consistent with our DART simulations shown in Figure 1, and they pointed out that the directional  
739 SIF emission is related to the canopy structure. [He et al. \(2017\)](#) developed a model to normalize the  
740 remotely sensed SIF to the hot spot direction by quantifying the fraction of sunlit and shaded leaves  
741 in the field of view, and consequently, the total SIF at canopy level could be estimated as a weighted  
742 sum of SIF from sunlit and shaded leaves. They reported that the calculated total SIF was better  
743 related with the simulated total GPP than the original SIF observation. According to these relevant  
744 studies, the demonstrated SIF directional correction is especially important for long-term,  
745 ground-based or satellite-based observations of SIF time series as the sun-view geometry has a big  
746 influence on the SIF values ([Guanter et al. 2012](#); [Joiner et al. 2012](#); [Liu et al. 2016](#); [He et al. 2017](#);  
747 [Pinto et al. 2017](#)). The downscaling approach proposed in this paper presents a practical method of  
748 reducing the anisotropy of SIF emissions, which consequently enables less biased understanding of  
749 the SIF information at canopy level.

## 750 **4.2 Improvements of APAR estimation by SIF downscaling**

751 APAR is a bridge linking SIF to GPP ([Berry et al. 2012](#); [Porcar-Castell et al. 2014](#)). Besides the SIF  
752 anisotropy at the canopy level, the SIF-APAR relationship also depends on the canopy components  
753 and structures.

754 [Du et al. \(2017\)](#) studied the response of SIF to  $APAR_{chl}$  using a simulated dataset and ground  
755 measurements, and found that the relationship between  $SIF_{Canopy}$  and  $APAR_{chl}$  is highly dependent on  
756 the canopy structure and chlorophyll content, especially for the red band. Our study pointed out that

757 corrections for the re-absorption and scattering that affects the SIF transfer from the PS level to  
758 canopy level is important for linking  $SIF_{\text{Canopy}}$  to  $APAR_{\text{chl}}$ . The study by [Guanter et al. \(2014\)](#) also  
759 found that there are differences between SIF-GPP models relationships for US croplands and  
760 European grasslands. According to the multi-species experiments used in our study (Figure 10), the  
761 RF-based downscaling of SIF is efficient to reduce the influence of the re-absorption and scattering  
762 effects within the canopy, and to reduce the species-dependency of the SIF- $APAR_{\text{chl}}$  models.

763 [Wieneke et al. \(2016\)](#) analyzed the value of  $F_{\text{yield}}$  at canopy level ( $SIF_{\text{Canopy}}/APAR$ ) for different  
764 agricultural fields captured in a *HyPlant* image, and found that  $F_{\text{yield}}$  varied with the crop type and  
765 with the time of image acquisition, i.e., the solar zenith and azimuth angles. The reason could be  
766 partly related to the re-absorption and scattering of SIF within the canopy. The results that we  
767 obtained using the *HyPlant* image further support the idea that SIF downscaling from canopy level to  
768 PS level can help to achieve more stable and reliable SIF-based APAR models.

### 769 **4.3 The variation of SIF spectral shape at canopy, leaf and PS levels**

770 Apart from the intensity of single-wavelength SIF, the spectral shape of SIF also contains  
771 important information ([Liu et al. 2015](#)). The two photosystems, PS I and PS II, contribute differently  
772 to the SIF emission. The PS II is responsible for the SIF emission at both the red and far-red bands,  
773 while the PS I only contributes to the far-red SIF emission and has a much smaller yield ([Pfündel](#)  
774 [1998](#); [Agati et al. 2000](#)). Therefore, the spectral shape of SIF is related to the energy distribution  
775 between PS I and PS II ([Porcar-Castell et al. 2014](#)). However, as the within-canopy re-absorption and  
776 scattering effects on SIF are quite different for the red band and the far-red band, the spectral shape  
777 of SIF at canopy, leaf and PS levels varies significantly ([Fournier et al. 2012](#); [Moya et al. 2006](#);

778 [Porcar-Castell et al. 2014](#)). [Romero et al. \(2018\)](#) developed a model based on the canopy reflectance,  
779 canopy transmittance and soil reflectance to retrieve the spectral shape of fluorescence emission at  
780 leaf level from the observed fluorescence at canopy level. [Ramos and Lagorio \(2004\)](#) proposed a  
781 physical model to obtain the fluorescence spectra at PS level by combining the leaf fluorescence  
782 emission and leaf reflectance. Based on the two studies above, it is possible to retrieve the SIF  
783 spectral shape at PS level from SIF observation at canopy level, but the absolute intensity of SIF  
784 emission at leaf level or PS level is not available.

785 In this paper, although we focused on the SIF downscaling at two spectrally narrow bands  
786 instead of full-wavelength, it is still possible to see the variation of SIF spectral shape at canopy, leaf  
787 and PS levels using the ratio of far-red and red SIF. For the wheat canopy introduced in the  
788 multi-species experiment, the averaged ratios of SIF at the far-red band (760 nm) and red band (687  
789 nm) are 1.63, 1.17 and 0.17 for the canopy level, leaf level and PS level, respectively. The significant  
790 decrease of the SIF ratios results from a much stronger re-absorption effect at the red band. The  
791 results are consistent with the Figure 8 in [Romero et al. \(2018\)](#).

#### 792 **4.4 Reliability of this study**

793 A practical solution based on RF regression was proposed to overcome the difficulties in the  
794 physical approach for SIF downscaling from canopy level to PS level. As an efficient machine learning  
795 algorithm, the RF regression model is able to give accurate prediction of parameters if it is properly  
796 trained. The RF model is made up of a large number of decision trees. Each decision tree is  
797 independently grown on a bootstrap sample, and hence, the trees are weakly correlated. Therefore,  
798 the risk of overfitting the training dataset, which is a significant problem for many machine learning

799 algorithms, can be reduced (Abdel-Rahman et al. 2013). The RF model is a black box and is totally  
800 reliant on the training dataset, which may reduce its robustness and applicability under certain  
801 conditions. For comparison, a simple multiple linear regression (MLR) method was also tested using  
802 the SCOPE simulation, but the results (Figure S4 in the Supplementary materials) were much worse  
803 than the RF model (as shown in Figure 7), which confirmed that the RF model was more efficient to  
804 estimate the SIF escape probability based on the information from reflectance.

805 A physical analysis based on the spectral invariant theory was carried out to improve the  
806 robustness of the SIF downscaling model and find out the most important variables. However, there  
807 are some limitations remaining in using the spectral invariant theory. In the spectral invariant theory,  
808 the leaf reflectance and transmittance are combined as the leaf single scattering albedo. In other  
809 words, the different transfer processes of the photons scattered downwards and upwards by leaves  
810 were ignored. Yang and Van der Tol (2018) analyzed the radiative transfer of incident light and  
811 emitted SIF considering the leaf reflectance and transmittance separately and got the same equation  
812 as Eq. (14). But they pointed out that the equation was not valid for the red band due to the difference  
813 between the leaf reflectance and transmittance. At the far-red band, the influence of the difference of  
814 leaf reflectance and transmittance becomes relatively small with the increasing interaction order. At  
815 the red band, however, the difference of leaf reflectance and transmittance is not ignorable because  
816 the single scattering dominates. Nevertheless, Yang and Van der Tol (2018) also found that the  $\varepsilon_{CL}$   
817 and  $\frac{BRF}{i_0\omega_L}$  were still proportional at the red band for individual leaves, but the slope of the  
818 relationship was influenced by the leaf structure and pigment composition. In our study, we did not  
819 rely on the physical analysis for SIF downscaling, but only used the spectral invariant theory to find  
820 out the key parameters to estimate the SIF escape probability. Therefore, the results of this study



821 were not directly influenced by the limitations of the spectral invariant theory, and the SIF  
822 downscaling at the red band was still reasonable and valid, although the accuracy was lower than  
823 that at the far-red band.

824 We used different data stemming from models, field and airborne observations to assess  
825 reliability of our approach. Although we could demonstrate consistency of downscaling results across  
826 levels and experiments, particularly results obtained from *HyPlant* data were less clear compared to  
827 modeling results. This is expected and related to the wealth of factors determining real  
828 measurements. Further, the atmospheric correction of airborne measured radiance data to retrieve  
829 surface reflectance and eventually calculate vegetation products such as fAPAR is a highly complex  
830 task. Particularly canopy structure can introduce uncertainties in estimated irradiance due to varying  
831 fractions of diffuse and direct irradiance components, thus causing errors in retrieved vegetation  
832 products (Damm et al 2015b).

833 Other assumptions applied might also limit the scope of our analysis. i) The training dataset was  
834 simulated with the SCOPE model. SCOPE provides relatively reliable simulations of SIF at PS, leaf and  
835 canopy levels, and has been widely used in studies dealing with SIF (Damm et al. 2015a, Verrelst et al.  
836 2016). However, SCOPE is a 1-D model and its simulations may only be reliable for canopies with a  
837 relatively simple structure, such as crops and grass, and not for more complicated canopies such as  
838 forest. The clumping effect was also neglected in the physical analysis. The performance of the  
839 proposed method for the cases across canopies still needs to be further tested. ii) The estimated SIF  
840 at PS level is not possible to be directly validated for ground or airborne measurements.  $APAR_{chl}$  or  
841  $fAPAR_{green}$  were, therefore, used to indirectly evaluate the reliability of estimated  $SIF_{PS}$ . But the  
842 measurements or estimates of  $APAR_{chl}$  or  $fAPAR_{green}$  also contain uncertainties. Moreover, the

843 influence of SIF yield was neglected. Therefore, the validation of our SIF downscaling must be  
844 elaborated in future work.

## 845 **5. Conclusions**

846 Remote sensing based SIF measurements at canopy level are largely affected by re-absorption  
847 and scattering within the leaves and canopies, so the downscaling of SIF from canopy level to PS level  
848 is important to better understand the link between SIF and GPP. A practicable solution based on  
849 physical analysis and RF regression for the estimation of SIF escape probability was proposed. The RF  
850 regression model was trained using SCOPE simulations. The results were evaluated using SCOPE and  
851 DART simulations, field experiments and *HyPlant* image. The results indicate that, for the far-red  
852 band, the SIF escape probability is dominated by the canopy scattering, while for the red band, the  
853 SIF escape probability is related to both canopy scattering and reabsorption within leaves. We  
854 conclude that accurate knowledge and correction of SIF escape probability is essential to reduce  
855 associated large uncertainty in the SIF-APAR relationship, and this is also expected to improve the  
856 SIF-based GPP estimation. Our suggested approach is based on the spectral invariant theory and  
857 relies on canopy directional reflectance at the red, red-edge and far-red bands to downscale canopy  
858 SIF to leaf or photosystem level. Although we could successfully demonstrate the reliability of our  
859 approach, we identified strong sensitivity of our results to data quality and assumptions in  
860 underlying models. We suggest advancing reliability of reflectance data retrievals in requested  
861 wavelength ranges and further assessing the impact of assumptions underlying our analysis.

862

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