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Abstract

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

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

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

1. Introduction

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

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

$$GPP = PAR \times fAPAR \times LUE \quad (1)$$

where PAR stands for the photosynthetically active radiation, fAPAR is the fraction of PAR absorbed by vegetation, and LUE is the light use efficiency, defined as the number of μmol of CO_2 absorbed per μmol of photons.

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

$$SIF_{PS}(\lambda) = PAR \times fAPAR \times F_{yield}(\lambda) \quad (2)$$

where λ is the wavelength, and F_{yield} is the quantum yield for chlorophyll fluorescence. If F_{yield} is constant, then SIF_{PS} is linearly related to the PAR absorbed by vegetation.

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

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

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

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

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

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

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

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

2. Materials and methods

2.1 Simulated datasets

2.1.1 SCOPE simulation

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 (~ 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 (Cab), 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	μg/cm^2	Leaf chlorophyll a + b content
C_{dm}	0.012	g/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	m^2 /m^2	Leaf area index
LIDF$_a$	1, -1, 0, 0, -0.35, 0	-	Leaf inclination parameter

$LIDF_b$	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

2.1.2 DART simulation

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

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

Parameter	Values	Unit	Description
C_{ab}	58	µg/cm²	Leaf chlorophyll a + b content
C_{dm}	0.0037	g/cm²	Dry matter content
C_w	0.0131	cm	Leaf water equivalent layer
N	1.518	-	Leaf mesophyll scattering parameter
LAI	4 (maize), 7 (spruce)	m^2/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

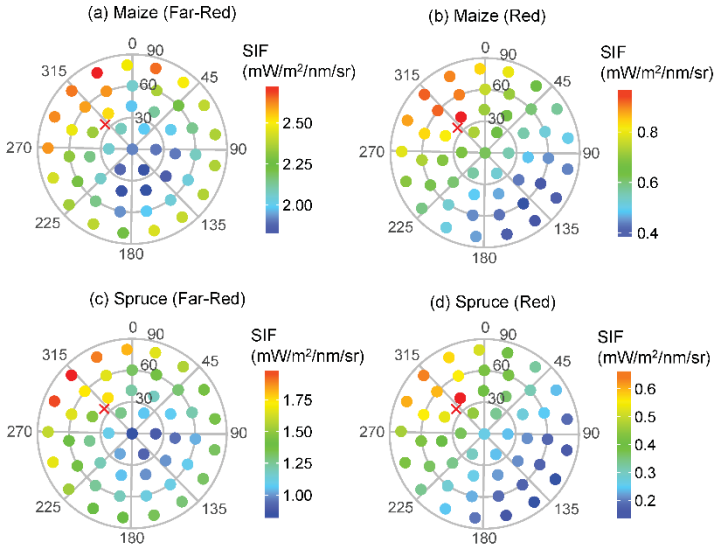


Figure 1. Multi-angular SIF at canopy level for maize and spruce at the far-red (740 nm) and red (687 nm) bands, as simulated by DART. The labels are the view azimuth (0° - 360°, 0° for the north) and zenith (0° - 90°) angles. The red cross indicates the solar position (zenith angle: 37.94°; azimuth angle: 311.89°). The incident PAR is 1185.76 W/m², and the temperature is 300 K.

2.2 Ground measurements

2.2.1 Multi-species experiments

A dataset comprising ground spectral measurements of different species, acquired at three sites, following three specific experimental settings was used to evaluate the performance of SIF downscaling for different canopy structures.

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

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

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

Details of the multi-species measurements described above are summarized in Table 3. All the spectral measurements were conducted using a customized Ocean Optics QE Pro spectrometer (Ocean Optics, Dunedin, FL, USA), characterized by a FWHM of 0.31 nm, a SSI of 0.155 nm, and a peak signal-to-noise ratio (SNR) higher than 1000. For more details of the experiments, please refer to Du 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 (μg/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° to 60° with an interval of 10° (a smaller interval of 2° 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 (μg/cm²)	SZA (°)
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 $APAR_{chl}$**

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

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

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

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

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

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

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

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

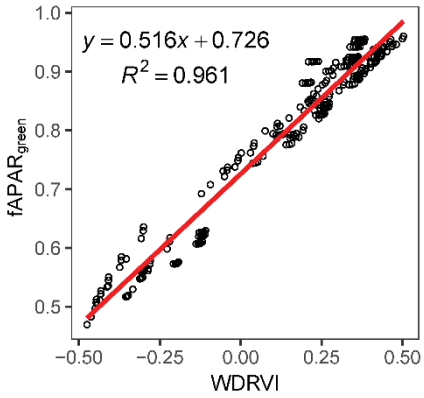


Figure 2. Linear regression of the fraction of photosynthetically active radiation absorbed by green leaves ($fAPAR_{green}$) on the wide dynamic range vegetation index (WDRVI) computed from SCOPE simulations for canopies with different leaf area indices, leaf chlorophyll contents and leaf inclination distributions.

Chlorophyll is the main absorbing compound for PAR in green leaves (Jacquemoud and Baret 1990; Porcar-Castell et al. 2014). According to Du et al. (2017), $fAPAR_{chl}$ can be approximated from $fAPAR_{green}$ with a linear function:

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

where the coefficient k is related to the leaf chlorophyll content. Analysis of SCOPE simulations conducted by Du et al. (2017) revealed that the value of k varies from 0.78 to 0.80 for the leaf chlorophyll content from 20 to 60 μg/cm². Since the leaf chlorophyll content of most of the samples was within the range 20 – 60 μg/cm² (except for one sample for which the value was 15.22 μg/cm²), we estimated $fAPAR_{chl}$ using k equal to 0.79 in this study.

The incident photosynthetically active radiation (PAR) was calculated using the radiance reflected from a white reference panel measured by a spectrometer. Consequently, the $APAR_{chl}$ can be calculated as:

$$APAR_{chl} = PAR \times fAPAR_{chl} \quad (6)$$

2.3 Airborne measurements

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

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

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

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

2.4 Physical analysis of SIF radiation transfer within the canopy

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

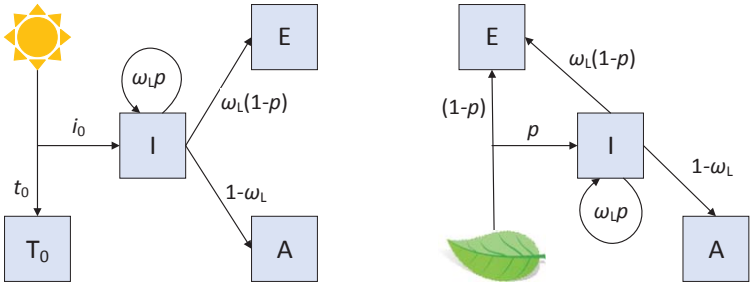


Figure 3. An illustration of the canopy absorption and scattering model for solar illumination (a) and SIF emission (b) assuming with non-reflecting soil background. State T_0 represents photons that go through the canopy without interacting with the canopy or being absorbed by the soil; state I represents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

335 the leaf scattering coefficient (single scattering albedo), i_0 is the canopy interceptance 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 $$a_i(\lambda) = i_0\left[\left(1-\omega_L(\lambda)\right) + \omega_L(\lambda)p\left(1-\omega_L(\lambda)\right) + \omega_L(\lambda)^2p^2\left(1-\omega_L(\lambda)\right) + \cdots\right] = i_0\frac{1-\omega_L(\lambda)}{1-p\omega_L(\lambda)} \quad (7)$$
345 where p is the recollision probability, ω_L is the leaf scattering coefficient (single scattering albedo),
346 and i_0 is the canopy interceptance of the incoming radiation. The canopy scattering can then be
347 expressed as:
348 $$s_i(\lambda) = i_0 - a_i(\lambda) = \frac{1-p}{1-p\omega_L(\lambda)} i_0\omega_L(\lambda) \quad (8)$$
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 $$1 - p = \frac{1}{\pi}\int_{4\pi}\rho(\Omega)\,|\mu|\,d\Omega \quad (9)$$
354 where $\rho(\Omega)$ is the gap fraction for direction Ω, 4π denotes the unit sphere, and μ is the cosine of
355 the polar angle of Ω. 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),

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

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

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

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

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

and the canopy scattering of SIF photons as:

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

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

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

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

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

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 interceptance and the leaf
383 scattering coefficient. In practice, the directional reflectance can be acquired concurrently with the
384 SIF measurements, but canopy interceptance and leaf scattering coefficients can not, in general, be
385 accurately estimated. The canopy interceptance 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 interceptance can be
387 expressed as (Chen and Black 1992; Ross 2012):

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

389 where θ is the SZA and $G(\theta)$ is the mean projection coefficient for foliages on a plane
390 perpendicular to θ. 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 θ.
392 For other values of the LIDF, the value of G ranges from 0 to 1 when θ varies from 0° to 90°, and
393 generally converges to 0.5 when θ is approximately 57.3° 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.

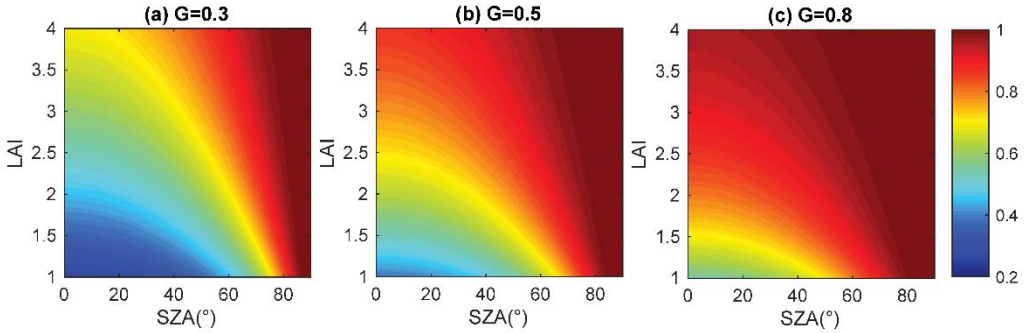
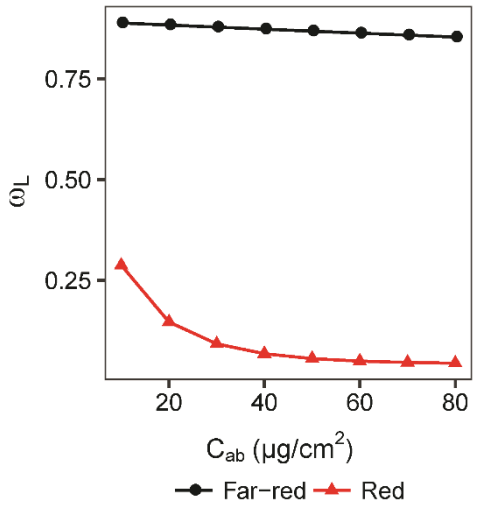


Figure 4. Values of the canopy interceptance of the incoming radiation (i_0) for different G function values, leaf area index (LAI) and solar zenith angle (SZA) combinations, calculated using Eq. (15). G function is the mean projection coefficient for foliages on a plane perpendicular to the solar zenith direction.

Since absorption by chlorophyll a molecules is very weak at the far-red band, leaf single scattering albedo (ω_L) is strongly influenced by chlorophyll content only in the red wavelengths of SIF emission. $\omega_L$at the far-red band is, therefore, almost independent of chlorophyll content and it is driven by a minor absorptance of leaf tissue biochemical compounds. Figure 5 shows the variations of ω_L at the far-red (760 nm) and red (687 nm) bands simulated by the Fluspect model for leaf chlorophyll content from 10 to 80 μg/cm^2. As expected, the value of ω_L at the far-red band is almost invariant, reaching values between 0.853 and 0.888, while it varies from 0.044 to 0.287 for the red band, where the absorption by chlorophyll is strong. It exhibits a large variation in the value of ω_L, especially for the chlorophyll content lower than 40 μg/cm^2.



412

413 Figure 5. Values of ω_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 ω_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 ε_{CL} and $\frac{\mathrm{BRF}}{i_0\omega_L}$ 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 ($\varepsilon_{LP} = \mathrm{SIF_{Leaves}}/\mathrm{SIF_{PS}}$) 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

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

$$\varepsilon_{LP}(\lambda) \approx f(\mathrm{Cab},\ \lambda) \tag{16}$$

Consequently, the SIF escape probability from the PS level to the canopy level (ε_{CP}) can be expressed as:

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

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

2.5 Estimation of ε_{CP} and ε_{CL} using the random forest approach

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

449 As shown in Section 2.4, the BRF has significant impact on ε_{CP}. Taking all other factors together

450 as f_{CP}, Eq. (17) can be modified thus:

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

452 where f_{CP} is the ratio of ε_{CP} to BRF. In the SCOPE simulations, $\varepsilon_{CP}(\lambda, \Omega)$ and $\mathrm{BRF}(\lambda, \Omega)$ 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, ε_{CL} can be expressed as,

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

457 We only estimated f_{CP} or f_{CL} with the random forest approach to increase robustness of estimated

458 ε_{CP} and ε_{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 Cab as it is less

465 impacted by the absorption saturation effect for a high Cab 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

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

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

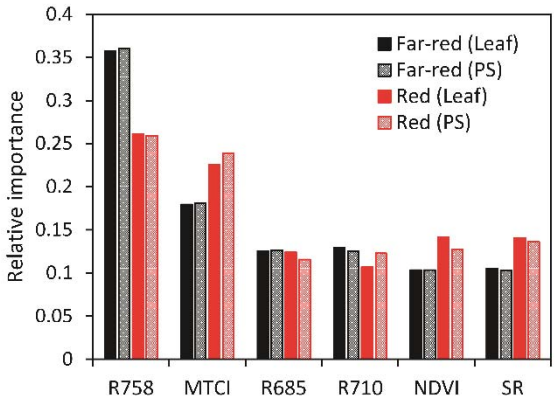
Equation	Reference
$NDVI=(R_{758}-R_{685}) / (R_{758}+R_{685})$	(Rouse et al. 1973)
$SR=R_{758} / R_{685}$	(Jordan 1969)
$MTCI=(R_{758}-R_{710}) / (R_{710}-R_{685})$	(Dash and Curran 2004)

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

3. Results

3.1 Selection of the inputs for the RF regression

To optimize the inputs for the RF regression, we tested the performance of the RF model with different combinations of the six potential input parameters explained in Section 2.5. Firstly, all the six potential parameters were used as the inputs for the RF regression to calculate their relative importance using the mean decrease accuracy (MDA) method based on the concept of out-of-bag (OOB) error. The OOB error is a parameter that represents the RF prediction error. It is considered as the mean prediction error on each training sample x_i, which uses only the trees that did not have x_i in their bootstrap sample (Breiman, 2001). To measure the importance of the j-th feature for training, the values of the j-th feature are permuted among the training data and the OOB error is computed for each perturbed data set. The importance score for the j-th feature is computed by averaging the difference in the OOB error before and after the permutation over all trees. Figure 6 shows the relative importance of the input variables of the RF model for SIF downscaling from canopy level to leaf level or PS level. These results indicate that the far-red directional reflectance and MTCI were found as the most important variables for the SIF downscaling model at both the far-red and red bands, while the importance of the directional reflectance at the red and red-edge bands, the NDVI, 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_{758}, R_{685} and R_{710} 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^2). To reduce the random errors, for each combination of input parameters, 30 RF

517 models were trained and the RRMSE and R^2 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_{758}, MTCI, R_{685}, R_{710}) were used, the RRMSE and R^2 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_{758}, MTCI, R_{685}, R_{710}) and using all six parameters was still significant

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

According to the results, R_{758}, MTCI, R_{685}, and R_{710} were selected as the input parameters of the 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 selected for the red band.

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

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

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

The SCOPE simulations were first used for accuracy assessments at the leaf and PS levels. 2/3 of the SCOPE simulations were randomly selected to train the RF model, and the remaining 1/3 was used for validation. Figure 7 shows a comparison of the far-red and red SIF estimated by the RF approach with the reference SIF simulated by SCOPE for the leaf and PS levels. In general, the estimated values of SIF at the leaf and PS levels matched well with the reference values. Most of the points were located near to the 1:1 line, and the values of the coefficient of determination (R^2) were 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 SIF, but the root-mean-square error (RMSE) was still as low as 3.613 mW/m^2/nm, resulting in the relative root-mean-square error (RRMSE) of 7.299%. The relationship of SIF at canopy level and leaf level, SIF at leaf level and PS level, SIF at canopy level and PS level from SCOPE simulations are also provided in the Supplementary materials (Figure S2) for comparisons.

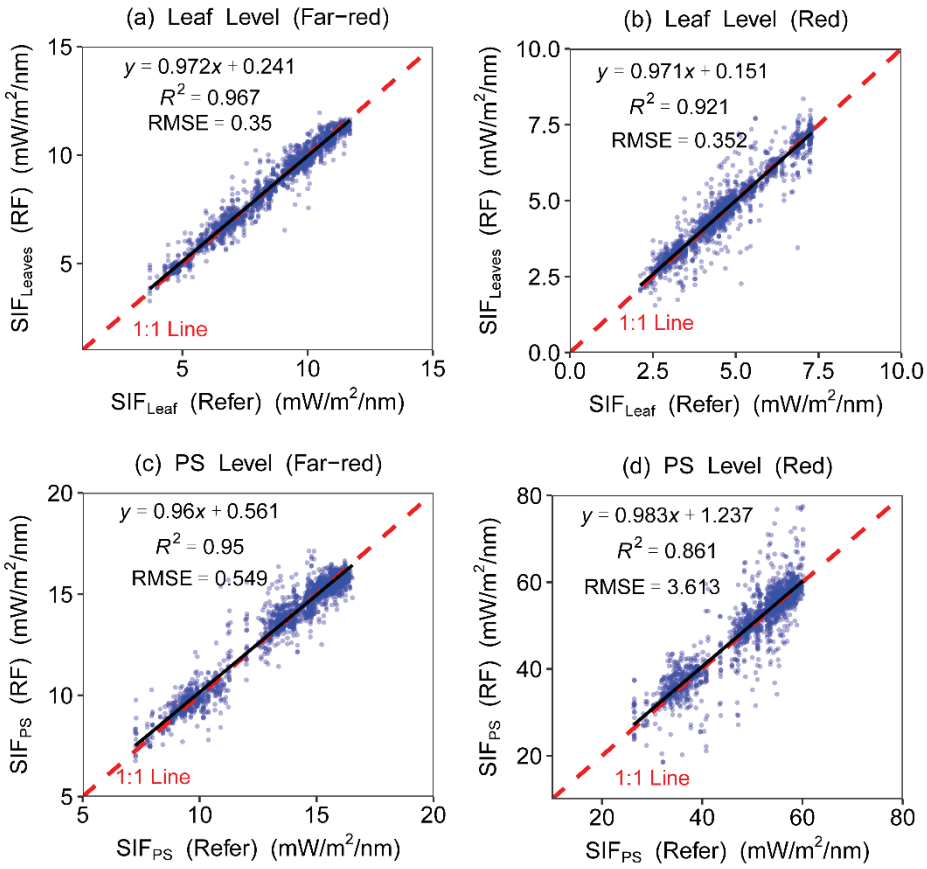


Figure 7. Comparison of far-red (760 nm) and red (687 nm) SIF estimated by the RF approach with reference SIF simulated by SCOPE for leaf and PS levels. R^2 is the coefficient of determination, and RMSE is the root-mean-square error.

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

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

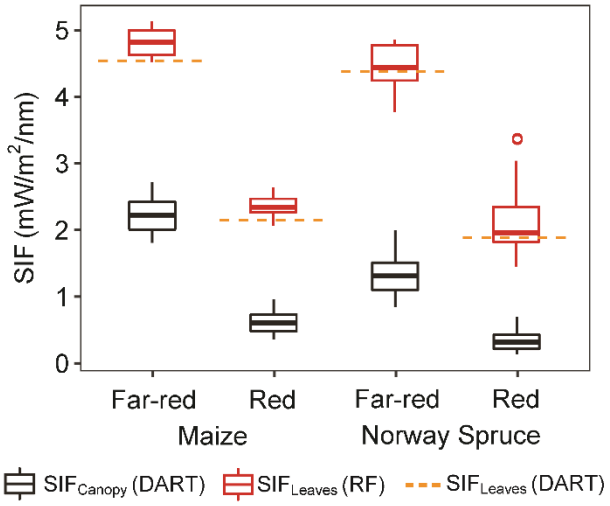


Figure 8. Boxplot of far-red (740 nm) and red (687 nm) SIF simulated by DART for maize and spruce canopies and corresponding downscaled leaf SIF using the Random Forest (RF) model. The orange dashed line shows the reference values of SIF at leaf level, as simulated in DART by Fluspect. The bottom and top of each box represent the first and third quartiles, respectively, the thick horizontal line in the box is the median, the whiskers show the maximum/minimum values within 1.5 times the interquartile range (IQR, the difference between the third and the first quartiles), and the circles show the outliers out of 1.5IQR. The units of mW/m²/nm/sr were applied to SIF at canopy level as well as leaf level to make the values comparable.

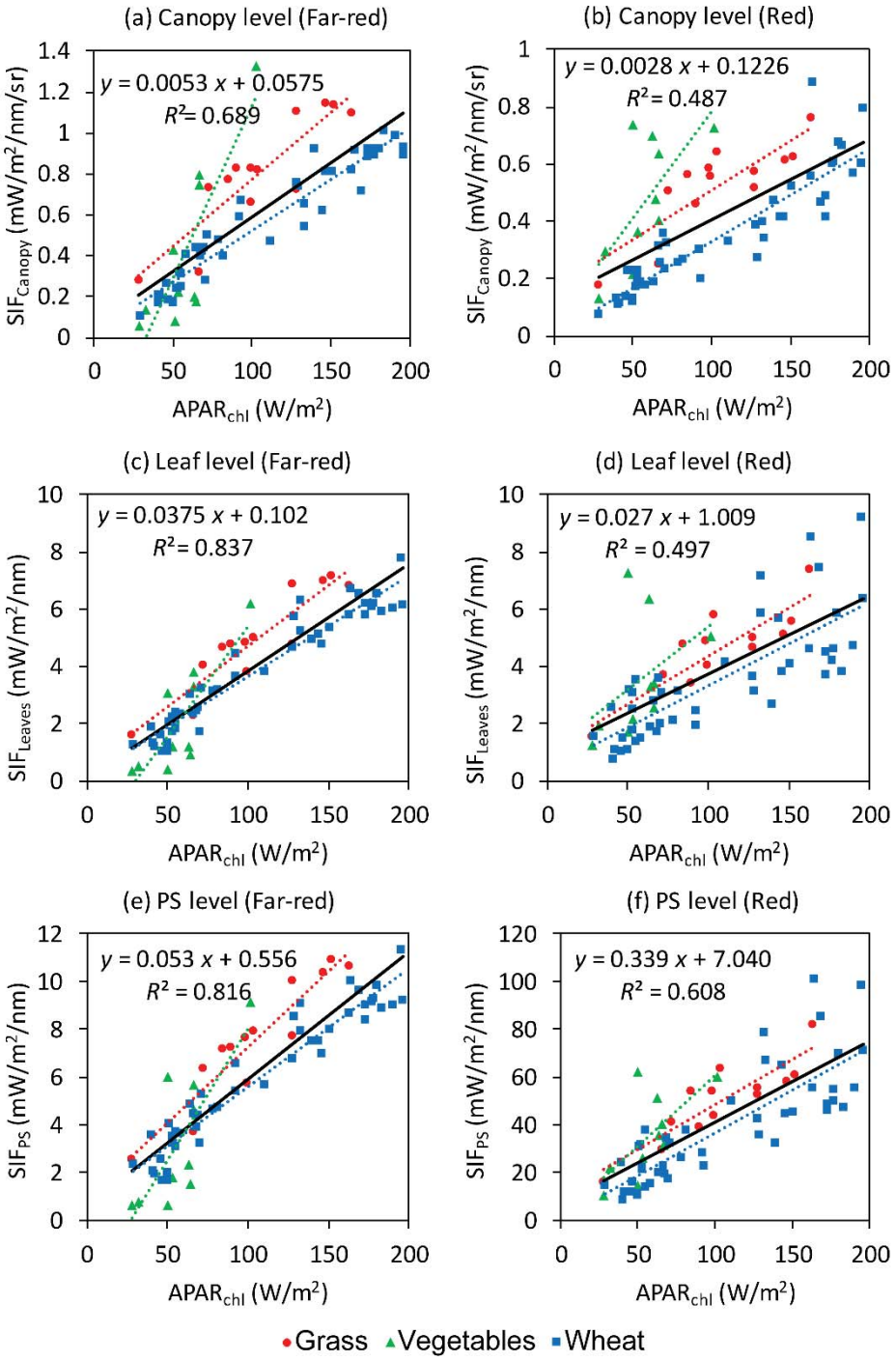
The evaluation carried out on datasets simulated by two different radiative transfer models using different vegetation representations and solar-viewing geometries revealed accurate and

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.

Table 7. Linear regression models of the SIF-$APAR_{chl}$ relationship for different species at canopy, leaf and photosystem (PS) levels. The 'CV of slopes' are the coefficients of variation of the slopes for 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

The linear regression models of the SIF-$APAR_{chl}$ relationship for different species at canopy, leaf and PS levels were summarized in Table 7, and the coefficients of variation (CV) of the slopes for different species at each level were also calculated. For grass and wheat, the relationships between SIF at all levels and APAR were close to linear. But for the vegetation, the relationship was some erratic, especially at the red band. The reason may partly due to the measurement errors. For both the far-red and red bands, the CV of slopes for different species decreased significantly when SIF was downscaled from canopy level to leaf or PS level. At the far-red band, both the CV of slopes and the R^2 of each model at the PS level were very close to that at the leaf level. At the red band, the CV of slopes at the PS level was some higher than that for the leaf level, but the R^2 of the regression model for all 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-$APAR_{chl}$ 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 $APAR_{chl}$ and values of the multi-angular observed SIF
638 at canopy level, leaf level or PS level in the form of boxplots. The $APAR_{chl}$ values were divided into
639 groups with an interval of $5W/m^2$. 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 $APAR_{chl}$ 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^2 for the relationship

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

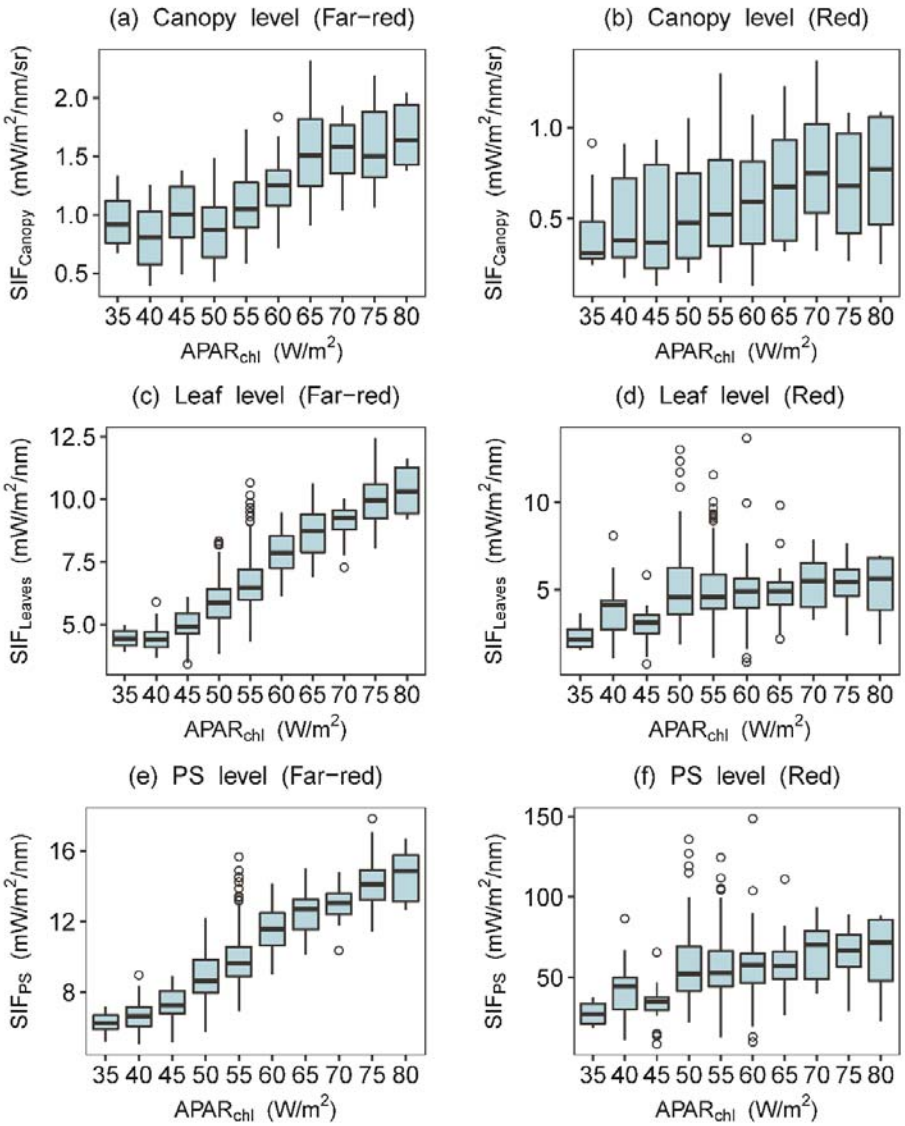
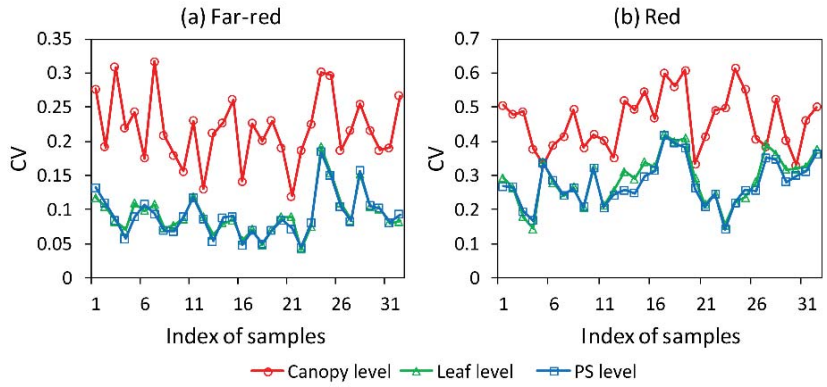


Figure 10. The relationship between $APAR_{chl}$ and multi-angular observations of SIF at canopy level (a, b) and estimated SIF at leaf level (c, d) or PS level (e, f) by the RF approach. The bottom and top of the boxes correspond to the first and third quartiles, the thick horizontal line in each box is the median, the whiskers show the maximum/minimum values within 1.5 IQR, and the circles show the outliers that lie outside 1.5 IQR. The multi-angular observations were conducted on a wheat canopy. The averaged number of observations per APAR interval is 49.



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

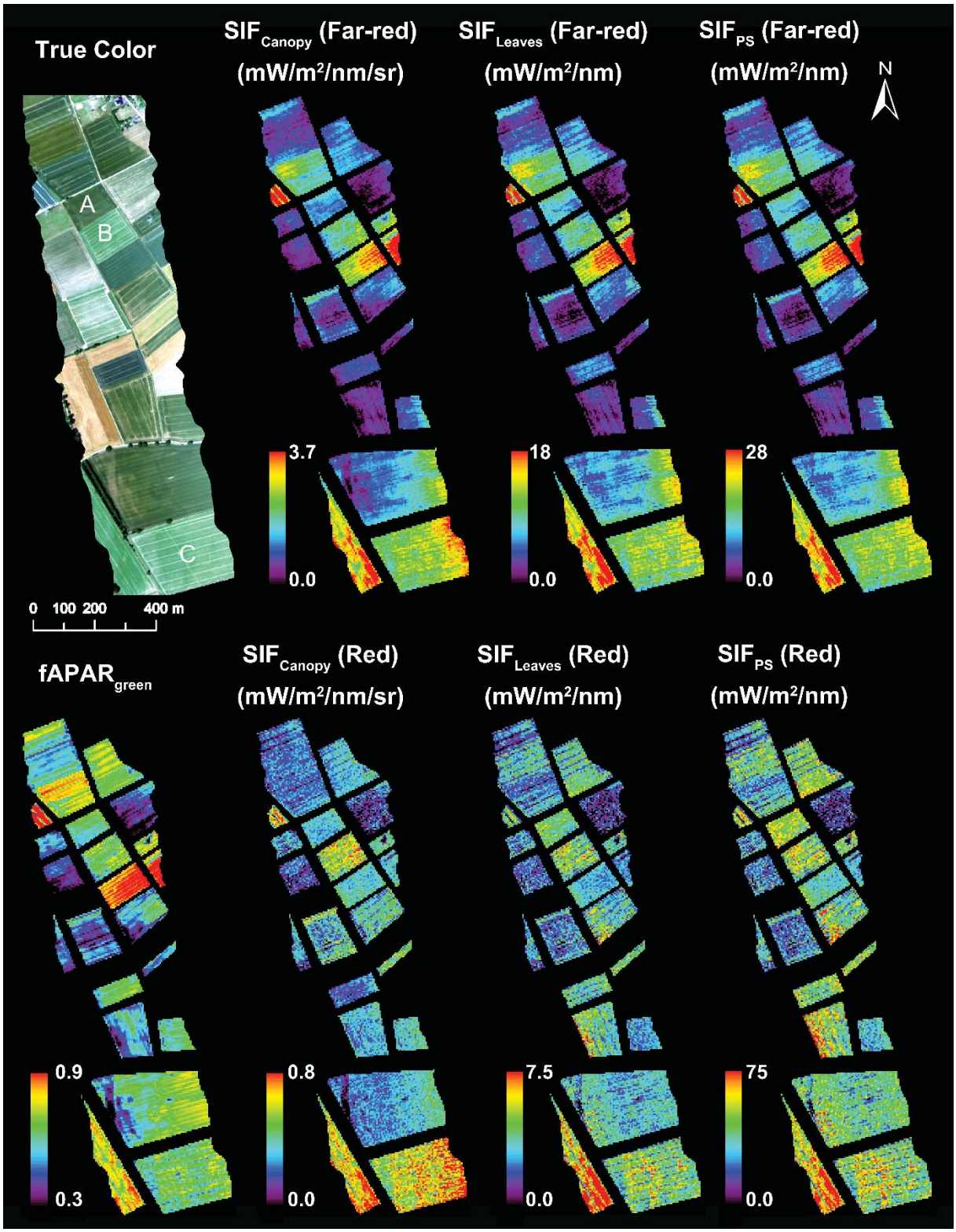
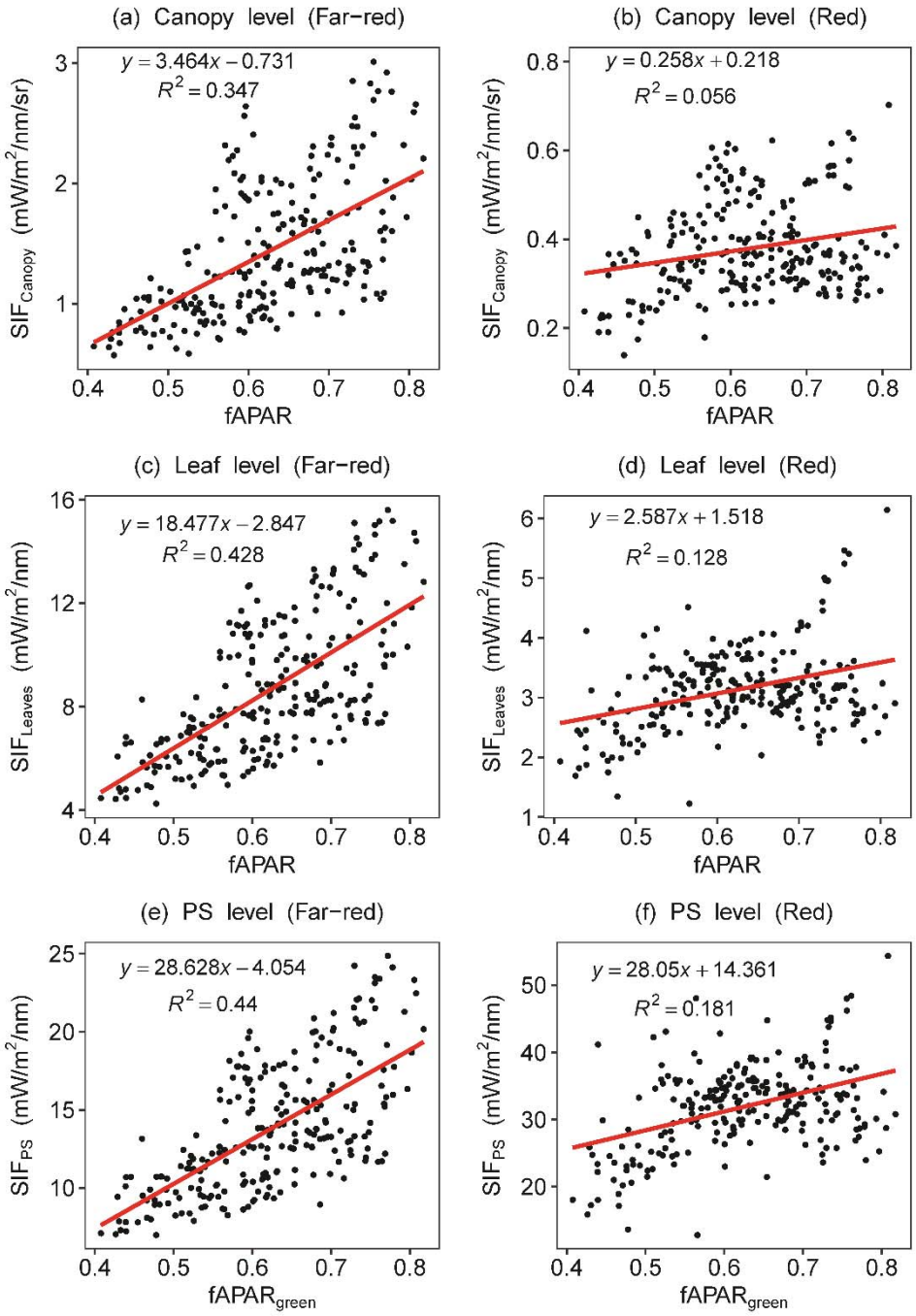


Figure 12. True color composited *HyPlant* image and values of $fAPAR_{green}$, SIF at canopy level (retrieved using the iFLD method), SIF at leaf level and PS level (estimated using the RF approach) at both the far-red (760 nm) and red (687 nm) bands. The image was acquired at 14:58 (local time) on

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



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 m × 50 m window.

693

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

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

716 SIF_{Canopy} and $fAPAR_{green}$ 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^2 for the linear relationship
718 between SIF and $fAPAR_{green}$ 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^2 for the leaf level and PS level were very similar, while for
720 the red band, the value of R^2 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

more homogeneous within each field.

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

4.2 Improvements of APAR estimation by SIF downscaling

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

Du et al. (2017) studied the response of SIF to $APAR_{chl}$ using a simulated dataset and ground measurements, and found that the relationship between SIF_{Canopy} and $APAR_{chl}$ is highly dependent on 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_{Canopy} to $APAR_{chl}$. 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-$APAR_{chl}$ models.

763 Wieneke et al. (2016) analyzed the value of F_{yield} at canopy level (SIF_{Canopy}/APAR) for different
764 agricultural fields captured in a *HyPlant* image, and found that F_{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 ε_{CL}
817 and $\frac{\mathrm{BRF}}{i_0\omega_L}$ 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

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

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

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

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

5. Conclusions

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

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