Far-red sun-induced chlorophyll fluorescence shows ecosystem-specific relationships to
gross primary production: An assessment based on observational and modeling
approaches

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Abstract

Sun-induced chlorophyll fluorescence (SIF) is a radiation flux emitted from
chlorophyll molecules and is considered an indicator of the actual functional state of plant
photosynthesis. The remote measurement of SIF opens a new perspective to assess actual
photosynthesis at ecologically relevant larger scales and provides an alternative approach to
study the terrestrial carbon cycle. Recent studies demonstrated the reliability of measured SIF
signals and showed significant relationships between SIF and gross primary production (GPP)
at ecosystem and global scales. Despite these encouraging results, understanding the complex
mechanisms between SIF and GPP remains challenging before SIF can be finally utilized to
constrain estimates of GPP. In this study, we present a comprehensive assessment of the
relationship between far red SIF retrieved at 760 nm (SIF$_{760}$) and GPP, and its transferability
across three structurally and physiologically contrasting ecosystems: perennial grassland, cropland and mixed temperate forest. We use multi-temporal imaging spectroscopy (IS) data acquired with the Airborne Prism Experiment (APEX) sensor as well as eddy covariance (EC) flux tower data to evaluate the relationship between SIF$_{760}$ and GPP$_{EC}$. We use simulations performed with the coupled photosynthesis-fluorescence model SCOPE to prove trends obtained from our observational data and assess apparent confounding factors such as physiological and structural interferences or temporal scaling effects. Observed relationships between SIF$_{760}$ and GPP$_{EC}$ were asymptotic and ecosystem-specific, i.e., perennial grassland ($R^2 = 0.59$, $r$RMSE = 27.1%), cropland ($R^2 = 0.88$, $r$RMSE = 3.5%) and mixed temperate forest ($R^2 = 0.48$, $r$RMSE = 15.88%). We demonstrate that asymptotic leaf level relationships between SIF$_{760}$-GPP$_{EC}$ became more linear at canopy level and scaled with temporal aggregation. We conclude that remote sensing of SIF provides a new observational approach to decrease uncertainties in estimating GPP across ecosystems but requires dedicated strategies to compensate for the various confounding factors impacting SIF-GPP relationships. Our findings help in bridging the gap between mechanistic understanding at leaf level and ecosystem-specific observations of the relationships between SIF and GPP.

**Keywords:** Sun-induced chlorophyll fluorescence, gross primary production, airborne-based spectroscopy, APEX, Fraunhofer line depth (FLD), eddy-covariance, SCOPE
1 Introduction

Plant photosynthesis is a key process in terrestrial ecosystems, mediating gas and energy exchanges in the atmosphere-biosphere system (Baldocchi et al. 2001; Ozanne et al. 2003). Products of photosynthesis provide a wealth of ecosystem services that are essential for human well-being, including food, fiber, energy and oxygen (Imhoff et al. 2004; Krausmann et al. 2013; Schröter et al. 2005). Photosynthesis as the underlying process for plant growth is a particularly interesting indicator of crop efficiency and agricultural management practices (Falloon and Betts 2010; Guanter et al. 2014; Trnka et al. 2004), both of which having important implications for yield forecasts and for the implementation of climate change adaptation strategies (IPCC 2013).

Observing the highly dynamic process of photosynthesis beyond the individual leaf or plant levels *in-situ* is based on measuring the carbon dioxide (CO$_2$) exchange between vegetation and atmosphere with eddy-covariance (EC) flux towers, and partitioning it into gross primary production (GPP) and ecosystem respiration (Baldocchi et al. 2001). Measurements of plant - light interactions using spectrometers installed on, for example, EC towers allow deriving information about the pigment status and provide an alternative approach to estimate GPP (Balzarolo et al. 2011; Gamon et al. 2010; Hilker et al. 2011). At landscape scale, photosynthesis can be assessed using process-based models (Sitch et al. 2003), greenness-based satellite observations (Running et al. 2004), or hybrid approaches combining *in-situ* observations and statistical modeling (Jung et al. 2011). All these approaches provide important insights to study photosynthesis but usually do not allow assessing photosynthesis at larger scales while preserving the high spatial variability present in ecosystems. EC flux tower measurements represent only smaller areas in preselected ecosystems (Drolet et al. 2008; Turner et al. 2005), are not spatially distributed according to carbon stocks (Schimel et al. 2014), and do not allow spatial differentiations within the
measured footprint (Barcza et al. 2009; Kljun et al. 2002). Combined large scale modeling and observational approaches based on vegetation greenness are spatially contiguous but face the complexity of naturally varying systems, including diverse interactions and complex feedbacks, which limit their predictive capabilities (Beer et al. 2010; Goetz and Prince 1999; Turner et al. 2005).

Over the last decade, significant progress has been made in measuring plant-light interactions and the process of photosynthesis. Remote measurements of sun-induced chlorophyll fluorescence (SIF), in particular, open a new perspective to assess photosynthesis at ecosystem scale. SIF is a radiation flux emitted from plant chlorophyll molecules a few nanoseconds after light absorption in the wavelength range from 600-800 nm and is considered an indicator for the functional status of actual plant photosynthesis (Baker 2008). Various studies demonstrated the possibility to measure SIF at certain wavelengths on ground (Guanter et al. 2013; Rascher et al. 2009), from airborne platforms (Damm et al. 2014; Guanter et al. 2007; Zarco-Tejada et al. 2012), and from satellites (Frankenberg et al. 2011; Guanter et al. 2014; Joiner et al. 2013). Recent research demonstrated SIF being sensitive to changes in photosynthesis, showing strong links to GPP at the level of leaves (Meroni et al. 2008; Middleton et al. 2002), plants (Damm et al. 2010; Rossini et al. 2010), canopies (Zarco-Tejada et al. 2013), and ecosystems (Frankenberg et al. 2011; Guanter et al. 2012).

Observed relationships between SIF and GPP are conceptually explained using an approximation of GPP based on Monteith’s light use efficiency concept (Monteith 1972):

\[ GPP = APAR \cdot LUE_p \]

where APAR is the absorbed photosynthetically active radiation expressed in radiance units and \( LUE_p \) is the efficiency of light utilization for photosynthesis and allows converting measured radiances into the number of fixed \( CO_2 \) molecules. SIF is expressed by expanding the GPP notation in Eq. (1) following Guanter et al., (2014):

\[ SIF = APAR \cdot LUE_f \cdot f_{esc} \]
where \( LUE_f \) is the light use efficiency of SIF (fluorescence yield), and \( f_{\text{esc}} \) accounts for a structural interference determining the fraction of SIF photons escaping the canopy. Relationships between SIF and GPP are mostly driven by the common APAR term. In addition, a covariance between both light use efficiencies, \( LUE_p \) and \( LUE_f \), is expected to occur in absence of the confounding impact of other protective mechanisms (Damm et al. 2010; Guanter et al. 2014).

The above outlined concept relating SIF and GPP simplifies a complex set of underlying mechanisms and violation of any assumptions made will directly confound the SIF-GPP relationship. In particular, the competition of three processes for de-exciting absorbed light energy, i.e., photochemistry, radiative energy loss (SIF), and non-radiative energy dissipation (commonly approximated as non-photochemical quenching, NPQ), causes complex and changing sensitivities of emitted SIF to actual rates of photosynthesis (Porcar-Castell et al. 2014; van der Tol et al. 2014; van der Tol et al. 2009a). This directly implies that the functional link between SIF and GPP depends on the rate of NPQ and, consequently, on ambient stress levels. At canopy scale, the three-dimensional structure causes gradients in light interception and light quality within canopies (Nobel et al. 1993; Stewart et al. 2003), additionally altering the rate of NPQ (Demmig-Adams 1998; Niinemets et al. 2003) and thus, impacting the SIF-GPP relationship. Canopy structure also increases the probability for the emitted SIF photons either to be re-absorbed by chlorophyll or to escape the canopy (Fournier et al. 2012; Knyazikhin et al. 2013), to some extent violating the assumption of \( f_{\text{esc}} \) to be constant. In addition to these structural and physiological effects, variations in SIF signals caused by, for example, instrumental (Damm et al. 2011) or atmospheric effects (Damm et al. 2014; Guanter et al. 2010), and retrieval uncertainties related to the estimation of surface irradiance (Damm et al. 2015) can potentially affect the apparent relationship between SIF and GPP. Proper understanding of confounding factors remains crucial to use SIF to constrain
estimates for GPP at ecosystem or continental scales (Garbulsky et al. 2014; Guanter et al. 2012; Parazoo et al. 2014).

Considering the above listed mechanisms, several aspects need to be addressed to further exploit SIF as a robust constraint for estimating GPP. We therefore aim at investigating the functional information content of SIF and its link to GPP considering three structurally and physiologically contrasting ecosystems, i.e., cropland, perennial grassland and mixed temperate forest. We use an innovative combination of multi-temporal imaging spectroscopy (IS) data, EC flux tower observations, and modeling approaches at the leaf and canopy levels i) to assess the relationship between far red SIF retrieved in the O$_2$-A band at 760 nm (SIF$_{760}$) and GPP across ecosystems, and ii) to investigate the impact of confounding factors on the SIF$_{760}$-GPP relationship, i.e., temporal scaling effects and structural and physiological interferences using a photosynthesis model. Our findings contribute to a better understanding of the information inherent in remotely measured SIF$_{760}$ and its functional relationship to GPP. Aspects discussed will help bridging the gap between small scale studies and observational attempts to estimate GPP globally.

2 Methods

2.1 Study sites

We investigated three contrasting ecosystems located on the Central Swiss Plateau in terms of structure, heterogeneity, species composition, and annual productivity. Two of these ecosystems were collocated in the agricultural area near the town of Oensingen (47°17'11" N, 7°44'01" E, 452 m.a.s.l.; Figure 1A). This area is characterized by relatively small agricultural parcels with grassland, clover fallow cropping, bean, maize, rapeseed, pea, sugar beet, winter barley, and winter wheat rotating as dominant crops. Two grassland fields, differently managed in terms of species composition, fertilization and harvesting activities (Ammann et
al. 2007), were investigated as representatives of the ecosystem type perennial grassland, as well as a cropland (one field with arable crop rotation) for the ecosystem type cropland. The forest area (47°28'42" N, 8°21'52" E; Figure 1B) is located on the south-facing slope of the Laegeren mountain, northwest of the city of Zurich. The temperate mixed forest is characterized by a relatively high species diversity and a complex canopy structure, with beech, ash, sycamore, and spruce being the dominant species (Eugster et al. 2007; Schneider et al. 2014).

Both test sites are well instrumented (i.e., with eddy-covariance flux towers, micrometeorological stations) and were extensively sampled during several airborne campaigns between 2009 and 2013 (Table 1).

2.2 Airborne spectroscopy

All three study sites were measured with the Airborne Prism EXperiment (APEX) sensor on several days between 2009 and 2013 (Table 1). APEX is an airborne dispersive pushbroom imaging spectrometer, covering the 400-2500 nm spectral region in 313 narrow continuous spectral bands. APEX allows capturing the O$_2$-A atmospheric absorption feature, and thus retrieving SIF$_{760}$, with a spectral sampling interval of 4.5 nm, a full width at half maximum (FWHM) of 5.7 nm, and a signal to noise ratio of approximately 450 in and 800 outside of the O$_2$-A feature for a 50% reflective target and a sun zenith angle of 30° (Jehle et al. 2010; Schaepman et al. 2015).
Radiance calibration of APEX images is performed using the approach of Hueni et al. (2009). Multitemporal comparison of images is secured by using consistent calibration and processing versions. Precise retrievals of SIF typically require data measured in sub-nanometer spectral resolution. However, the feasibility of using APEX like instruments (i.e., FWHM ~5nm) for SIF\textsubscript{760} retrievals was theoretically assessed in Damm et al. (2011) and experimentally demonstrated in recent work (Zarco-Tejada et al. 2009; Zarco-Tejada et al. 2013). The use of calibrated APEX radiance data for the fluorescence retrieval is described in Section 2.4 and Appendix-B. Vegetation indices (see Section 2.5) were calculated using Hemispherical-Conical-Reflectance-Factor data obtained after atmospheric correction using ATCOR-4 (Richter and Schläpfer 2002). Resulting SIF\textsubscript{760} and vegetation indices were projected in the same map projection using parametric geocoding (Schläpfer and Richter 2002). Details about APEX data calibration are listed in Appendix-A.

2.3 Field spectroscopy

ASD (PANalytcs, Boulder, US) field spectrometer data were acquired for validation purposes within one hour of the APEX overflight during four campaigns. In total, 23 agricultural fields covering various crops, including carrot, maize, pea, rye, sugar beet, wheat, white clover, were systematically sampled by measuring reflected and emitted radiances in four homogeneous 3 m\textsuperscript{2} plots per field (Table 2). Incident light was quantified before and after measuring each plot using a Spectralon reference panel.

< Table 2 >

2.4 SIF\textsubscript{760} retrieval

Emitted SIF was analytically separated from the reflected radiance flux measured with ground and airborne-based spectrometers (see Appendix-B). We applied the Fraunhofer Line
Depth (FLD) approach (Plascyk 1975), which serves as a standard for SIF retrievals using medium resolution instruments (Meroni et al. 2009). The FLD method uses atmospheric absorption bands, characterized by lower incident light compared to wavelength regions outside of these bands. This configuration allows evaluating the in-filling of the absorption bands by SIF (Damm et al. 2014). In this study, we used the broad O$_2$-A oxygen absorption band around 760 nm for the SIF$_{760}$ retrieval. For the ground data, surface irradiance was estimated from white reference measurements, while perturbing atmospheric absorption and scattering effects were assumed to be negligible on the 1 m pathway between canopy and sensor (c.f., Damm et al., (2014) for details on the set-up for SIF$_{760}$ retrieval on the ground). For the airborne measurements, we compensated atmospheric absorption and scattering using the atmospheric radiative transfer model MODTRAN5 (Berk et al. 2005). Details of the SIF$_{760}$ retrievals using airborne data are provided in Appendix-B.

2.5 Derivation of additional spectral indices

The relationship between two vegetation indices and GPP was investigated in parallel to judge the performance of the new remote observation of SIF compared to commonly used remote sensing approaches. The photochemical reflectance index (PRI) (Gamon et al. 1992) was found to be sensitive to pigment changes related to the xanthophyll cycle and is frequently used to quantify LUE$_p$ and GPP (Cheng et al. 2013; Drolet et al. 2008; Hilker et al. 2009). The PRI was calculated as

$$PRI = \frac{R_{531}-R_{570}}{R_{531}+R_{570}}, \quad (3)$$

while $R_\lambda$ accounts for the surface reflectance at the wavelength $\lambda$.

We further tested the soil adjusted Modified Chlorophyll Absorption Ratio Index 2 (MCARI2) (Haboudane et al. 2004) that was found to be strongly related to green LAI, thus potential photosynthesis, and is calculated as:
Continuous turbulent fluxes of CO$_2$ were measured at the agricultural and forest sites between 2009 and 2013 using the EC technique (Baldocchi 2003). At each site, the EC instrumentation consisted of an open-path infrared gas analyzer (IRGA) (model LI-7500, LI-COR Inc., Lincoln, NE, USA) and a three-dimensional sonic anemometer-thermometer (models HS, R3 and R2, Gill Instruments, Lymington, UK). EC measurements were made at a frequency of 20 Hz and processed to half-hourly averages using the eth-flux EC software for the forest and cropland (Mauder et al. 2008) or a comparable custom-made EC software for the grassland (Ammann et al. 2007). Post-processing included corrections for damping losses (Eugster and Senn 1995), air density fluctuations (Webb et al. 1980), data screening for optical sensor contamination, stationary or low turbulence conditions (Foken and Wichura 1996), and statistical outliers. Standardized gap filling and partitioning of CO$_2$ fluxes was performed using the methodology from Lasslop et al. (2010) for the forest and cropland, and using the methodology from Falge et al. (2001) for the grassland. Measurements of photosynthetic photon flux density (PPFD) quantified in µmol m$^{-2}$ s$^{-1}$ were converted to radiance units (mW m$^{-2}$ sr$^{-1}$ nm$^{-1}$), representing the photosynthetic active radiation (PAR) to be consistent with Monteith’s LUE concept and the SIF radiance units.

2.7 Leaf area index measurements

The Leaf Area Index (LAI) of the grassland and cropland was measured at the time of APEX flights, using an optical non-destructive approach based on LAI-2000 leaf area meter observations (Li-Cor, Lincoln, USA). The LAI of the forest was estimated using digital
hemispherical photographs at two subplots following the VALERIE sampling scheme, while
subsequent analysis were applied to obtain the LAI (Schneider et al. 2014).

2.8 Statistical analysis of SIF$_{760}$ - GPP relationship

SIF$_{760}$ values were manually extracted from APEX-SIF$_{760}$ maps for areas representing
the footprint of eddy-flux measurements (Figure 1). For the perennial grassland and cropland,
we selected all pixels with SIF$_{760}$ values $\geq 0$ mW m$^{-2}$ sr$^{-1}$ nm$^{-1}$ in respective fields although the
EC tower footprint can be slightly smaller than the entire field. The increased number of
resulting pixels allows reducing data noise and covering small spatial variations within the
footprint. Using the pixels of the entire field is justified by the large homogeneity of the
underlying fields (Figure 1A). For the forest site Laegeren, all pixels representing an area that
covered 70% of all footprint occurrences were selected, irrespective of spatial footprint
changes due to changing wind conditions. Using the same area for all years reduces variations
in SIF due to changes in biomass and canopy structure but also reduces the representativeness
of selected pixels for actual spatial EC footprints.

We used a hyperbolic model to relate GPP to SIF$_{760}$ and to both vegetation indices.
Although the hyperbolic model only empirically approximates the data behavior, it is
supported by theoretical arguments for the SIF$_{760}$-GPP relationship that are outlined hereafter.
The photosynthetic efficiency LUE$_{p}$ is often described as a hyperbolic function of APAR
following the Michaelis-Menten theory (Michaelis and Menten 1913):

$$LUE_p = \frac{c \cdot LUE_{p,max}}{c + APAR}$$

(5)

where c is a coefficient in radiance units and LUE$_{p,max} \cdot c$ represents GPP$_{max}$. Following Eqs.
(1) and (5), GPP rises asymptotically with APAR to GPP$_{max}$. This equation is used in many
models for partitioning GPP, e.g., Falge et al. (2001). Substituting LUE$_{p}$ from Eq. (5), and
APAR $= SIF_{760} / (LUE_{f} \cdot f_{esc})$ from Eq. (2), into Eq. (1) results in
\[ GPP = GPP_{\text{max}} \frac{\text{SIF}_{760}}{\text{SIF}_{760} + b}, \] (6)

where the coefficient \( b \) represents \( c \cdot \text{LUE}_{f} \cdot f_{\text{esc}} \), accounting for the difference between \( \text{LUE}_p \) and \( \text{LUE}_f \). \( GPP_{\text{max}} \) is a value that is asymptotically reached, representing the photosynthetic capacity or GPP of the canopy at light saturation. It must be noted that Eq. (6) is a simplification of the complex relationships between GPP and SIF\(_{760}\), and thus performs best if \( c \cdot \text{LUE}_f \cdot f_{\text{esc}} \) remains constant, or SIF\(_{760}\) corresponds to APAR. A constant \( \text{LUE}_f \) is a reasonable first approximation for vegetation that is only moderately stressed, meaning that variations in \( \text{LUE}_f \) are substantially smaller than variations in \( \text{LUE}_p \) (van der Tol et al. 2014).

Moderate stress relates to any kind of environmental conditions (warm temperature, strong irradiance, reduced water availability) that cause only short term and slight changes in photochemical and non-photochemical protections. However, \( c \) and \( f_{\text{esc}} \) are known to vary across ecosystems and \( \text{LUE}_f \) changes under environmental stress. In order to evaluate their impacts on the SIF-GPP relationships as expressed in Eq. (6), we carried out simulations with the Soil-Canopy Observations of Photosynthesis and Energy balance (SCOPE) model SCOPE version 1.53 (van der Tol et al. 2009b) (see Section 2.9). The goodness of fit for the hyperbolic model was quantified using non-linear regression analysis and was quantitatively described using the root mean square error normalized by the mean of measured data (rRMSE) and the coefficient of determination \( R^2 \) defined as the correlation between data and the best fit-curve determined by non-linear regression.

2.9 SCOPE simulations

SCOPE uses semi-empirical models for \( \text{LUE}_p \) (Collatz et al. 1991) and \( \text{LUE}_f \) (van der Tol et al. 2014) embedded in a radiative transfer scheme for the canopy (van der Tol et al. 2009b). The radiative transfer model at leaf level (Fluspect) is an extension of PROSPECT (Jacquemoud and Baret 1990) and includes a fluorescence component. The radiative transfer
within the canopy is calculated following Verhoef (1984) in the optical domain (SAIL), following Verhoef et al. (2007) in the thermal domain, and Miller et al. (2005) for the fluorescence emissions (FluorSAIL). SCOPE requires a number of vegetation structural and physiological parameters as well as weather information as input. The model simulates GPP and spectrally distributes SIF with a spectral resolution and a spectral sampling interval of 1.0 nm each. Simulated PPFD values (µmol m\(^{-2}\) s\(^{-1}\)) were also converted to radiance units (PAR).

We carried out three simulations using SCOPE. In the first simulation, we calculated leaf level LUE\(_{f}\) and LUE\(_{p}\) of a typical C3 cropland as function of varying APAR. For the second simulation at canopy level, we calculated LUE\(_{f}\) and LUE\(_{p}\) as function of varying APAR for differently structured canopies. We took the standard SCOPE parameters for a typical C3 cropland and varied APAR and the structural parameters LAI, leaf inclination angle (LIDF) and the fraction of brown pigments (Cs). Both simulation experiments provide theoretical evidence on the relationships between LUE\(_{f}\) and LUE\(_{p}\), between SIF\(_{760}\) and GPP and their respective relationships to APAR. For the third canopy level simulation, SCOPE was initialized using time series of mid-day (solar noon) meteorological data (PAR, air temperature), a seasonal cycle of LAI, and the model’s default soil and vegetation parameters for a C3 cropland (c.f., the SCOPE user manual). The purpose of this simulation was to evaluate seasonal SIF\(_{760}\)-GPP relationships at various temporal aggregation levels. For better readability, we use the following notation through the manuscript: SIF\(_{760, o}\) for APEX-SIF, SIF\(_{760, L}\) and SIF\(_{760, C}\) for SCOPE simulated leaf and canopy SIF, GPP\(_{EC}\) for flux tower GPP and GPP\(_{L}\), GPP\(_{C}\) to relate to simulated GPP at leaf and canopy level.

3 Results

3.1 SIF\(_{760}\) maps
Two examples of SIF\textsubscript{760, O} maps obtained from APEX are shown in Figures 2 and 3. The appearance of SIF\textsubscript{760, O} emissions in vegetated areas demonstrates that measured SIF\textsubscript{760, O} signals originated solely from vegetation and were not contaminated by non-fluorescent non-vegetation surfaces. Retrieved SIF\textsubscript{760, O} values range between 0 and 3 mW m\textsuperscript{-2} sr\textsuperscript{-1} nm\textsuperscript{-1} and showed a high agreement ($r^2 = 0.7$, rRMSE = 28.9\%) with in-situ measured reference data. Details of the SIF\textsubscript{760, O} validation are discussed in Appendix-C.

< Figure 2 >

< Figure 3>

3.2 Relationships of $\text{GPP}_{\text{EC}}$ with SIF\textsubscript{760, O}, PRI and MCARI2

Relating instantaneous measurements of SIF\textsubscript{760, O} and $\text{GPP}_{\text{EC}}$ from several years revealed an asymptotic relationship with saturating $\text{GPP}_{\text{EC}}$ in presence of moderate to high SIF\textsubscript{760, O} (Figure 4A, Table 3). This general behavior was consistent for all investigated vegetation types. The fitted hyperbolic model shows a moderate to high goodness of fit for the grassland ($R^2 = 0.59$, rRMSE = 27.1\%), cropland ($R^2 = 0.88$, rRMSE = 3.5\%) and forest ($R^2 = 0.48$, rRMSE = 15.88\%). The saturation of $\text{GPP}_{\text{EC}}$ appeared earlier for the cropland (SIF\textsubscript{760, O} ~0.5 mW m\textsuperscript{-2} sr\textsuperscript{-1} nm\textsuperscript{-1} ) than for the grassland and forest (SIF\textsubscript{760, O} > 1.0 mW m\textsuperscript{-2} sr\textsuperscript{-1} nm\textsuperscript{-1}). An independent assessment considering a linear model to describe the relationship between SIF\textsubscript{760, O} and $\text{GPP}_{\text{EC}}$ revealed a consistently lower goodness of fit, justifying the use of a hyperbolic model (data not shown).

Statistical analysis showed that a hyperbolic model represents well the relationship between both vegetation indices (PRI and MCARI2) and $\text{GPP}_{\text{EC}}$ for the grassland with a notable variation in LAI (range between 0.5 and 4.8 m\textsuperscript{2} m\textsuperscript{-2}). However, a hyperbolic model does not allow well representing the relationship between PRI and MCARI2 with $\text{GPP}_{\text{EC}}$ for the forest and cropland, both showing only a small variation in LAI (less than ±0.3 m\textsuperscript{2} m\textsuperscript{-2}).
(Figure 4B-C, Table 3). The goodness of fit for the hyperbolic model describing the PRI and GPPEC data for grassland ($R^2 = 0.95$, rRMSE = 8.6%) was even higher compared to SIF$_{760,\, O}$, but lower for forest ($R^2 = 0.09$, rRMSE = 21.79%) and cropland ($R^2 = 0.008$, rRMSE = 11.76%). With MCARI2, the goodness of fit for the hyperbolic model for grassland was high ($R^2 = 0.98$, rRMSE = 5.5%) but low for cropland ($R^2 = 0.005$, rRMSE = 10.29%) and forest ($R^2 = 0.34$, rRMSE = 17.98%). Again, considering a linear relationship between both vegetation indices and GPPEC revealed no consistent improvement compared to the use of a hyperbolic model (data not shown).

3.3 Assessment of factors determining SIF$_{760}$ GPPEC relationships

The asymptotic relationship between SIF$_{760,\, O}$ and GPPEC (Figure 4A) represented instantaneous measurements of different canopies at different times and days over several years, covering a range of different light conditions, phenological stages of the forest, and various amounts of green biomass for both investigated grasslands (crosses in Figure 5A-C that indicate EC measurements during APEX overpasses). Relationships between SIF$_{760,\, O}$ and GPPEC are consequently a complex function of light absorption in the canopy (APAR), of the efficiency of light utilization (i.e., expressed as photosynthetic capacity and quantum efficiency of photosynthesis), and of structural effects including fractions of non-photosynthetic vegetation components. Both grass canopies were measured before and after mowing, resulting in a large range in LAI (0.5-4.8 m$^2$ m$^{-2}$) and GPPEC (4-27 µmol m$^{-2}$ s$^{-1}$) for similar PAR values. The forest LAI of 5.0 m$^2$ m$^{-2}$ was more constant over the years due to the consistent timing of flights; however, senescence (e.g., lower canopy chlorophyll content and light absorption) might explain the decrease in GPPEC of 15 µmol m$^{-2}$ s$^{-1}$ in September for
comparable irradiance conditions (Figure 5C). Investigated crops (winter wheat, barley and pea) were characterized by small variations in LAI (2.2-2.5 m$^2$ m$^{-2}$) and chlorophyll contents, corresponding to small variations in GPP_{EC} (5 µmol m$^{-2}$ s$^{-1}$) while observed under comparable irradiance conditions. During the time of observation, the barley and wheat canopies were in the ripening phase with a pronounced ear layer.

The validity of the asymptotic relationship between SIF$_{760, O}$ and GPP$_{EC}$ was tested using simulations made with the SCOPE model. We emphasize that the regression coefficient $b$ in Eq. (6) includes terms that vary in the model ($b= c \cdot$LUE$_f$ f$_{esc}$): the fluorescence efficiency LUE$_f$ varies with irradiance conditions (predominantly APAR), the fraction f$_{esc}$ depends on vegetation structure, while c=GPP$_{max}$/LUE$_{p,max}$ varies between sites and over time during the season. We first analysed how LUE$_f$ and LUE$_p$, and consequently, SIF$_{760}$ and GPP, vary at leaf (i.e., SIF$_{760, L}$ and GPP$_L$) and canopy levels (i.e., SIF$_{760, C}$ and GPP$_C$) using the model of van der Tol et al. (2014) that is embedded in SCOPE. For the leaf level, Figure 6A shows a decrease of LUE$_p$ with increasing APAR, consistent with Eq. (5). The relation between APAR and LUE$_f$ appears more complex: LUE$_f$ first increases with increasing APAR under low light conditions, reaches a climax at intermediate light, and then decreases with increasing APAR under higher APAR values (> 50 mW m$^{-2}$ sr$^{-1}$ nm$^{-1}$) (Figure 6B). The initial increase in LUE$_f$ is caused by the decline in photochemical quenching of the excitons, whereas the decrease of LUE$_f$ is caused by the growing number of non-photochemical quenching traps that dissipate light energy before it can be emitted as fluorescence light (van der Tol et al. 2009a). It is important to note that the range of LUE$_p$ is nearly an order of magnitude greater compared to the range of LUE$_f$ (Figure 6C). Although LUE$_f$ is not constant, we can still conclude that the difference in both LUE terms causes an earlier saturation of leaf-level GPP$_L$ (Figure 6D).
compared to leaf-level SIF\textsubscript{760,L} (Figure 6E) with APAR, leading to an asymptotic relationship between SIF\textsubscript{760,L} and GPP\textsubscript{L} (Figure 6F). Our canopy level simulations confirm these trends (Figure 7A-D). The in-field measured asymptotic relationships between SIF\textsubscript{760,O} and GPP\textsubscript{EC} are consequently caused by the covariance of GPP\textsubscript{EC} and SIF\textsubscript{760,O} with APAR, the photosynthetic capacity with APAR, and the different value ranges of LUE\textsubscript{f} and LUE\textsubscript{p}. Additionally, our canopy level simulations suggest that structure impacts the SIF\textsubscript{760,O} - GPP\textsubscript{EC} relationship. Figure 7D shows an example that changing LAI, leaf inclination angles, or the fraction of senescent plant material determine the curvature of the hyperbolic SIF\textsubscript{760,C} - GPP\textsubscript{C} relationships.

The modelled SIF\textsubscript{760,L,C} - GPP\textsubscript{L,C} curves (Figures 6D and 7D) also indicate that under reduced light intensity GPP and SIF\textsubscript{760} are almost linearly related, while GPP tends to saturate under higher light intensities. Changes in APAR at canopy level are caused by either sun elevation or, in the case of a constant solar angle, by canopy structure (i.e., shading, fractional vegetation cover). In complex structured canopies with many foliage layers, the saturation of GPP with APAR may not be observable because variations of APAR are less related to PAR falling on the leaves but rather to the variation of leaf area exposed to light. Model simulations suggest that in complex canopies SIF\textsubscript{760} saturates with APAR before GPP due to $f_{esc}$ being lower with high APAR (data not shown). This structural effect reduces the curvature of the hyperbolic leaf level GPP\textsubscript{L} - SIF\textsubscript{760,L} relationship at canopy level (compare Figures 6F and 7F). Furthermore, the effect of structure and APAR covary in time since canopy structure (i.e., LAI) varies in concert with APAR during a seasonal cycle, especially for crops. We
expect that this covariance makes the relationship between GPP and SIF\textsubscript{760} more linear at the canopy level, especially if observations are aggregated over time.

To evaluate the structure related alleviation of the hyperbolic relationship between SIF\textsubscript{760} and GPP at canopy level in response to temporal aggregation, we modelled an annual course of GPP\textsubscript{C} and SIF\textsubscript{760, C} considering varying environmental conditions (Figure 8A-B), i.e., PAR ranging from 0-500 mW m\textsuperscript{-2} sr\textsuperscript{-1} nm\textsuperscript{-1}, air temperature ranging from 0-32\degree C using data collected during 2009 at a Nitro-Europe flux tower site (Speulderbos, The Netherlands) and canopy properties, i.e., LAI ranging from 1.5-3.0 m\textsuperscript{2} m\textsuperscript{-2} (Figure 8C). The LAI data are synthetic but have a realistic seasonal cycle. For daily noon values of modelled SIF\textsubscript{760, C} and GPP\textsubscript{C}, an asymptotic behaviour can be observed while GPP\textsubscript{C} tends to saturate compared to SIF\textsubscript{760, C}. The SIF\textsubscript{760,C}-GPP\textsubscript{C} relationship tends to become linear when monthly or quarterly averages are considered (Figure 8D).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure8}
\caption{Figure 8}
\end{figure}

This visual trend can be confirmed by statistical measures: for daily aggregated values, the hyperbolic model (rRMSE = 17.4\%, R\textsuperscript{2} = 0.70) performed slightly better than the linear model (rRMSE = 18.5\%, r\textsuperscript{2} = 0.68). In case of monthly aggregated data, both the hyperbolic and linear models performed similarly, while the linear model gave better results (RMSE = 9.0, r\textsuperscript{2} = 0.90) than the hyperbolic model (rRMSE = 9.4\%, R\textsuperscript{2} = 0.88) for quarterly aggregated data.

4 Discussion

Significant relationships between remotely measured SIF and ecosystem GPP have been reported in the past (Frankenberg et al. 2011; Guanter et al. 2014); however, sufficient
process understanding for using SIF as proxy for GPP across ecosystems is still limited (Porcar-Castell et al. 2014). Below we discuss how our observational and modeling approaches help bridging the gap between mechanistic understanding at the leaf level and ecosystem-specific observations and, thus, provide insights on mechanisms determining the complex relationship between SIF and GPP.

4.1 Insights from the observational approach

Our results showed ecosystem-specific asymptotic relationships between SIF$_{760,\text{O}}$ and GPP$_{\text{EC}}$ for the three investigated ecosystems: mixed temperate forest, cropland and perennial grassland. The varying SIF-GPP relationships across ecosystems were consistent with results recently reported from combined satellite observations and model predictions (Ganter et al. 2012). Our results showed that the relationships of both tested vegetation indices, PRI and MCARI2, to GPP$_{\text{EC}}$ experienced a higher variability across ecosystems compared to SIF$_{760,\text{O}}$. SIF$_{760,\text{O}}$ showed an ecosystem-specific and overall moderate to good relationship ($R^2$ between 0.48 and 0.88) to GPP$_{\text{EC}}$ for the three ecosystems. Both vegetation indices showed only strong relationships for the grassland ($R^2 = 0.95$ and 0.98) that notably changed in LAI during the various observations. It is important to note that we do not further elaborate on the underlying mechanisms relating vegetation indices and GPP$_{\text{EC}}$, and that it is unclear if hyperbolic models best describe their relationships to GPP$_{\text{EC}}$ based on mechanistic principles. The intention of evaluating the relationships between GPP$_{\text{EC}}$ and both vegetation indices was to provide a base to judge the performance of SIF$_{760,\text{O}}$ in relation to these commonly used remote observations.

The diversity of sampled conditions and used data sources provide further evidence on the robustness of observed SIF$_{760,\text{O}}$-GPP$_{\text{EC}}$ relationships. Our measurements represent various canopies characterized by different biomasses sampled over several years. Although most observations were acquired under similar light condition and physiological states, a few measurements represented lower light conditions and other physiological states. This suggests
that observed relationships are rather robust across different representations of APAR, LUE$_p$, and LUE$_f$. Furthermore, we use data from different sources, i.e., four EC flux towers, the APEX imaging spectrometer, and modeling at leaf and canopy levels, to reduce the uncertainties associated with each method of measurements and to get a better understanding of the SIF$_{760}$, O-GPP$_{EC}$ relationship at ecosystem level.

Flux tower measurements are representative of a certain source area (footprint) from the ecosystem which changes constantly based on wind direction and turbulent state of the atmosphere. Depending on the heterogeneity of the ecosystem, GPP$_{EC}$ signals can vary in response to changing footprints (Barcza et al. 2009; Kljun et al. 2004), although this variation should be rather small if the vegetation is homogeneous. Remote measurements of SIF$_{760}$ are likely representative of the upper layer of the ecosystem, thus, vertical canopy heterogeneity potentially leads to a mismatch when compared to GPP$_{EC}$ which integrates over the different layers of the ecosystems. This is expected to be especially the case in structurally complex ecosystems such as forests. Although the upper layer in forest ecosystems substantially contributes to the total rate of GPP$_{EC}$, there are still many layers of leaves or needles within the canopy photosynthesizing at different rates depending on their sun/shade exposure. In addition, understory vegetation in forest ecosystems can significantly contribute to GPP$_{EC}$ at different rates depending on the ecosystem and time of year. Even homogeneous vegetation canopies like crops or grasslands can show vertical heterogeneity. This is especially the case at peak biomass during ripening or senescence. During such phenological stages, the top layer of cereal crops consists of less fluorescing components (i.e., ears) and cereal crops or grasslands can contain a higher fraction of brown pigments resulting in low SIF$_{760}$, O values, while the entire canopy can still produce high photosynthetic rates and thus GPP$_{EC}$ (Damm et al. 2010). Indeed most of the crops investigated in our study were in the ripening phase with a pronounced ear layer.
This resulted in relatively low SIF$_{760}$ values and in high GPP$_{EC}$ and thus, in a more pronounced asymptotic relationship (c.f., Figure 4A, Figure 7F) compared to results reported for other crops (Guanter et al. 2013; Guanter et al. 2014). Further research is needed to better understand the impact of vertical heterogeneity on GPP$_{EC}$ and SIF$_{760}$ observations and their respective relationships.

Despite the technical aspects causing variations in retrieved SIF$_{760}$, canopy structure causes inherent variations in measured SIF$_{760}$ values, and thus, impacts SIF$_{760}$-GPP relationships. The combination of complex canopy architecture and the distribution of absorbing and scattering elements determine vegetation canopies to act as photon traps (Knyazikhin et al. 2013; Lewis and Disney 2007). Parts of emitted SIF$_{760}$ photons from inner-canopy leaves are re-absorbed, while others escape the canopy in direction of the sensor. The probability of photons escaping the canopy is a function of canopy structure, which implies sensitivity to measured SIF$_{760}$ intensities for canopy structure. In Eq. (2), this sensitivity was approximated with the term $f_{esc}$. In our analysis, we minimized the impact of $f_{esc}$ by observing always the same forest area representative for the EC tower footprint. In less complex structured crop and grass canopies, we expect $f_{esc}$ to be less important. However, future research is required to quantify the impact of $f_{esc}$ and to propose strategies to compensate its influence on SIF$_{760}$ retrievals.

### 4.2 Insights from the modeling approach

From a theoretical point of view, radiative energy loss competes with photochemistry and non-radiative energy dissipation for absorbed photons. Considering that GPP and SIF$_{760}$ can be conceptualized according to Eqs. (1) and (2), SIF$_{760}$ must show under certain environmental conditions a sensitivity to photochemistry (Porcar-Castell et al. 2014; van der Tol et al. 2009a; van der Tol et al. 2009b). This relationship is confirmed by our observational data and other studies at leaf (Amoros-Lopez et al. 2008) and canopy levels (Damm et al. 2010).
Our modeling results, however, indicated that the relationship between \( \text{LUE}_f \) and \( \text{LUE}_p \) is subject to change, hence, impacting the sensitivity of \( \text{SIF}_{760} \) to track changes in GPP (Figures 6C and 7C).

The asymptotic relationship between \( \text{SIF}_{760} \) and GPP theoretically predicted and observed at leaf and canopy levels can be related in particular to the different value ranges of both efficiency terms (\( \text{LUE}_p \) and \( \text{LUE}_f \)) (Figures 6C and 7C), while a complex set of mechanisms causes an ecosystem dependency for \( \text{SIF}_{760}\text{-GPP} \) relationships. The photosynthetic capacity of the entire ecosystem in combination with its vertical heterogeneity determines differences in GPP and \( \text{SIF}_{760} \) and thus, the slope and curvature of their respective relationships. Furthermore, the initial slope of the asymptotic \( \text{SIF}_{760}\text{-GPP} \) relationship, which has a value of \( \frac{\text{LUE}_{p,max}}{\text{LUE}_f f_{esc}} \), is determined by a combination of the photosynthetic efficiency and canopy structure. Canopy structure and related shadowing effects alter the average light interception and quality at leaf level (Nobel et al. 1993; Stewart et al. 2003) and, consequently, the overall productivity of the canopy. In the case of reduced APAR caused by canopy shadowing, the overall apparent stress level in the canopy and, consequently, the rate of certain photoprotective mechanisms such as non-radiative energy dissipation is reduced (Cheng et al. 2015; Demmig-Adams 1998; Niinemets et al. 2003) and observed GPP and \( \text{SIF}_{760} \) fall in a range where they are more linearly related (c.f., Figure 6F and 7F). In addition, canopy level simulations show that the fraction of senescent plant material impacts the curvature of the hyperbolic relationship.

Recent literature reports linear relationships between satellite-based SIF and modeled GPP (Frankenberg et al. 2011; Guanter et al. 2012; Guanter et al. 2014), while we found asymptotic relationships. Both results are not contradicting if one considers the temporal aggregation applied to the data. Our results are based on instantaneous measurements while monthly averages were calculated for the satellite data to minimize noise effects (Frankenberg et al. 2011; Guanter et al. 2014). It is known from previous research that temporal averaging
tends to linearize the response between GPP and APAR (Ruimy et al. 1995), as saturating light conditions tend to be only a small fraction of averaged diurnal/monthly data. Aggregating $GPP_{EC}$ and APAR over different time scales also showed this effect (data not shown). Because of the rather linear relationship between $SIF_{760}$ and APAR, we expect that temporal aggregation tends to linearize the $SIF_{760}$-GPP relationship as well. A recent study presenting continuous measurements of GPP and $SIF_{760}$ over a temperate deciduous forest support this hypothesis (Yang et al. 2015). The increasing number of experiments using autonomous spectrometer systems in combination with flux towers (Balzarolo et al. 2011) will likely provide more experimental results that supports this finding. Our simulations provide further evidence that the covariance of structure and APAR during a seasonal cycle additionally tends to linearize the relationship between GPP and $SIF_{760}$, if observations are aggregated over time.

The dependency of $SIF_{760}$-GPP relationships on temporal aggregation requires special attention since it has implications on the usage of SIF to constrain GPP. In principle, conclusions and results obtained from temporally aggregated and instantaneous measurements are valid if consistently related to the underlying temporal aggregation level. Generalizing conclusions obtained at various aggregation levels bears the risk for mis-interpretations, e.g., when vegetation models are refined or empirically re-calibrated using observations or for projections of GPP using observational SIF data.

4.3 Requirements for the use of SIF to assess GPP across ecosystems

The changing relationship between $SIF_{760}$ and $GPP_{EC}$ with vegetation type challenges the usage of $SIF_{760}$ as a robust constraint to estimate GPP. Specific strategies are required to account for ecosystem (or species) specific sensitivities of SIF in general and $SIF_{760}$, in particular. This includes i) integration platforms to combine observations and process
understanding, and ii) accurate observations of additional vegetation and environmental variables.

Process-based models as data integration platform in combination with comprehensive observations to sufficiently measure important environmental factors and vegetation properties are considered as flexible and powerful framework. Parazoo et al. (2014), for example, proposed the combination of ensemble dynamic global vegetation models (DGVMs) in combination with SIF as observational constraint. Lee et al. (2015) suggest incorporating SIF in a climate model to utilize SIF as observational constraint of photosynthesis simulations and subsequent calculations of carbon, water and energy cycle information. Yet other studies propose using SIF to obtain physiological vegetation parameters, i.e., Vcmax for improved parameterizations of photosynthesis models to eventually model GPP (Zhang et al. 2014). The European space agency's (ESA) Earth Explorer 8 opportunity mission Fluorescence Explorer (FLEX) suggests a combination of comprehensive observations (i.e., SIF over the full emission spectrum, vegetation ecosystems, and actual environmental conditions) and process-based models (Guanter et al. 2012).

Additional information is required to use SIF in process-based models, as one has to account for varying photosynthetic efficiencies of plants and prevailing stress responses. According to the conceptualization of GPP and SIF as given in Eqs. (1) and (2), extracting and evaluating the exact relationship between LUEp and LUEf is essential but requires normalizing APAR and calculating both yields (Damm et al. 2010; Govindjee 2004; Louis et al. 2005). Retrievals of APAR can be considered challenging (Garbulsky et al. 2010; Gitelson and Gamon 2015; Hanan et al. 2002) as available approaches often utilize a-priori knowledge of prevailing land cover or plant distribution functions and rely on the inversion of physical-based models or simple band ratios (Hilker et al. 2008). Research is required to provide high quality information on APAR not perturbed by light absorption of non-photosynthetic active
canopy elements (stems, branches, twigs) c.f., Zhang et al., (2013; 2012) that demonstrate attempts to improve estimates of APAR. Observed SIF$_{760, O}$ - GPP$_{EC}$ relationships are additionally confounded by non-radiative energy dissipation. The PRI was designed to monitor pigment changes related to the xanthophyll cycle (Gamon et al. 1992) and provides access to this superimposing process. However, reported sensitivities of PRI for other effects, i.e., structure (Barton and North 2001), pigment pool sizes (Gamon and Berry 2012), illumination effects (Damm et al. 2015) and the results obtained in this study question the applicability of the PRI at canopy level. Alternative approaches, such as the development of a canopy PRI as suggested by several groups (Hernandez-Clemente et al. 2011; Kovac et al. 2013; Wu et al. 2010) or the usage of pigment compositions and other functional plant traits, might represent interesting strategies and should be elaborated in future research. Structural sensitivities of canopy leaving SIF signals are critical and require further research. The application of spectrally invariant correction factors, e.g., the directional area scattering factor (Knyazikhin et al. 2013) or more advanced physically-based retrieval schemes using combined atmosphere-canopy models (Damm et al. 2015; Laurent et al. 2013) might provide potential strategies to compensate for canopy structural effects on retrieved SIF$_{760}$. Another important source of information that allows improving the usage of SIF as constraint of GPP is to consider SIF emissions over the entire emission spectrum between approximately 600 and 800 nm. Recent research successfully demonstrated the complementary information content of red-fluorescence retrieved in the O$_2$-B band at 688 nm (SIF$_{688}$) compared to SIF$_{760}$ because of the different contributions from photosystem I and II (Rossini et al. 2015). Yet other studies highlighted the potential to improve predictions of LUE$_p$ and GPP using both SIF$_{688}$ and SIF$_{760}$ (Cheng et al. 2013).
5 Conclusions

Remote sensing of SIF provides a new observational approach to assess terrestrial GPP. Compared to traditional greenness-based remote sensing parameters, we found SIF$\textsubscript{760}$ to be more consistently related to GPP$\textsubscript{EC}$. These results in combination with the more direct mechanistic link between SIF$\textsubscript{760}$ and photosynthesis suggest that using SIF$\textsubscript{760}$ provides a strategy to decrease uncertainty in estimating GPP across ecosystems.

Our observational and modeling approaches revealed asymptotic and ecosystem-specific relationships for SIF$\textsubscript{760}$ and GPP$\textsubscript{EC}$. We identified a set of interlinked mechanisms determining SIF$\textsubscript{760}$-GPP$\textsubscript{EC}$ relationships to be ecosystem specific, i.e., the photosynthetic capacity and efficiency of ecosystems, the confounding impact of non-radiative energy dissipation (NPQ), as well as ecosystem structure and the fraction of non-photosynthetic vegetation components. We demonstrated that SIF$\textsubscript{760}$-GPP$\textsubscript{EC}$ relationships scale with temporal aggregation due to a covariance of canopy structure and APAR over the seasonal cycle.

We suggest going beyond empirical and ecosystem-specific relationships, instead using instantaneous observations, comprehensively providing information on the full SIF emission, vegetation status and functioning, as well as environmental conditions, in combination with process-based models. Such approaches, e.g., suggested for ESA’s potential “Fluorescence Explorer” (FLEX) Earth Explorer mission, provide a flexible framework to account for the various influencing factors identified and to successfully apply SIF as constraint of unbiased global GPP estimates.

Furthermore, research is required to improve the comparison between observations of GPP$\textsubscript{EC}$ and SIF. Both observations stem from conceptually contrasting technologies, i.e., measurements of gas exchange vs. plant-light interactions, and provide independent and complementary access to study ecosystem photosynthesis. Despite the need to harmonize horizontally differing footprints, the vertical heterogeneity of ecosystems including the
varying contributions from different ecosystem layers must be better understood to harmonize and successfully integrate both measurements.

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Appendix-A: APEX data calibration

The calibration of APEX images is based on the APEX Processing and Archiving Facility (PAF), which is the combined software and hardware designed to generate calibrated level 1 at-sensor radiances from APEX raw image streams (Hueni et al. 2009). Calibration coefficients for the radiometric, geometric and spectral calibrations are generated from system calibrations at the APEX Calibration Home Base (CHB) at DLR Oberpfaffenhofen (Gege et al. 2009). These CHB data are stored and processed within the APEX Calibration Information System (CAL IS), producing the so-called calibration cubes holding coefficients for each spatio-spectral pixel (Hueni et al. 2013).

For the multi-temporal dataset employed within this study, all flight lines were reprocessed from the original raw image streams to ensure that the same version of the processor was applied. The APEX PAF and CAL IS have significantly evolved over the timeframe of the dataset with calibrations getting more accurate over the years. To ensure consistency, all data were calibrated using coefficients obtained in May 2013.

The processor was specifically configured to retain the highest information content in the VNIR channel, including i) no spectral resampling to compensate for spectral shifts and misregistrations (D'Odorico et al. 2010; D'Odorico et al. 2011), ii) no compensation of spectral shift related changes in radiometry (Hueni et al. 2015), and iii) no spatial misregistration correction. The calibration was thus effectively reduced to a linear dark current correction over time, a de-smearing of the visible-NIR channel to compensate for sensor smear effects, the application of radiometric gains and offsets followed by a destriping routine working in the spatial dimension only to remove pushbroom related along track striping. Calibrated radiance data were directly used for the fluorescence retrieval (see Section 2.4), while the feasibility to use APEX for SIF\textsubscript{760} retrievals was theoretically demonstrated in
a study of Damm et al. (2011). Resulting SIF$_{760}$ maps were afterwards geo-rectified using a parametric geocoding approach (Schläpfer and Richter 2002).
Appendix-B: Retrieval of SIF_{760} from airborne data

The quantification of SIF measured with ground or airborne-based spectrometers requires separating emitted SIF from the reflected radiance flux. The Fraunhofer Line Depth (FLD) approach, introduced by Plascyk (1975), serves as a de facto standard for medium resolution instruments such as APEX (Meroni et al. 2009) and was applied in our study. The FLD method uses atmospheric absorption bands, characterized by lower incident light compared to wavelength regions outside of these bands. This configuration increases the spectral information and allows the separation of SIF from reflected radiation. In this study, we used the broad O_2-A oxygen absorption band around 760 nm and quantified the infilling of SIF_{760} using radiance measurements inside (subscript i) and outside (subscript o) of the O_2-A band.

For the airborne case, only atmospheric components can be simulated with MODTRAN-5 assuming perfect knowledge of the acquisition conditions. The reflectance terms for diffuse and direct irradiance as well as the SIF_{760} contribution are usually unknown. Assuming Lambertian surface reflectance behavior, which introduces some inaccuracies but allows formulating the radiative transfer (RT) for radiance measurements at sensor level ($L^{AtS}$) to obtain SIF_{760}, both measurements inside and outside of the absorption band can be expressed as:

$$L^{AtS}_j = \frac{(E_j^0 \cos \theta_i)}{\pi} \left[ (\rho_{so}^i + (\tau_{oo}^i + \tau_{sd}^i) j \frac{\tau_{ss}^i}{1 - \rho_{dd}^i}) \right] + \frac{SIF_{j}}{1 - \rho_{dd}^i}, j = i, o$$  \quad (B1)

where $E_j^0$ is the top-of-atmosphere irradiance including diffuse and direct irradiance components, $\theta_i$ is the illumination zenith angle, $\rho_{so}$ is the path scattered radiance, $\tau_{ss}$ is the direct transmittance for sunlight, $\tau_{oo}$ is the direct transmittance in view direction, $\tau_{sd}$ is the diffuse transmittance of the atmosphere for sunlight, $\tau_{do}$ is the hemispherical-directional transmittance in view direction, and $\rho_{dd}$ is the spherical albedo. If these atmospheric
components are obtained from MODTRAN-5 simulations (Damm et al. 2015; Verhoef and Bach 2003a, b, 2007), the radiative transfer equation (Eq. B1) only contains four unknowns, namely $R_i$, $R_o$, $SIF_i$, and $SIF_o$. The 3FLD method (Maier et al. 2003), which is an adaptation of the original FLD method proposed by (Plascyk 1975), was used to linearly relate $R$ and $SIF$ inside and outside of the O$_2$-A absorption band. SIF can be finally retrieved with:

$$SIF_{760} = \frac{X_j(E_j + X_o(\rho_{do}^j))}{E_j} - X_j(E_i + X(\rho_{di}^j))$$  

$$X_j = \left( E_j - \left( \frac{\rho_0^j \cos \theta_{jun}^j}{\rho_0^j \cos \theta_{jou}^j} \right) \right), \quad j = i, o$$

$$E_j = \left( \frac{\rho_0^j \cos \theta_{jun}^j}{\rho_0^j \cos \theta_{jou}^j} \right) \left( \tau_{do}^j + \tau_{di}^j \right) \cdot \left( \tau_{as}^j \cdot \tau_{ds}^j \right)$$

$$R_i = AR_o$$

$$SIF_i \left( (\tau_{as}^i) + (\tau_{ds}^i) \right) = BSIF_o \left( (\tau_{as}^o) + (\tau_{ds}^o) \right)$$

where $B$ is the factor relating $SIF_i$ and $SIF_o$ and was fixed to a value of 0.8, justified by simulations and experiments (Rascher et al., 2009; Alonso et al., 2008), $X_j$ equals the at-sensor radiance (reflected plus emitted radiation) without path radiance contribution and $E_j$ expresses surface irradiance as measured at the sensor level. $A$ is the factor relating $R_i$ and $R_o$, and was derived from linear interpolation of $R$ of the left (758 nm) and right (771 nm) O$_2$-A band shoulder with

$$A = \frac{R_{758} + R_{771} \omega_2}{R_{758}}$$

$$\omega_1 = \frac{771 - 760}{771 - 758}, \quad \omega_2 = \frac{760 - 758}{771 - 758}$$

Because APEX suffered from slight spectral smile effects (D’Odorico et al. 2010), updated center wavelength positions were involved in the convolution approach. The spectral shift quantification for each pixel across track was based on the Cr method as described in
Meroni et al. (2010). The method assumes a high correlation between a measured and a convolved spectrum and iteratively minimizes a cost function, which is 1 minus the Pearson correlation coefficient (r), calculated for both signals. Remaining artifacts of the spectral shift correction and slightly inaccurate estimates of atmospheric properties cause SIF\textsubscript{760} retrieval uncertainties. We therefore applied a semi-empirical correction as described in Damm et al., (2014) for each scan line across the track. This technique employs reference surfaces, which are free of any SIF\textsubscript{760} emission (e.g., bare soil) to adjust the upward transmittance term inside the absorption feature $\tau_i^{ao}$. The retrieval of SIF\textsubscript{760} from top-of-canopy radiance data measured on ground follows the same approach as described in Eqs. B2-B7 under the assumption that the surface irradiance can be approximated with the measurement of a reference panel and that $\rho_{so}$, $\tau_{do}$ and $\tau_{do}$ can be set to 0. Furthermore, the spectral resolution of APEX can be considered suboptimal for SIF\textsubscript{760} retrievals, although Damm et al. (2011) demonstrate that APEX with its spectral resolution of 5.4 nm at 760 nm is sensitive for SIF\textsubscript{760}. However, retrieved SIF\textsubscript{760} values are too high and in an absolute sense incorrect. We used reference SIF\textsubscript{760} data obtained in parallel to the airborne acquisitions using the ASD field spectrometers (Section 2.3) to estimate the actual offset. The observed scaling factor of 1.93 was afterwards applied to the retrieved SIF\textsubscript{760} values to transfer them to a realistic value range.
Appendix-C: SIF retrieval accuracy

We applied a quantitative accuracy evaluation of resulting SIF$_{760}$ maps using ground measured SIF$_{760}$ values (Figure C1). Considering all reference data acquired during five campaigns, a good linear relationship was achieved between ground and airborne-based SIF$_{760}$ values ($r^2 = 0.71$), but with a proportionality factor much higher than 1 (Figure C1-A). This experimentally obtained systematic overestimation of APEX SIF$_{760}$ is comparable to simulation results documented in Damm et al. (2011). Further, we found slightly changing correlations between the different years (several linear models in Figure C1-A), which are likely caused by canopy structural effects, spectral and radiometric performances of used ground instruments, or slight deviations of the performance of APEX over time.

To compensate for the overestimation of APEX SIF$_{760}$, we applied an empirical correction factor of 1.93 derived from the comparison of reference data and APEX, which resulted in a rRMSE of 28.9% (Figure C1-B).

The Laegeren site was covered with three adjacent flight lines having an overlap of approximately 10% (c.f., Figure 3). This configuration provides the opportunity to quantitatively evaluate the consistency of SIF retrievals obtained from different measurements and view zenith angles (i.e., ± 13.5°). The comparison of SIF$_{760}$ retrievals obtained from flight lines 1 and 2 reveals a moderate linear relationship for homogeneous agricultural surfaces ($r^2 = 0.81$, rRMSE = 5.7%). We observed a systematic underestimation of flight line 1 compared to flight line 2 (factor 0.6) for a view zenith angle difference of ~26° for SIF$_{760}$, indicating either a directionality of SIF$_{760}$ emissions or an insufficient decoupling of surface HCRF affected by reflectance anisotropy. With increasing surface heterogeneity, scattering increases
and the agreement of retrieved SIF from both flight lines slightly decreases (i.e., for forested areas: $r^2$ of 0.5 and rRMSE of 8.8%). This lower correlation can be mainly associated to slight geometric mis-registrations (i.e., max. 2 pixel ~ 4.0 m) in combination with surface heterogeneity (e.g., shaded and sunlit tree crowns) and emission anisotropy of SIF$_{760}$. Also negative SIF$_{760}$ values are present in the SIF$_{760}$ maps and caused by sensor noise and, especially for forests, due to shadowing effects (Damm et al. 2015).
Appendix-D: Technical aspects determining the SIF\textsubscript{760} retrieval accuracy

A rigorous evaluation of the SIF\textsubscript{760} retrieval accuracy is crucial to judge the reliability of our assessment on the relationship between SIF\textsubscript{760} and GPP\textsubscript{EC} across ecosystems. Furthermore, additional factors imposing variations on SIF\textsubscript{760} retrieved from airborne spectroscopy data that cannot be related to the physiological origin of SIF\textsubscript{760} needs to be critically discussed to justify the proposed approach.

Ground-based measurements of SIF\textsubscript{760} were made using field spectrometers to validate the airborne retrievals. Field spectroscopy provides a good reference for validating airborne retrievals, as it is likely not affected by biases resulting from atmospheric composition estimates (e.g., aerosol load) due to the simultaneous measurement of irradiance fluxes at canopy level using a reference panel. The reliability of the applied field spectroscopic approach to measure SIF\textsubscript{760} was previously demonstrated using field studies (Damm et al. 2010; Liu and Cheng 2010; Meroni et al. 2009; Rascher et al. 2009) and theoretical assessments (Damm et al. 2011). It must be noted that field spectroscopic approaches are subject to uncertainties particularly for heterogeneous vegetation canopies. Damm et al. (2015) discussed retrieval errors caused by illumination effects, likely introducing slight errors in reference SIF\textsubscript{760}. This source of uncertainty must be considered when judging the accuracy of APEX SIF\textsubscript{760}. The nevertheless good agreement between ground and airborne observations indicated that atmospheric absorption and scattering effects could be sufficiently compensated and thus, demonstrated the reliability of retrieved SIF\textsubscript{760} measurements. In particular, the empirical correction applied, making use of high spatial resolution airborne IS data in combination with reference surfaces not emitting SIF\textsubscript{760}, allowed to bypass retrieval uncertainties caused by atmospheric effects (Damm et al. 2014).

Instrumental effects in combination with retrieval methods were found to cause systematic differences in SIF\textsubscript{760} retrievals (Damm et al. 2011): the comparatively low
resolution of APEX around the O$_2$-A band used to retrieve SIF$_{760}$ (i.e., ~5.4 nm) resulted in an overestimation of APEX SIF$_{760}$ compared to retrievals from high resolution instruments. Indeed, maximum APEX SIF$_{760}$ values are 6 mW m$^{-2}$ sr$^{-1}$ nm$^{-1}$, while typical SIF$_{760}$ values obtained from high resolution instruments range between 0 and 3 mW m$^{-2}$ sr$^{-1}$ nm$^{-1}$ (Guanter et al. 2013). Considering SIF$_{760}$ values retrieved from ASD data in original resolution (3 nm), APEX showed an overestimation of 110.2%, which confirmed that low spectral resolution resulted in an overestimation of SIF$_{760}$. The reasoning for this absolute error is given by the sub-optimal spectral resolution of APEX with 5.4 nm at 760 nm, causing a reduced sensitivity for SIF$_{760}$ on the one hand and a wider distance of the O$_2$-A shoulder values used to parameterize the 3FLD approach on the other hand. The bias was corrected using the ASD reference data and does not impact the results of our analysis. Further, the relative variation of SIF$_{760}$ is unaffected by the bias.

Surface heterogeneity complicates the retrieval of SIF$_{760}$. According to Damm et al. (2015), SIF$_{760}$ retrievals for forest sites are especially subject to uncertainties due to assumptions on surface irradiance. Crown shapes and associated surface orientations determine the intensity and quality of irradiance, including fractional amounts of diffuse and direct irradiance. To account for pixel wise changes in surface irradiance, high resolution digital object models (DOM) (e.g., derived from LiDAR observations) are required. In absence of such a high resolution DOM’s, crowns are assumed to be flat, which results in uncertainties of up to 58% in case of cast shadows (Damm et al. 2015). Since we used averaged observations over larger areas representing flux tower footprints and most of our data were flown under comparable illumination conditions (i.e., around solar noon), we expect these potential biases to be less influential in this analysis.
Tables

Table 1: Date and time of APEX flights and corresponding eddy covariance flux tower measurements for the three investigated ecosystems (i.e., grassland, cropland, mixed temperate forest)

<table>
<thead>
<tr>
<th>Date</th>
<th>Time [UTC]</th>
<th>Location</th>
<th>Ecosystem</th>
<th>Flux tower</th>
</tr>
</thead>
<tbody>
<tr>
<td>17.06.2009</td>
<td>9:50</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
</tr>
<tr>
<td>17.06.2009</td>
<td>10:30</td>
<td>Oensingen</td>
<td>cropland</td>
<td>1 tower</td>
</tr>
<tr>
<td>17.06.2009</td>
<td>10:30</td>
<td>Oensingen</td>
<td>grassland</td>
<td>2 tower</td>
</tr>
<tr>
<td>25.06.2010</td>
<td>10:30</td>
<td>Oensingen</td>
<td>cropland</td>
<td>1 tower</td>
</tr>
<tr>
<td>25.06.2010</td>
<td>10:30</td>
<td>Oensingen</td>
<td>grassland</td>
<td>2 tower</td>
</tr>
<tr>
<td>26.06.2010</td>
<td>15:00</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
</tr>
<tr>
<td>26.06.2010</td>
<td>10:30</td>
<td>Oensingen</td>
<td>cropland</td>
<td>1 tower</td>
</tr>
<tr>
<td>26.06.2010</td>
<td>10:30</td>
<td>Oensingen</td>
<td>grassland</td>
<td>2 tower</td>
</tr>
<tr>
<td>29.06.2010</td>
<td>10:30</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
</tr>
<tr>
<td>26.06.2011</td>
<td>10:30</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
</tr>
<tr>
<td>28.06.2011</td>
<td>10:30</td>
<td>Oensingen</td>
<td>cropland</td>
<td>1 tower</td>
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<td>28.06.2011</td>
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<td>1 tower</td>
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<td>16.06.2012</td>
<td>10:25</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
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<td>Oensingen</td>
<td>cropland</td>
<td>1 tower</td>
</tr>
<tr>
<td>16.06.2012</td>
<td>11:00</td>
<td>Oensingen</td>
<td>cropland</td>
<td>1 tower</td>
</tr>
<tr>
<td>12.07.2013</td>
<td>7:30</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
</tr>
<tr>
<td>03.09.2013</td>
<td>10:50</td>
<td>Laegeren</td>
<td>forest</td>
<td>1 tower</td>
</tr>
</tbody>
</table>
Table 2: Availability of reference SIF\textsubscript{760} data obtained from field spectroscopy measurements to validate APEX based SIF\textsubscript{760} retrievals

<table>
<thead>
<tr>
<th>Date, time [UTC]</th>
<th>Location</th>
<th>Measured crops</th>
<th>Nr. points</th>
</tr>
</thead>
<tbody>
<tr>
<td>17.06.2009, 10:30</td>
<td>Oensingen</td>
<td>maize, rye, pea, sugar beet, wheat, white clover</td>
<td>29 points</td>
</tr>
<tr>
<td>25.06.2010, 10:30</td>
<td>Oensingen</td>
<td>maize, pea, sugar beet, wheat, white clover</td>
<td>15 points</td>
</tr>
<tr>
<td>16.06.2012, 9:00</td>
<td>Oensingen</td>
<td>carrot, maize, winter wheat</td>
<td>11 points</td>
</tr>
<tr>
<td>16.06.2012, 11:00</td>
<td>Oensingen</td>
<td>carrot, maize, winter wheat</td>
<td>10 points</td>
</tr>
</tbody>
</table>
Table 3: Goodness of fit for the hyperbolic model describing the relationship between GPP$_{EC}$ and SIF$_{760, O}$, PRI, and MCARI2 for the three ecosystem types perennial grassland, cropland, and mixed temperate forest. Calculated statistics are based on all data acquired from 2009-2013 as described in Table 1.

<table>
<thead>
<tr>
<th>Optical variable</th>
<th>Ecosystem</th>
<th>Regression coefficient</th>
<th>Relative RMSE [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIF</td>
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<td>0.88</td>
<td>3.55</td>
</tr>
<tr>
<td></td>
<td>grass</td>
<td>0.59</td>
<td>27.08</td>
</tr>
<tr>
<td></td>
<td>forest</td>
<td>0.48</td>
<td>15.88</td>
</tr>
<tr>
<td>PRI</td>
<td>crops</td>
<td>0.008</td>
<td>11.76</td>
</tr>
<tr>
<td></td>
<td>grass</td>
<td>0.95</td>
<td>8.60</td>
</tr>
<tr>
<td></td>
<td>forest</td>
<td>0.09</td>
<td>21.79</td>
</tr>
<tr>
<td>MCARI2</td>
<td>crops</td>
<td>0.005</td>
<td>10.29</td>
</tr>
<tr>
<td></td>
<td>grass</td>
<td>0.98</td>
<td>5.50</td>
</tr>
<tr>
<td></td>
<td>forest</td>
<td>0.34</td>
<td>17.98</td>
</tr>
</tbody>
</table>
Figure 1: Study sites. A: Oensingen agricultural site. B: Laegeren forest site. The white rectangles represent in A the boundary of investigated fields that comprise most of the flux-tower footprints, and in B a coarse outline of the footprint area of the flux-tower. The white crosses show the locations of the flux-towers. Background: RGB images from Google-Earth.
Figure 2: APEX reflectance and SIF$_{760}$ image for the Oensingen site acquired on the 26.06 2010, 10:30 UTC. A: top-of-canopy hemispherical-conical reflectance data as true color composite. B: SIF$_{760}$ map. The white boxes indicate the approximate position of the flux tower.
Figure 3: APEX reflectance and SIF$_{760}$ image for the Laegeren site acquired on the 26.06 2010, 15:10 UTC. A: top-of-canopy hemispherical-conical reflectance data as true color composite. B: SIF$_{760}$ map. The black arrows indicate the flight direction of flight line 1 to 3 (FL1-FL3). The white line marks a transect along the overlapping region of FL1 and FL2. The white boxes indicate the approximate position of the flux tower.
Figure 4: Relationships between GPP$_{EC}$ from the eddy-covariance measurements and SIF$_{760, O}$ instantaneously measured between 2009 and 2013 (see Table 1) with the airborne spectrometer APEX (A), PRI index (B), and MCARI2 index (C) for three vegetation types (black dots: perennial grassland; dark grey rectangles: cropland including winter wheat, pea, and barley; grey triangles: mixed temperate forest). The solid curves correspond to a hyperbolic model fitted to the measured data. The dashed curves show the extrapolated behavior.
Figure 5: Daily light response curves from eddy flux measurements for A: cropland, B: perennial grassland, and C: mixed temperate forest. Data were acquired between 2009 and 2013 (see Table 1). Grey curves represent a fitted hyperbolic model to approximate the behavior of measured PAR-GPP values. Crosses show GPP_EC measurements that were used for the SIF_{760} - GPP_EC comparison based on the time of APEX flights. PAR values are binned in 20 mW m^{-2} sr^{-1} nm^{-1} increments.
Figure 6: Leaf level relationships between photosynthetic (LUE$_p$) and fluorescence yield (LUE$_f$) for a typical C3 crop. Dependency of LUE$_p$ (A) and LUE$_f$ (B) on APAR. C: Relationship between LUE$_p$ and LUE$_f$. D: Relationship between APAR and GPP$_L$. GPP$_L$ was calculated as APAR*LUE$_p$. E: Relationship between APAR and SIF$_{760}$. SIF$_{760}$ was calculated as APAR*LUE$_f$ assuming a constant relationship between the SCOPE output SIF$_{total,L}$ (integral between 640-850nm) and SIF$_{760,L}$. F: Relationship between SIF$_{760,L}$ and GPP$_L$. All data were simulated using SCOPE. The grey areas indicate illumination conditions comparable to APEX flights.
Figure 7: Canopy level relationships between photosynthetic (LUE\textsubscript{p}) and fluorescence yield (LUE\textsubscript{f}) for different canopy representations of a C3 cropland in SCOPE. Dependency of LUE\textsubscript{p} (A) and LUE\textsubscript{f} (B) on APAR, LUE\textsubscript{p} was calculate as GPP\textsubscript{C}/APAR and LUE\textsubscript{f} was directly obtained from SCOPE. C: Relationship between LUE\textsubscript{p} and LUE\textsubscript{f}. D: Relationship between APAR and GPP\textsubscript{C}, GPP\textsubscript{C} was directly obtained from SCOPE. E: Relationship between APAR and SIF\textsubscript{760,C}, SIF\textsubscript{760,C} was directly obtained from SCOPE. F: Relationship between SIF\textsubscript{760,C} and GPP\textsubscript{C}. The black dashed line corresponds to a C3 cropland with LAI = 3.0, fraction of brown pigments (Cs) = 0.0%, and a spherical (sp) leaf inclination distribution function (LIDF). For the grey line Cs was changed to 20%, for the black dashed line, the LAI was changed to 1.0, and for the grey dashed/dotted line, the LIDF was changed to plagiophile (pg). The grey areas indicate illumination conditions comparable to APEX flights.
Figure 8: Impact of temporal scaling on the SIF$_{760,C}$-GPP$_C$ relationship. SIF$_{760,C}$ and GPP$_C$ data were simulated using SCOPE. Model input parameters air temperature (A), PAR (B) and LAI (C) were measured within the NitroEurope project (http://www.nitroeurope.eu/) at the Speulderbos forest site, Netherlands. D: Relationship between SIF$_{760,C}$ and GPP$_C$ including a fitted hyperbolic model for daily averages (grey dots and grey line), monthly averages (dark grey triangles and line), and quarterly data (black dots and black dashed line).
Figure C1: Comparison of ground and airborne-based SIF$_{760}$ retrievals from various crops. Data were acquired during four campaigns between 2009 and 2012 in the agricultural site Oensingen (see Table 2). Left: Fitted linear regression lines for the four considered campaigns are overlaid in black. The dashed line corresponds to the 1:1 line. Right: SIF retrievals from APEX after applying an empirical correction factor (1.93). The black line represents the fitted linear model, the dashed line corresponds to the 1:1 line.
Figure A shows the relationship between $SIF_{760,0}$ [mW m$^{-2}$ sr$^{-1}$ nm$^{-1}$] and GPP$^{EC}$. Figure B depicts the correlation between PRI [-] and GPP$^{EC}$ [µmol m$^{-2}$ s$^{-1}$]. Figure C illustrates the connection between MCARI 2 [-] and GPP$^{EC}$ [µmol m$^{-2}$ s$^{-1}$].