

## Supporting Information (SI)

### From Remotely-Sensed SIF to Ecosystem Structure, Function, and Service:

#### *Part I - Harnessing Theory*

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25 **Table S1. List of symbols and their definitions**

26 **a. Leaf-level variables and parameters (varying with canopy depth  $L$ )**

Symbols (units)	Definition
$A_n$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ )	Net Photosynthesis
$C_c$ (Pa)	Chloroplastic $\text{CO}_2$ partial pressure
$C_i$ (Pa)	Intercellular $\text{CO}_2$ partial pressure
$F_e$ ( $\mu\text{mol photons m}^{-2} \text{ s}^{-1} \text{ nm}^{-1}$ ) <sup>#</sup>	The Chl $a$ F emission irradiance of a single leaf at $\lambda_F$
$g_m$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1} \text{ Pa}^{-1}$ )	Mesophyll conductance of $\text{CO}_2$
$g_s$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1} \text{ Pa}^{-1}$ )	Stomatal conductance of $\text{CO}_2$
$I$ ( $\mu\text{mol photons m}^{-2} \text{ s}^{-1} \text{ nm}^{-1}$ ) <sup>#</sup>	The excitation irradiance at $\lambda_I$ (i.e., the incident solar irradiance illuminating a leaf at canopy depth $L$ )
$J_a$ ( $\mu\text{mol electrons m}^{-2} \text{ s}^{-1}$ )	The actual linear electron transport rate (ETR)
$J_{max}$ ( $\mu\text{mol electrons m}^{-2} \text{ s}^{-1}$ )	The maximum electron transport rate
$J_{max25}$ ( $\mu\text{mol electrons m}^{-2} \text{ s}^{-1}$ )	$J_{max}$ at 25°C
$J_p$ ( $\mu\text{mol electrons m}^{-2} \text{ s}^{-1}$ )	The potential electron transport rate
$k_{PAR}$ (unitless)	The extinction coefficient of PAR under Beer's law
$k_{\lambda_F}$ (unitless) <sup>#</sup>	The extinction coefficient of Chl $a$ F emission under Beer's law
$L$ ( $\text{m}^2$ leaf area $\text{m}^{-2}$ ground area)	Canopy depth ( $L = 0$ and $L = LAI$ at the top and bottom of the canopy respectively)
$NPQ$ (unitless)	non-photochemical quenching of PSII
$O$ (Pa)	The oxygen partial pressure
$p$ ( $\text{mol m}^{-2}$ leaf area)	The total concentration of light-harvesting photosynthetic pigments associated with both PSII and PSI per unit leaf area
$PAR$ ( $\mu\text{mol photons m}^{-2} \text{ s}^{-1}$ )	The photosynthetically active radiation ( $PAR = \int_{400}^{700} I(L, \lambda_I) d\lambda_I$ )

$q_{LII}$ (unitless)	The fraction of open PSII reaction centers under the lake model
$q_{LI}$ (unitless)	The fraction of open PSI reaction centers under the lake model
$q_7$ (unitless)	The fraction of the oxidized PSI donor P700 <sup>+</sup>
$R_d$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ )	Day respiration
$T_l$ ( $^{\circ}\text{C}$ )	Leaf temperature
$TPU$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ )	The triose phosphate utilization rate
$V_{cmax}$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ )	The maximum carboxylation rate of Rubisco
$V_{cmax25}$ ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ )	$V_{cmax}$ at 25 $^{\circ}\text{C}$
$\beta$ (unitless) <sup>#</sup>	The relative contribution of pigments associated with PSII to the overall absorption cross section at $\lambda_I$ ( $1 - \beta$ denotes that of PSI)
$\sigma$ ( $\text{m}^2 \text{ mol}^{-1}$ ) <sup>#</sup>	The overall leaf-level effective absorption cross section of photosynthetic pigment (which has taken into consideration pigment packaging inside the leaf) at $\lambda_I$
$\sigma_{\Omega\uparrow}$ ( $\text{m}^2 \text{ mol}^{-1}$ )	The effective specific absorption cross section of photosynthetic pigment for excitation radiance $I$ at the excitation wavelength $\lambda_I$ incident at the direction of $\theta_I$ projected to the direction of $\Omega \uparrow$
$\sigma_{\Omega\downarrow}$ ( $\text{m}^2 \text{ mol}^{-1}$ )	The effective specific absorption cross section of photosynthetic pigment for excitation radiance $I$ at the excitation wavelength $\lambda_I$ incident at the direction of $\theta_I$ projected to the direction of $\Omega \downarrow$ .
$\tau$ (unitless) <sup>#</sup>	The transmittance of irradiance
$\tau_f$ (unitless) <sup>#</sup>	The partitioning of Chl $a$ F emission in the backward direction
$\rho$ (unitless) <sup>#</sup>	The reflectance of irradiance
$\rho_f$ (unitless) <sup>#</sup>	The partitioning of Chl $a$ F emission in the forward direction
$\omega$ (unitless) <sup>#</sup>	The leaf scattering coefficient ( $\omega = \rho + \tau$ )
$\alpha$ (unitless) <sup>#</sup>	The absorptance of irradiance, i.e., the product of $p$ and $\sigma$

$\alpha_{vis}$ (unitless)	The broadband absorption efficiency (i.e., $\alpha$ integrated over the PAR spectral range)
$\alpha_T$ (unitless)	non-returned fraction of the glycolate carbon recycled in the photorespiratory cycle
$\varepsilon_\alpha$ (unitless) <sup>#</sup>	The self-absorption probability of ChlaF emission ( $\varepsilon_\alpha + \varepsilon_\downarrow + \varepsilon_\uparrow = 1$ )
$\varepsilon_\downarrow$ (unitless) <sup>#</sup>	The downward escape probability of ChlaF emission
$\varepsilon_\uparrow$ (unitless) <sup>#</sup>	The upward escape probability of ChlaF emission
$\varepsilon_{\Omega\downarrow}$ (unitless) <sup>#</sup>	The directional escape probability (downward direction) of ChlaF emission at sun-canopy-sensor geometry $\Omega$
$\varepsilon_{\Omega\uparrow}$ (unitless) <sup>#</sup>	The directional escape probability (upward direction) of ChlaF emission at sun-canopy-sensor geometry $\Omega$
$\Phi_{PSII}$ (unitless)	The photochemical quantum yield of PSII
$\Phi_{PSI}$ (unitless)	The photochemical quantum yield of PSI
$\Phi_{FII}$ (unitless)	The quantum yield of PSII ChlaF emission
$\Phi_{FI}$ (unitless)	The quantum yield of PSI ChlaF emission
$\Gamma^*$ (Pa)	The chloroplastic CO <sub>2</sub> compensation point (a linear function of oxygen concentration, von Caemmerer, 2000)

27 Note: m<sup>-2</sup> refers to “per unit leaf area”.

28 <sup>#</sup> highlight variables that are wavelength-dependent (i.e., spectrally-varying).

29

### 30 **b. Canopy-level variables**

<b>Symbols (units)</b>	<b>Definition</b>
$F_{eT}$ ( $\mu\text{mol photons m}^{-2}$ ground area $\text{s}^{-1} \text{nm}^{-1}$ ) <sup>#</sup>	Total ChlaF emission at $\lambda_F$
$F_\uparrow$ ( $\mu\text{mol photons m}^{-2}$ ground area $\text{s}^{-1} \text{nm}^{-1}$ ) <sup>#</sup>	Upward ChlaF irradiance at $\lambda_F$ leaving top-of-canopy (TOC)
$F_\downarrow$ ( $\mu\text{mol photons m}^{-2}$ ground area $\text{s}^{-1} \text{nm}^{-1}$ ) <sup>#</sup>	Downward ChlaF irradiance at $\lambda_F$ leaving bottom-of-canopy (BOC)
$F_{\Omega\uparrow}$ ( $\mu\text{mol photons m}^{-2}$ ground area $\text{s}^{-1} \text{nm}^{-1} \text{sr}^{-1}$ ) <sup>#</sup>	Directional (sun-canopy-sensor geometry $\Omega \uparrow$ ) TOC ChlaF radiance at $\lambda_F$

Symbols (units)	Definition
$F_{\Omega\downarrow}$ ( $\mu\text{mol photons m}^{-2}$ ground area $\text{s}^{-1} \text{ nm}^{-1} \text{ sr}^{-1}$ ) <sup>#</sup>	Directional (sun-canopy-sensor geometry $\Omega \downarrow$ ) BOC Chl <i>a</i> F radiance at $\lambda_F$
$f^{esc}$ (unitless) <sup>#</sup>	The fluorescence escape probability (i.e., the fraction of $F_{eT}$ escaping from TOC, $f^{esc} = \frac{F_{\uparrow}}{F_{eT}}$ )
$f_{\Omega\uparrow}^{esc}$ (unitless) <sup>#</sup>	The directional fluorescence escape probability from TOC at (sun-canopy-sensor geometry $\Omega \uparrow$ ), $f_{\Omega\uparrow}^{esc} = \frac{F_{\Omega\uparrow}}{F_{eT}}$
$GPP_T$ ( $\mu\text{mol CO}_2 \text{ m}^{-2}$ ground area $\text{s}^{-1}$ )	The total GPP integrated over canopy depth
$J_{aT}$ ( $\mu\text{mol m}^{-2}$ ground area $\text{s}^{-1}$ )	The total actual ETR integrated over canopy depth
LAI ( $\text{m}^2$ leaf area $\text{m}^{-2}$ ground area)	leaf area index
$\bar{p}$ ( $\text{mol m}^{-2}$ leaf area)	The mean photosynthetic pigment content of the canopy
$R_{\Omega\uparrow}$ (unitless) <sup>#</sup>	The directional reflectance at TOC
$\bar{\beta}$ (unitless)	The canopy-mean broadband $\beta$ (i.e., integrated over the PAR spectral range 400 to 700nm)
$\bar{\sigma}$ ( $\text{m}^2$ leaf area $\text{mol}^{-1}$ )	The canopy-mean broadband $\sigma$ (i.e., integrated over the PAR spectral range 400 to 700nm)
$\bar{\Phi}_{PSII}$ (unitless)	The canopy-level photochemical quantum yield of PSII
$\bar{\Phi}_{FII}$ (unitless)	The canopy-level fluorescence quantum yield of PSII (i.e., SIF yield)

31 Note:  $\text{m}^{-2}$  refers to either “per unit leaf area” or “per unit ground area”, specified in each variable.

32 <sup>#</sup> highlight variables that are wavelength-dependent.

33

### 34 c. Other variables and parameters

Symbols (units)	Definition
$a, b$	Empirical parameter for calculating $q_{LII}$ as a function of $PAR$
$a_N, b_N$	Empirical parameter for calculating $NPQ$ as a function of $PAR$

<b>Symbols (units)</b>	<b>Definition</b>
$i_0$	The canopy directional interceptance (depending on canopy gap fraction)
$K_c$ (Pa)	Michaelis-Menten constant for RuBP carboxylation
$K_o$ (Pa)	Michaelis-Menten constant for RuBP oxygenation
$k_D$ (s <sup>-1</sup> )	The rate constant for internal conversion (constitutive or unregulated heat dissipation)
$k_{DF}$ (unitless)	The ratio of $k_D$ to $k_F$
$k_F$ (s <sup>-1</sup> )	The rate constant for ChlaF emission
$k_N$ (s <sup>-1</sup> )	The rate constant of NPQ for PSII
$k_{PMII}$ (s <sup>-1</sup> )	The maximal (intrinsic) rate constant for photochemical quenching of PSII
$k_{PMI}$ (s <sup>-1</sup> )	The maximal (intrinsic) rate constant of photochemical quenching of PSI
$k_7$ (s <sup>-1</sup> )	The rate constant of NPQ by P700 <sup>+</sup>
$NPQ_0$ (unitless)	$NPQ$ at TOC
$NPQ_7$ (unitless)	The non-photochemical quenching capacity of P700 <sup>+</sup>
$PAR_0$ (μmol photons m <sup>-2</sup> s <sup>-1</sup> )	The incoming PAR at TOC
$q_{LII0}$ (unitless)	$q_{LII}$ at TOC
$r_s$ (unitless) <sup>#</sup>	The soil reflectance
$S_0$	The ground state of chlorophyll
$S_1$	The first excited state of chlorophyll
$s_{II}$ (unitless) <sup>#</sup>	The spectral shape function (elementary distribution) of ChlaF emission of PSII, integrated to unity
$s_I$ (unitless) <sup>#</sup>	The spectral shape function (elementary distribution) of ChlaF emission of PSI, integrated to unity
$x$ (unitless)	The fraction of total electron transport of mesophyll and bundle sheath allocated to mesophyll
$\lambda_F$ (nm)	The ChlaF emission wavelength

<b>Symbols (units)</b>	<b>Definition</b>
$\lambda_{Fmax}$ (nm)	The maximum wavelength of ChlaF emission
$\lambda_{Fmin}$ (nm)	The minimum wavelength of ChlaF emission
$\lambda_I$ (nm)	The excitation light wavelength
$\lambda_{Imin}$ (nm)	The minimum wavelength of excitation light
$\Phi_{PSII_m}$ (unitless)	The maximal photochemical quantum yield of PSII (can be considered as constant $\sim c. 0.83$ across species, Björkman and Demmig, 1987; Johnson et al., 1993)
$\Phi_{PSI_m}$ (unitless)	The maximal photochemical quantum yield of PSI
$\theta$ (unitless)	The curvature parameter (to compute the potential electron transport rate $J_p$ in FvCB)
$\theta_I$	A generic vector representing direction of the excitation radiance
$\Omega \uparrow$	A vector representing the sun-canopy-sensor geometry, including: solar zenith angle (SZA), view zenith angle (VZA) away from TOC towards the sky, and relative azimuth angle (RAA) between the sun and sensor above the canopy
$\Omega \downarrow$	A vector representing the sun-canopy-sensor geometry, including: solar zenith angle (SZA), view zenith angle (VZA) away from BOC towards the ground, and relative azimuth angle (RAA) between the sun and sensor below the canopy
$\varepsilon_{\downarrow 0}$ (unitless) <sup>#</sup>	The downward escape probability of ChlaF emission for an infinitesimally thin leaf layer at BOC
$\varepsilon_{\uparrow 0}$ (unitless) <sup>#</sup>	The upward escape probability of ChlaF emission for an infinitesimally thin leaf layer at TOC

35 Note: m<sup>-2</sup> refers to “per unit leaf area”.

36 <sup>#</sup> highlight variables that are wavelength-dependent.

37

38

Table S2. Summary of existing process-based models that have SIF-simulating capability.

Model	Leaf-level parameterization of Chl <sub>a</sub> F emission		Canopy RTM of SIF	Sun-canopy -sensor geometry	$\lambda_F$	Application	Pros	Cons	C E ^	Ref
	Leaf RTM	Biochemical								
<b>3D (horizontally) heterogeneous canopy - small scale scenes</b>										
DART <sup>#</sup>	Fluspect	None	Explicit modeling based on 3D ray-tracing	Full spectra	<ul style="list-style-type: none"> <li>Natural landscapes</li> <li><i>DART only</i>: including urban landscapes</li> </ul>	<ul style="list-style-type: none"> <li>Suitable for small scale scenes with fine complex composition and structure</li> <li><i>DART only</i>: Integration with Lidar</li> </ul>	<ul style="list-style-type: none"> <li>Computationally still too demanding to be applied at large scale (&gt;100m), but more efficient approaches may emerge.</li> <li>Requiring accurate leaf/canopy structural/functional info as priori input, which are often challenging to obtain</li> <li>No leaf-level Chl<sub>a</sub>F emission formulation included (except FLiES)</li> <li>No vertical heterogeneity in vegetation structure</li> <li>Not yet thoroughly validated with in-situ data</li> </ul>			
FluorWPS	Fluspect	As a function of PAR <sup>&amp;</sup>								
FluorFLIGHT <sup>#</sup>	Fluspect	None								
FLiES	FluoMODLeaf	F <sub>v</sub> CB + $k_N$								
FluorRTER	Fluspect	None	Explicit modeling based on SRTE			<ul style="list-style-type: none"> <li>Computationally more efficient than the ray-tracing approach</li> <li>Potential for large-scale applications</li> </ul>				
<b>1D (horizontally) homogeneous canopy - point to landscape scale</b>										
SCOPE	Fluspect	F <sub>v</sub> CB + $k_N$	<ul style="list-style-type: none"> <li>Explicit modeling based on SAIL 4-stream approach</li> <li>Multi-layer canopy (nlayer = 10LAI)<sup>s</sup></li> </ul>	Full spectra	<ul style="list-style-type: none"> <li>Process interpretation</li> <li>Benchmarking for both 3D and global TBMs/LSMs</li> </ul>	<ul style="list-style-type: none"> <li>Computationally more efficient than 3D models</li> <li>Vertical heterogeneity in biochemical and/or biophysical properties</li> </ul>	<ul style="list-style-type: none"> <li>Not suitable for horizontally heterogeneous canopy, e.g., crops with row structure, forests with complex architecture</li> <li>Requiring accurate site-specific leaf/canopy structural/functional info as priori input, which are often challenging to obtain</li> <li><math>k_N</math> formulation empirical and susceptible to uncertainties in F<sub>v</sub>CB</li> <li>Impact of biotic stress not represented</li> </ul>			(Van der Tol et al., 2009, 2014; van der Tol et al., 2019; Yang et al., 2017; Yang, Prikaziuk, et al., 2021)



**ID (horizontally) homogeneous canopy - global scale TBMs or LSMs**

BETHY + SCOPE	Fluspect	FvCB +*	<ul style="list-style-type: none"> <li>Multi-layer canopy (nlayer = 60)</li> </ul>	<ul style="list-style-type: none"> <li>Not explicitly represented</li> </ul>	<ul style="list-style-type: none"> <li>Single wavelength</li> </ul>	<ul style="list-style-type: none"> <li>Global (forward) simulations of SIF for comparison with in-situ and/or satellite SIF retrievals</li> </ul>	<ul style="list-style-type: none"> <li>Computationally most efficient for large-scale simulations</li> </ul>	<ul style="list-style-type: none"> <li>Uncertainties in model structure (formulations) and parameters of FvCB, <math>k_N</math>, SIF parameterizations for global PFTs</li> <li>Simplified SIF leaf-to-canopy RTM formulations</li> <li>Depend on external simulations of SCOPE for deriving simple conversion factors or parameterizations to account for escape probability at certain viewing angle(s) and specific wavelength</li> </ul>	(Koffi et al., 2015)		
JSBACH	None	FvCB + $QLII$	<ul style="list-style-type: none"> <li>Multi-layer canopy (nlayer = 3)</li> <li>Assuming a constant exponential attenuation factor of ChlaF emission, calibrated to SCOPE simulations</li> </ul>	<ul style="list-style-type: none"> <li>Only output nadir and/or hemispherically-integrated TOC SIF (calibrated to SCOPE ensemble simulations)</li> </ul>	<ul style="list-style-type: none"> <li>A conversion factor calibrated to SCOPE ensemble simulations</li> <li><i>BETHY only</i>: No info provided on wavelength adjustment</li> </ul>	<ul style="list-style-type: none"> <li>Data assimilation by ingesting SIF measurements to constrain parameters and/or variables related to GPP simulations</li> </ul>	<ul style="list-style-type: none"> <li>Vertical heterogeneity in biochemical/biophysical properties (for some models)</li> </ul>		(Thum et al., 2017)		
SiB*	None	FvCB +*	<ul style="list-style-type: none"> <li>One "big-leaf" model NOT separating sunlit and shaded portions</li> <li>Assuming a factor accounting for leaf to canopy scaling calibrated to SCOPE simulations</li> </ul>	<ul style="list-style-type: none"> <li><i>BETHY only</i>: No info provided</li> <li><i>JSBACH only</i>: No SIF magnitude, as no wavelength separation</li> </ul>						(Haynes et al., 2020)	
ORCHIDEE	None		<ul style="list-style-type: none"> <li>A simplified empirical model calibrated to SCOPE ensemble simulations</li> </ul>								(Bacour et al., 2019)
BEPS	None		<ul style="list-style-type: none"> <li>Two "big-leaf" model accounting for sunlit and shaded portions</li> <li>Exponential attenuation factor of ChlaF emission as a function of LAI and clumping index</li> <li>Scattering factor of ChlaF emission as a function of LAI</li> </ul>								(Cui et al., 2020; Qiu et al., 2019)
CLM*	None		<ul style="list-style-type: none"> <li>Two "big-leaf" model accounting for sunlit and shaded portions</li> <li>CLM4: Assuming a factor accounting for leaf to canopy scaling calibrated to SCOPE simulations</li> <li>CLM5: Separate calculation of canopy-level escape probability for sunlit and shaded portions according to Zeng et al. (2019)</li> </ul>	<ul style="list-style-type: none"> <li>Empirically represented</li> <li>Only output nadir and/or hemispherically-integrated TOC SIF</li> </ul>							(Lee et al., 2015; Raczka et al., 2019; Li et al., 2022)

<sup>&</sup>Based on Rosema et al. (1998)

<sup>#</sup>Radiation transfer Model Intercomparison (RAMI) participating model

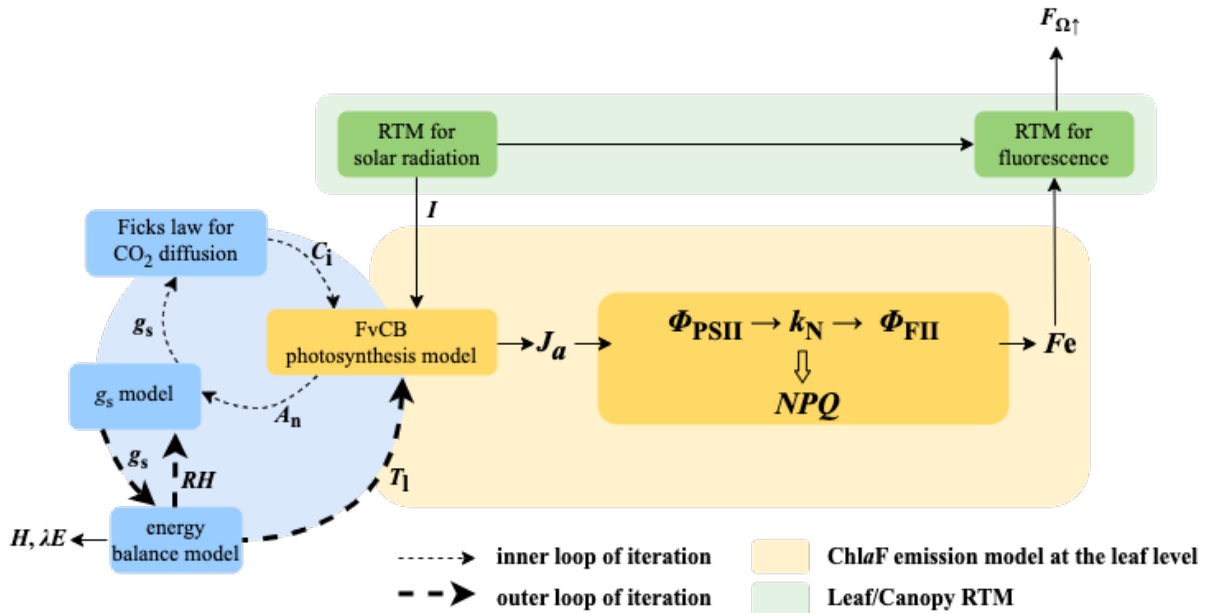
\*Subjective to version differences and/or formulation variants

<sup>^</sup>CE denotes computational efficiency; models are broadly sorted in increasing order of CE, color-coded in a warm (low CE) to cold (high CE) spectrum.

<sup>§</sup>nlayer denotes number of canopy layer

**Table S3. Model configuration and parameter setup in SCOPE2.1 for simulations of canopy-level escape probability  $f_{\Omega\uparrow}^{esc}$  and reflectance  $R_{\Omega\uparrow}$  for a C3 crop canopy in Fig. 3b.**

Parameter/Variable	Abbreviation	Values (units)
<i>Canopy structural properties</i>		
Leaf area index	LAI	3
Leaf angle distribution	LIDF	Spherical
<i>Leaf structural and physiological properties</i>		
Chlorophyll a + b content	Cab	40 ( $\mu\text{g cm}^{-2}$ )
Carotenoid content	Cca	10 ( $\mu\text{g cm}^{-2}$ )
Dry matter content	Cdm	0.0120 ( $\text{g cm}^{-2}$ )
Water content	Cw	0.0090 (cm)
Brown pigments	Cs	0 (-)
Leaf structure parameter	N	1.5 (-)
Anthocyanin content	Cant	1 ( $\mu\text{g cm}^{-2}$ )
Protein content	Cp	0 ( $\mu\text{g cm}^{-2}$ )
Carbon-based constituents	Cbc	0 ( $\mu\text{g cm}^{-2}$ )
Carboxylation capacity at 25°C	$V_{cmax25}$	60 ( $\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ )
Ball-Berry slope	$g_1$	8 (-)
Ball-Berry intercept	$g_0$	0.01 (-)
<i>Illumination and viewing conditions</i>		
Incoming shortwave radiation	Rin	600 ( $\text{Wm}^{-2}$ )
Solar zenith angle	SZA	30
View zenith angle	VZA	0



1

2 **Figure S1.** Graphical illustration of the leaf-level calculation of ChlaF emission (yellow) and its  
 3 coupling with energy balance (blue) and leaf/canopy-level radiative transfer modeling (RTM,  
 4 green). Note we intend to display details disproportionately for different processes. This is  
 5 because we intend to highlight the FvCB+  $k_N$  strategy (section 2.4 in the main text) in modeling  
 6 the leaf-level ChlaF emission, i.e.,  $F_e$ , while paradigms of the nested loop of energy balance and  
 7 photosynthesis-stomatal conductance model, and leaf/canopy RTM are historically well  
 8 established (based on laws of physics). The FvCB+  $k_N$  modeling strategy of ChlaF emission is  
 9 built upon the assumption of balanced light and carbon reaction under steady state, and is  
 10 implemented by SCOPE (van der Tol et al., 2014). Here  $T_l$ ,  $H$ , and  $\lambda E$  represent leaf  
 11 temperature, sensible heat flux, and latent heat flux at the leaf level, respectively. All other  
 12 symbols are defined in Table S1.

13 **SI – 1. Rationale for considering both PSII and PSI in SIF research**

14 ChlaF emissions from both PSII and PSI need to be considered in SIF research for the following  
 15 reasons:

- 16 - In typical PAM fluorometry, it is generally assumed PSI does not contribute to variable  
 17 ChlaF, which is the difference between ChlaF yield observed during the application of  
 18 saturating pulse and that observed after the saturating pulse is switched off and the  
 19 electrons from the acceptors of PSII have been drained off (Baker, 2008). This  
 20 assumption stems from a convenient assumption that P700<sup>+</sup> quenches the excitation  
 21 energy non-photochemically as efficiently as its reduced state quenches the excitation  
 22 photochemically (Kitajima & Butler, 1975). However, this assumption has been  
 23 increasingly challenged in experiments (Franck et al., 2002; E. E. Pfündel et al., 2013;  
 24 Schreiber & Klughammer, 2021; Trissl, 1997) and modeling (Lazár, 2013) studies which  
 25 showed that P700<sup>+</sup> does not quench non-photochemically as efficiently as P700 does  
 26 photochemically.

- 27 - Even if we accept the assumption that PSI does not contribute to variable fluorescence,  
 28 we still cannot assume the Chl $a$ F emission of PSI is negligibly small in the context of  
 29 general SIF applications. PSI uses a bidirectional (symmetrical) mechanism for charge  
 30 separation whereas PSII employs a unidirectional (asymmetrical) mechanism. As a  
 31 result, PSI is photochemically more efficient than PSII is (for details, see Caffarri et al.,  
 32 2014). However, PSI photochemical efficiency is not 100%.  $\Phi_{PSIm}$  is between 0.94 to  
 33 0.98 (Hogewoning et al., 2012) while  $\Phi_{PSII m}$  is about 0.83 across species (Björkman &  
 34 Demmig, 1987; JOHNSON et al., 1993). More importantly, SIF currently can only be  
 35 observed at specific wavelengths such as Franhauser lines, O<sub>2</sub>A and O<sub>2</sub>B bands. We have  
 36 no guarantee that  $s_I$  is much smaller than  $s_{II}$  at these specific wavelengths (see Eq 3).  
 37 - In typical PAM fluorometry, PSII and PSI are assumed to receive equal allocation of  
 38 absorbed energy, i.e.,  $\beta = 0.5$  (Baker, 2008). However, under stress when consumption of  
 39 ATP increases (see discussions next section), more energy may be allocated to PSI than  
 40 PSII (i.e.,  $\beta < 0.5$ ), potentially increasing PSI fluorescence.  
 41 Therefore, PSI cannot be ignored in SIF research until further evidence proves otherwise.

## 42 SI – 2. Formulation of directional SIF: $F_{\Omega \uparrow}$ and $F_{\Omega \downarrow}$

$$\begin{aligned}
 & F_{\Omega \uparrow}(\lambda_F) \\
 &= \int_0^{LAI} p(L) \varepsilon_{\Omega \uparrow}(L, \lambda_F) \int_{\lambda_{Imin}}^{\lambda_F} \{ \Phi_{FII}(L) s_{II}(\lambda_F) \beta(L, \lambda_I) + \Phi_{FIS_I}(\lambda_F) [1 - \beta(L, \lambda_I)] \} \int \sigma_{\Omega \uparrow}(\theta_I, L, \lambda_I) I(\theta_I, L, \lambda_I) d\theta_I d\lambda_I dL \\
 &+ \varepsilon_{\Omega \uparrow}(LAI, \lambda_F) \int r_s \varepsilon_{\Omega \uparrow}(\theta_I, \lambda_F) F_{\theta \downarrow}(\lambda_F) d\theta_I
 \end{aligned}$$

43  
 44 (S1)

$$\begin{aligned}
 & F_{\Omega \downarrow}(\lambda_F) \\
 &= \int_0^{LAI} p(L) \varepsilon_{\Omega \downarrow}(L, \lambda_F) \int_{\lambda_{Imin}}^{\lambda_F} \{ \Phi_{FII}(L) s_{II}(\lambda_F) \beta(L, \lambda_I) + \Phi_{FIS_I}(\lambda_F) [1 - \beta(L, \lambda_I)] \} \int \sigma_{\Omega \downarrow}(\theta_I, L, \lambda_I) I(\theta_I, L, \lambda_I) d\theta_I d\lambda_I dL \\
 &+ \varepsilon_{\Omega \downarrow}(LAI, \lambda_F) \int r_s \varepsilon_{\Omega \downarrow}(\theta_I, \lambda_F) F_{\theta \uparrow}(\lambda_F) d\theta_I
 \end{aligned}$$

46  
 47 (S2)

48  
 49 Here  $F_{\Omega \uparrow}$  is the radiance of SIF at  $\lambda_F$  traveling in the direction of  $\Omega \uparrow$  away from TOC towards  
 50 the sky, while  $F_{\Omega \downarrow}$  is the radiance of SIF at  $\lambda_F$  traveling in the direction of  $\Omega \downarrow$  away from BOC  
 51 towards the soil surface.  $\varepsilon_{\Omega \uparrow}$  and  $\varepsilon_{\Omega \downarrow}$  are the escape probability of a SIF photon emitted at the  
 52 canopy depth of  $L$  into the direction of  $\Omega \uparrow$  and  $\Omega \downarrow$  at TOC and BOC, respectively.  $\sigma_{\Omega \uparrow}$  and  
 53  $\sigma_{\Omega \downarrow}$  are the effective specific absorption cross section of photosynthetic pigment for excitation  
 54 radiance  $I$  at the excitation wavelength  $\lambda_I$  incident at the direction of  $\theta_I$  projected to the direction  
 55 of  $\Omega \uparrow$  and  $\Omega \downarrow$  respectively.  $r_s$  is the spectral reflectance of the soil surface. All directional  
 56 integrals of  $\theta_I$  occur on a sphere.

57

## 58 SI – 3. Derivation of Eq 3

59 Gu et al. (2019) expressed  $\Phi_{FII}$  as a function of photochemical quenching (i.e.,  $q_{LII}$ ) and  
 60  $NPQ$ .

$$\Phi_{FII} = \frac{1 - \Phi_{PSII_m}}{(1 + k_{DF})[(1 + NPQ)(1 - \Phi_{PSII_m}) + q_{LII}\Phi_{PSII_m}]} \quad (S3)$$

Here  $\Phi_{PSII_m}$  is the maximal photochemical quantum yield of PSII.  $k_{DF}$  is the ratio of rate constant for constitutive (unregulated) heat dissipation ( $k_D$ ) to that for Chl $a$ F emission ( $k_F$ ). Note that  $\Phi_{FII}$ ,  $q_{LII}$ ,  $NPQ$  form a closed equation for PSII, and knowing any two of them is sufficient to resolving the third, assuming  $\Phi_{PSII_m}$  and  $k_{DF}$  are constants.

Here we derive a similar expression for  $\Phi_{FI}$ . A couple of uncertainties affect the derivation of  $\Phi_{FI}$ . The first uncertainty is whether PSI undergoes regulated heat dissipation. In the PAM fluorometry literature, the quantity known as  $NPQ$  is virtually always implied for PSII because it has been generally believed PSII does not experience non-photochemical quenching in the same way as PSII does. Surprisingly, Ballottari et al., (2014) found that zeaxanthin efficiently quenched fluorescence in PSI particles extracted from an *Arabidopsis thaliana* mutant, implying that a PSII-type NPQ process also occurs in PSI. However, Tian et al., (2017) demonstrated that in wide type *Arabidopsis thaliana*, no zeaxanthin-dependent NPQ existed in PSI. In this review, based on the findings of Tian et al., (2017), we assume that in vivo, physiologically relevant environmental conditions, no PSII-type NPQ occurs in PSI.

The second uncertainty is related to the capacity of the oxidized electron donor of PSI reaction center (P700<sup>+</sup>) in dissipating PSI excitation energy into heat. It is accepted that the oxidized electron donor of PSII reaction center (P680<sup>+</sup>), whose sustained existence results in photodamage (Jegerschoeld et al., 1990), is incapable of non-photochemically dissipating excitation. However, P700<sup>+</sup> has been shown to protect PSI by dissipating excess excitation energy into harmless heat (Bukhov & Carpentier, 2003; Sonoike, 2011). A convenient assumption that was first made by Kitajima & Butler (1975) states that P700<sup>+</sup> quenches the excitation energy non-photochemically as efficiently as its reduced state quenches the excitation photochemically. A consequence of this assumption is that the variable fluorescence in PAM fluorometry comes only from PSII as the fluorescence yield from PSI does not change between the minimal and maximal fluorescence measurements, which simplifies the interpretation of PAM fluorometry parameters. However, this assumption has been increasingly challenged in experimental (Franck et al., 2002; E. E. Pfündel et al., 2013; Schreiber & Klughammer, 2021; Trissl, 1997) and modeling (Lazár, 2013) studies which showed that P700<sup>+</sup> does not quench non-photochemically as efficiently as P700 does photochemically. We accept this contemporary view of P700<sup>+</sup> to derive  $\Phi_{FI}$ .

Based on these considerations, we express  $\Phi_{FI}$  as the following:

$$\Phi_{FI} = \frac{k_F}{k_F + k_D + q_{LI}k_{PMI} + q_7k_7} \quad (S4)$$

Here  $q_{LI}$  is the fraction of open reaction centers of PSI,  $q_7$  the fraction of the oxidized PSI donor,  $k_{PMI}$  the maximal (intrinsic) rate constant of photochemical quenching of PSI, and  $k_7$  the rate constant of NPQ by P700<sup>+</sup>. Instead of using the cumbersome P700<sup>+</sup> as subscript, we have simply used '7' to denote it in  $q_7$  and  $k_7$ . We assume that PSII and PSI share the same  $k_F$  and  $k_D$  values.

98 To transform Eq S4 into a form analogous to Eq S3, we note that the maximal photochemical  
 99 quantum yield of PSI ( $\Phi_{PSIm}$ ) is given by

$$101 \quad \Phi_{PSIm} = \frac{k_{PMI}}{k_F + k_D + k_{PMI}} \quad (S5)$$

102 From Eq S5,

$$103 \quad \frac{k_{PMI}}{k_F + k_D} = \frac{\Phi_{PSIm}}{1 - \Phi_{PSIm}} \quad (S6)$$

104 Analogous to  $NPQ$  for PSII, we define the corresponding NPQ of P700<sup>+</sup> ( $NPQ_7$ ) as

$$105 \quad NPQ_7 = \frac{k_7}{k_F + k_D} \quad (S7)$$

106 Note that, however,  $NPQ$  for PSII dynamically responds to changes in environmental  
 107 conditions, whereas  $NPQ_7$  is a parameter constant. Thus the NPQ dynamics of PSI is entirely  
 108 determined by the oxidized fraction of PSI donor  $q_7$ . Using Eqs S6-S7, Eq S4 becomes

$$109 \quad \Phi_{FI} = \frac{1 - \Phi_{PSIm}}{(1 + k_{DF})[(1 + q_7 NPQ_7)(1 - \Phi_{PSIm}) + q_{LI} \Phi_{PSIm}]} \quad (S8)$$

110 Eq S8 shows that  $\Phi_{FI}$ ,  $q_7$ , and  $q_{LI}$  are uniquely coupled for PSI and knowing any two of the  
 111 three is sufficient to resolve the third. Insert Eq S3 and S8 into Eq 2c, we have the complete  
 112 equation for  $F_{\uparrow}$  in Eq 3 in the main text.

#### 114 **SI – 4. Rationale of parameter constants treatment in Eq 3**

115 For non-stressed plants,  $\Phi_{PSII}$  is constant ( $\sim$ c. 0.83) across species (Björkman & Demmig,  
 116 1987; JOHNSON et al., 1993). PSI is photochemically more efficient than PSII (Nelson, 2009),  
 117 and thus  $0.83 < \Phi_{PSIm} < 1$ . This means that for a fully relaxed leaf in the dark, the combined  
 118 quantum yield of fluorescence whose rate constant is  $k_F$ (s<sup>-1</sup>) and internal conversion  
 119 (constitutive or unregulated heat dissipation) whose rate constant is  $k_D$ (s<sup>-1</sup>) is at most 0.17.  $k_{DF}$   
 120 (unitless) is the ratio of  $k_D$  to  $k_F$ .  $k_D$  and  $k_F$  are physical properties of chlorophyll molecules and  
 121 their environments.  $k_D$  is an intrinsic property of chlorophyll molecules and can be determined  
 122 by the collision of the excited chlorophyll molecules with solvent molecules whereas  $k_F$  is  
 123 determined by the lifetime of the chlorophyll's first excited singlet state. Because plants have no  
 124 active mechanisms to regulate  $k_D$  and  $k_F$  and because the unstressed  $\Phi_{PSII}$ , which equals  
 125  $k_{PMII}/(k_D + k_F + k_{PMII})$  where  $k_{PMII}$  is the maximal rate constant for photochemistry of  
 126 PSII, is constant, it is reasonable to assume  $k_F$  and  $k_D$  and therefore  $k_{DF}$  are constant (Gu et al.,  
 127 2019). However, the precise values of  $k_F$  and  $k_D$  and thus  $k_{DF}$  in vivo are currently unknown.  
 128 The maximum fluorescence emission rate of chlorophyll a extracts in ether is 30%,  
 129 corresponding to a  $k_{DF}$  of 2, but this value probably does not represent in vivo  $k_{DF}$  of

130 chlorophyll in thylakoids. E. Pfündel, (1998) suggested a maximal PSII fluorescence quantum  
 131 yield of PSII of 0.09, which would correspond to  $k_{DF} = 10$ . Tesa et al., (2018) found that at  
 132 75K, which made photochemical and nonphotochemical quenching impossible, the fluorescence  
 133 quantum yield of an intact holly leaf was about 5%, resulting a  $k_{DF}$  of 19, a value used in Gu et  
 134 al., (2019). But their measurements did not account for the self-absorption of fluorescence by  
 135 leaf tissues and thus would lead to an overestimation of  $k_{DF}$ . If we assume 50% of the total  
 136 fluorescence was measured in Tesa et al., (2018), corresponding to a self-absorptance of 0.5, a  
 137  $k_{DF} = 10$  would also be obtained. The precise value of  $NPQ_7$  is also uncertain. To estimate its  
 138 magnitude, we accept, for the moment, the assumption of Kitajima & Butler, (1975) that PSI is  
 139 an equal photochemical and non-photochemical quencher ( $k_{PMI} = k_7$ ), the rate constant of  
 140 non-photochemical quenching by P700<sup>+</sup>), and further,  $\Phi_{PSIm} = 0.98$  (Hogewoning et al., 2012;  
 141 Nelson & Junge, 2015), then  $NPQ_7 = 49$ , according to Eq. S6. The actual value of  $NPQ_7$  is  
 142 likely less than 49 because recent studies have shown that P700<sup>+</sup> does not quench non-  
 143 photochemically as efficiently as P700 does photochemically (Franck et al., 2002; Lazár, 2013;  
 144 E. E. Pfündel et al., 2013; Schreiber & Klughammer, 2021; Trissl, 1997), which implies  $k_7$  is less  
 145 than  $k_{PMI}$ .  $k_D$ ,  $k_F$  and therefore  $k_{DF}$  are assumed to be constant for both PSII and PSI.

146 It is difficult to measure  $s_{II}$  and  $s_I$  directly (even though might vary across species,  
 147 canopy positions and physiological states) because PSII and PSI fluorescence emission overlap  
 148 and because the foliar self-absorption depends on fluorescence wavelength. However, complexes  
 149 of PSII and PSI can be isolated from leaves and their fluorescence emissions have been  
 150 measured (Croce et al., 1996; Franck et al., 2002). Such measurements represent the best  
 151 estimates for  $s_{II}$  and  $s_I$  so far.

## 152 **SI – 5. Derivation of the balanced relationships between light and carbon reactions at the** 153 **leaf level**

154 To develop a strategy for modeling the regulatory light reaction variables (e.g.,  $NPQ$ ,  $q_{LII}$ )  
 155 consistent with our empirical knowledge and theoretical understanding of photosynthesis, we  
 156 consider the constraints set by the condition of balance between the light and carbon reactions,  
 157 specifically by the requirement that the actual electron transport rate  $J_a$  estimated by the light  
 158 reaction model equals that derived from the Farquhar-von Caemmerer-Berry (FvCB)  
 159 biochemical model of photosynthesis (Farquhar et al., 1980). We use C<sub>3</sub> species and the lake  
 160 model as an example. The balance relationships for C<sub>4</sub> species or the puddle model can be  
 161 similarly derived.

162 Within the FvCB framework, the potential electron transport rate  $J_p$  is empirically  
 163 calculated by BERNACCHI et al., (2003) at the leaf level:

$$164 \quad J_p = \frac{\Phi_{PSII} \beta \alpha_{vis} PAR + J_{max} - \sqrt{(\Phi_{PSII} \beta \alpha_{vis} PAR + J_{max})^2 - 4\theta J_{max} \Phi_{PSII} \beta \alpha_{vis} PAR}}{2\theta}$$

165 (S9)

166 Here  $\theta$  is an empirical curvature parameter and  $J_{max}$  is the maximum electron transport rate. The  
 167 subscript  $p$  is used to differentiate the potential ETR of FvCB from the actual ETR  $J_a$  at the leaf  
 168 level.  $\alpha_{vis}$  is broadband absorption efficiency. Eq S9 is a root of the following quadratic equation:



169  $\theta J_p^2 - (\Phi_{PSII m} \beta \alpha_{\bar{v}is} PAR + J_{max}) J_p + J_{max} \Phi_{PSII m} \beta \alpha_{\bar{v}is} PAR = 0$  (S10)

170 which can be rewritten as:

171  $\theta J_p^2 - J_{max} J_p - (J_p - J_{max}) \Phi_{PSII m} \beta \alpha_{\bar{v}is} PAR = 0$  (S11)

172 Or equivalently,

173  $J_p = \frac{J_{max} - J_p}{J_{max} - \theta J_p} \Phi_{PSII m} \beta \alpha_{\bar{v}is} PAR$  (S12)

174 Eq S12 shows that the FvCB model for potential ETR is a recursive model as  $J_p$  occurs on both  
175 sides. It assumes the photochemical quantum yield of PSII is a function of ETR.

176 **When the carboxylation is limited by RuBP regeneration,**  $J_p$  becomes  $J_a$ . Comparing  
177 Eq S12 with Eqs 16-17 in Gu et al., (2019), we see that

178  $\Phi_{PSII} = \frac{\Phi_{PSII m}}{\frac{1+NPQ}{q_{LII}}(1 - \Phi_{PSII m}) + \Phi_{PSII m}} = \frac{J_{max} - J_p}{J_{max} - \theta J_a} \Phi_{PSII m}$  (S13)

179 If defining  $q_{LN} = \frac{q_{LII}}{1 + NPQ}$ , we have:

180  $q_{LN} = \frac{1}{1 + \frac{1-\theta}{1-\Phi_{PSII m}} \frac{J_a}{J_{max}-J_a}}$  (S14)

181 **When Rubisco limits carboxylation,** the carboxylation rate supported by the actual ETR  
182 equals the Rubisco-limited carboxylation rate. Therefore,

183  $A_n + R_d = \frac{J_a C_c}{4C_c + 8\Gamma^*} = \frac{V_{cmax} C_c}{C_c + K_c(1 + \frac{O}{K_o})}$  (S15)

184 Eq S15 omits the cyclic electron transport around PSI and the Mehler reaction (water-water  
185 cycle) (Yin et al., 2009). Thus,

186  $J_a = \frac{4C_c + 8\Gamma^*}{C_c + K_c(1 + \frac{O}{K_o})} V_{cmax}$  (S16)

187 Combining Eq 17 in Gu et al., (2019) and Eq S16, and solving for  $q_{LN}$ , we have:

188  $q_{LN} = \frac{q_{LII}}{1 + NPQ} = \frac{1 - \Phi_{PSII m}}{\Phi_{PSII m} \left( f_R \frac{\beta \alpha_{\bar{v}is} PAR}{4V_{cmax}} - 1 \right)}$  (S17)

189 Here  $f_R$  denotes

190  $f_R = \frac{C_c + K_c(1 + \frac{O}{K_o})}{C_c + 2\Gamma^*}$  (S18)

191 **When TPU limits carboxylation,**

$$192 \quad \frac{J_p C_c}{4C_c + 8\Gamma^*} = \frac{3TPU \cdot C_c}{C_c - (1 + 3\alpha_T)\Gamma^*} \quad (S19)$$

193 Here  $TPU$  is the rate of triose phosphate utilization and  $\alpha_T$  is the non-returned fraction of the  
 194 glycolate carbon recycled in the photorespiratory cycle. Therefore,

$$195 \quad J = \frac{4C_c + 8\Gamma^*}{C_c - (1 + 3\alpha_T)\Gamma^*} 3TPU \quad (S20)$$

196 Combining Eq 16 in Gu et al., (2019) and Eq S20 leads to:

$$197 \quad q_{LN} = \frac{q_{LII}}{1 + NPQ} = \frac{1 - \Phi_{PSII_{max}}}{\Phi_{PSII_{max}} \left( f_T \frac{\beta \alpha_{vis} PAR}{3TPU} - 1 \right)} \quad (S21)$$

198 Here  $f_T$  is given by

$$199 \quad f_T = \frac{C_c - (1 + 3\alpha_T)\Gamma^*}{C_c + 2\Gamma^*} \quad (S22)$$

200  $V_{cmax}$ ,  $J_{max}$  and  $TPU$  are classic FvCB model parameters and have played key roles in  
 201 photosynthesis and carbon cycle modeling. Eqs S14, S17, S21 show that they are intimately  
 202 linked to regulatory light reaction variables via  $q_{LII}$  and  $NPQ$ .

## 203 **SI – 6. Derivation of the toy model for $F_{\uparrow}(\lambda_F)$ : Eq 8**

204 We start from Eq 2c in the main text, by invoking several assumptions, which are necessary to  
 205 simplify Eq 2c. Note that simplification is necessary in this context, but we are vigilant to the  
 206 underlying assumptions and overall validity of the corollary. First, we assume a single value of  
 207  $\Phi_{FII}$  and  $\Phi_{FI}$ , denoted as  $\bar{\Phi}_{FII}$  and  $\bar{\Phi}_{FI}$  respectively, can effectively represent a whole canopy  
 208 under steady state (**A1**). This is because the vertical heterogeneity in their leaf-scale variations  
 209 can be largely attenuated once aggregated to the canopy scale (Chang et al., 2021), due to the  
 210 compensation effect between photochemical and non-photochemical quenching, i.e.,  $q_{LII}$  and  
 211  $NPQ$  for PSII, as well as  $q_7$  and  $q_{LI}$  for PSI. Note that this assumption may not hold under non-  
 212 steady state when photochemistry and non-photochemistry are decoupled, a property exploited in  
 213 PAM fluorometry. We also assume  $\bar{p}$  can effectively represent the mean photosynthetic pigment  
 214 content of the canopy (**A2**). Moreover, we assume that  $\beta$  and  $\sigma$  are relatively stable vertically,  
 215 and can be effectively represented as a canopy-mean value, denoted as  $\bar{\beta}$  and  $\bar{\sigma}$  respectively (**A3**).  
 216 No doubt these assumptions and simplifications can cause uncertainty but the alternative, which  
 217 is to model vertical variations of these variables, can be equally or more uncertain, and will make  
 218 any attempt to infer ecosystem structure and function from the observed  $F_{\uparrow}(\lambda_F)$  exceedingly  
 219 difficult. Further, we omit the small error that may be caused by a possible fluorescence  
 220 wavelength  $\lambda_F$  shorter than the upper wavelength of the excitation irradiance (e.g., around the  
 221 O<sub>2</sub>B band) and use  $PAR(L) = \int_{400}^{700} I(L, \lambda_I) d\lambda_I$  (**A4**). Accepting these assumptions, Eq 3 in  
 222 the main text becomes:

223  $F_{\uparrow}(\lambda_F) = [\bar{\Phi}_{FII}S_{II}(\lambda_F)\bar{\beta} + \bar{\Phi}_{FISI}(\lambda_F)(1 - \bar{\beta})]\bar{\sigma}\bar{p} \int_0^{LAI} [\varepsilon_{\uparrow}(L, \lambda_F) + \varepsilon_{\uparrow}(LAI, \lambda_F)r_s(\lambda_F)\varepsilon_{\downarrow}(L, \lambda_F)]PAR(L)dL$   
 224 (S23)

225 To derive an analytical solution of the leaf-to-canopy integration, i.e., the integral of LAI, we  
 226 here employ Beer's law to describe the attenuation of ChlaF emission and PAR inside a canopy:

$$\begin{cases} \varepsilon_{\uparrow}(L, \lambda_F) = \varepsilon_{\uparrow 0}(\lambda_F)e^{-k_{\lambda_F}L} & \text{(a)} \\ \varepsilon_{\downarrow}(L, \lambda_F) = \varepsilon_{\downarrow 0}(\lambda_F)e^{-k_{\lambda_F}(LAI-L)} & \text{(b)} \\ PAR(L) = PAR_0e^{-k_{PAR}L} & \text{(c)} \end{cases}$$

227 (S24)

229 Here  $\varepsilon_{\uparrow 0}$  and  $\varepsilon_{\downarrow 0}$  denote the upward/downward escape probability of ChlaF emission for an  
 230 infinitesimally thin leaf layer at TOC/BOC respectively;  $PAR_0$  denotes incident light intensity at  
 231 TOC;  $k_{\lambda_F}$  and  $k_{PAR}$  denote the extinction coefficients of ChlaF emission and PAR under Beer's  
 232 law, respectively. Inserting Eqs S24 to S23 lead to Eq 8 in the main text (also shown below for  
 233 clarify):

$$F_{\uparrow}(\lambda_F) = \varepsilon_{\uparrow 0}(\lambda_F) \underbrace{\left\{ \frac{1 - e^{-(k_{PAR} + k_{\lambda_F})LAI}}{(k_{PAR} + k_{\lambda_F})LAI} + \frac{\varepsilon_{\downarrow 0}(\lambda_F)r_s(\lambda_F)[e^{-2k_{\lambda_F}LAI} - e^{-(k_{PAR} + k_{\lambda_F})LAI}]}{(k_{PAR} - k_{\lambda_F})LAI} \right\}}_{\text{Structure}} \times \underbrace{[\bar{\Phi}_{FII}S_{II}(\lambda_F)\bar{\beta} + \bar{\Phi}_{FISI}(\lambda_F)(1 - \bar{\beta})]}_{\text{Mean ChlaF yield}} \times \underbrace{\overbrace{\bar{p}LAI}^{\text{Pigment}} \times \bar{\sigma}PAR_0}_{\text{Light harvesting}}$$

234 (8)  
 235  
 236

237 We note that Eq 8 can be applied to a leaf by setting  $LAI = 1$  and  $r_s = 0$ . At the leaf level, the  
 238 light transmittance  $\tau$  is related to light extinction coefficient at the leaf level, i.e., by  $\tau = e^{-k}$ ;  
 239 thus  $\tau_{\lambda_F} = e^{-k_{\lambda_F}}$  and  $\tau_{PAR} = e^{-k_{PAR}}$ . The corresponding  $F_{\uparrow}(\lambda_F)$  is then given by:

$$F_{\uparrow}(\lambda_F) = \varepsilon_{\uparrow 0} \underbrace{\frac{\tau_{\lambda_F}\tau_{PAR} - 1}{\ln(\tau_{\lambda_F}\tau_{PAR})}}_{\text{Structure}} \times \underbrace{[\bar{\Phi}_{FII}S_{II}(\lambda_F)\bar{\beta} + \bar{\Phi}_{FISI}(\lambda_F)(1 - \bar{\beta})]}_{\text{Mean F yield}} \times \underbrace{\overbrace{\bar{p}}^{\text{Pigment}} \times \bar{\sigma}PAR}_{\text{Light harvesting}}$$

240 (S25)  
 241  
 242

## 243 SI – 7. Derivation of the redox state-based models to infer the actual canopy ETR from

244  $F_{\uparrow}(\lambda_F)$ : Eq 9

245 The relevance of SIF for monitoring photosynthesis rests on the fact that ChlaF emission is  
 246 directly coupled to the linear ETR from PSII to PSI (Gu et al., 2019). This refers to the actual

247 ETR (denoted as  $J_a$  at the leaf level) instead of the potential ETR (i.e.,  $J_p$  at the leaf level) in the  
 248 commonly used FvCB model. As photochemistry, non-photochemical heat dissipation, and  
 249 ChlaF emission form a closed system according to the principle of energy conservation, the  
 250 relationship between the canopy-level actual ETR  $J_{aT}$  and  $F_{\uparrow}(\lambda_F)$  can be expressed in terms of  
 251 either redox states of PSII (i.e.,  $q_{LII}$ ) or  $NPQ$ . For simplicity, we assume the contribution of  
 252 soil reflected SIF is negligible (i.e.,  $r_s = 0$ , **A5**).

253 We first extend the  $q_{LII}$ -based  $J_a$  equation at the leaf level derived in Gu et al., (2019; Eq  
 254 21 therein) to the canopy level (denoted as  $J_{aT}$ ), leading to Eq 6 in the main text (also copied  
 255 below for clarity):

$$\begin{aligned}
 J_{aT} &= \int_0^{LAI} J_a(L) dL \\
 &= \frac{\Phi_{PSII m}(1 + k_{DF})}{1 - \Phi_{PSII m}} \int_0^{LAI} p(L) q_{LII}(L) \int_{\lambda_{Fmin}}^{\lambda_{Fmax}} \int_{\lambda_{Imin}}^{\lambda_F} \Phi_{FII}(L) s_{II}(\lambda_F) \beta(L, \lambda_I) \sigma(L, \lambda_I) I(L, \lambda_I) d\lambda_I d\lambda_F dL
 \end{aligned}
 \tag{6}$$

259 Next we invoke **A4** as in the derivation of Eq 8 (SI-6 above), which leads to:

$$\begin{aligned}
 J_{aT} &= \int_0^{LAI} J_a(L) dL \\
 &= \int_0^{LAI} q_{LII}(L) \frac{\Phi_{PSII m}(1 + k_{DF})}{1 - \Phi_{PSII m}} \Phi_{FII}(L) \beta(L) p(L) \sigma(L) PAR(L) dL
 \end{aligned}
 \tag{S26}$$

263 Further we invoke assumptions **A1-3** defined above. Moreover, we use the following function to  
 264 capture the first order variation of  $q_{LII}$  with  $PAR$  within a canopy (Han et al., 2022):

$$q_{LII}(L) = a[PAR(L)]^b = aPAR_0^b e^{-bk_{PAR}L} = q_{LII0} e^{-bk_{PAR}L}
 \tag{S27}$$

266 Here,  $a$  and  $b$  are two empirical coefficients, and Eq S27 is used to describe the light attenuation  
 267 with  $L$ .  $q_{LII0}$  is the fraction of open PSII reaction centers of a leaf at TOC. We insert Eqs S27  
 268 and S24c into Eq S26. After integration, we obtain

$$J_{aT} = \frac{aPAR_0^{b+1} \bar{p} \bar{\sigma} \bar{\beta} \Phi_{PSII m}(1 + k_{DF}) [1 - e^{-(b+1)k_{PAR}LAI}]}{(1 - \Phi_{PSII m})(b + 1)k_{PAR}} \bar{\Phi}_{FII}
 \tag{S28}$$

270 Next, we derive an estimate of  $\bar{\Phi}_{FII}$  from  $F_{\uparrow}(\lambda_F)$ , using Eq 8 in the main text. To do so, we  
 271 assume the ratio of  $\bar{\Phi}_{FI}$  to  $\bar{\Phi}_{FII}$  (and also the ratio of  $\bar{\Phi}_{FI}$  to  $\bar{\Phi}_{FII}$ ) is a constant (**A6**).

$$272 \quad \frac{\bar{\Phi}_{FI}}{\bar{\Phi}_{FII}} = \zeta \quad (S29)$$

273 Applying this ratio to Eq 8 and solving for  $\bar{\Phi}_{FII}$ , we have

$$274 \quad \bar{\Phi}_{FII} = \frac{F_{\uparrow}(\lambda_F)(k_{\lambda_F} + k_{PAR})}{PAR_0 [s_{II}(\lambda_F)\bar{\beta} + \zeta s_I(\lambda_F)(1 - \bar{\beta})] \bar{p}\bar{\sigma}\varepsilon_{\uparrow 0} \{1 - e^{-[k_{\lambda_F} + k_{PAR}]LAI}\}} \quad (S30)$$

275 Combining Eqs S28 and S30, we obtain the following  $q_L$ -based relationship between  $J_{aT}$  and  
276  $F_{\uparrow}(\lambda_F)$ , i.e., Eq 9 in the main text (also included below for clarity).

$$277 \quad J_{aT} = \underbrace{\left( \frac{k_{\lambda_F}}{k_{PAR}} + 1 \right) [1 - e^{-(b+1)k_{PAR}LAI}]}_{\text{Structure}} \times \underbrace{\frac{\Phi_{PSII_m}(1 + k_{DF})}{1 - \Phi_{PSII_m}}}_{\text{Constant}} \times \underbrace{\frac{\overbrace{aPAR_0^b}^{\text{Redox state}}}{b+1}}_{\text{ChlaF weighting factor}} \times F_{\uparrow}(\lambda_F)$$

278 Note that in Eq 9, the physiology is represented by the redox state term of PSII of the canopy,  
279 which is collectively expressed as a function of the fraction of open PSII reaction centers of a  
280 leaf at the canopy top ( $aPAR_0^b$ ).

281

## 282 **SI – 8. Derivation of the redox state-based models to infer canopy-level GPP from $F_{\uparrow}(\lambda_F)$ :** 283 **Eq 10**

284 At the leaf level, once  $J_a$  is known, photosynthesis can be calculated by assuming all electrons  
285 from PSII are consumed either in carboxylation ( $\text{CO}_2$  assimilation) or oxygenation  
286 (photorespiration) and no other electron sinks exist and the light-carbon reactions are in perfect  
287 balance (**A7**). This assumption is fairly accurate in normal conditions but may be violated when  
288 plants are under stress (Tcherkez & Limami, 2019). To calculate photosynthesis, one must  
289 further decide whether the carboxylation is limited by the supply of reducing power NADPH or  
290 energy currency ATP. In typical applications of the FvCB model, NADPH is assumed to be  
291 limiting (**A8**). These assumptions are adopted here to calculate photosynthesis of the canopy  
292 denoted as  $GPP_T$ , and hence leads to Eq 7 in the main text (also copied below for clarity).

$$GPP_T \left\{ \begin{aligned} &= \int_0^{LAI} \frac{C_c(L) - \Gamma^*(L)}{4C_c(L) + 8\Gamma^*(L)} J_a(L) dL \\ &= \frac{\Phi_{PSII_m}(1 + k_{DF})}{1 - \Phi_{PSII_m}} \int_0^{LAI} \frac{C_c(L) - \Gamma^*(L)}{4C_c(L) + 8\Gamma^*(L)} q_{LII}(L) \int_{\lambda_{Fmin}}^{\lambda_{Fmax}} \int_{\lambda_{Imin}}^{\lambda_F} \Phi_{FII}(L) s_{II}(\lambda_F) \beta(L, \lambda_I) \sigma(L, \lambda_I) I(L, \lambda_I) d\lambda_I d\lambda_F dL \quad (C3) \text{ (a)} \\ &= \int_0^{LAI} \frac{1-x}{3} J_a(L) dL \\ &= \frac{\Phi_{PSII_m}(1 + k_{DF})}{1 - \Phi_{PSII_m}} \frac{1-x}{3} \int_0^{LAI} q_{LII}(L) \int_{\lambda_{Fmin}}^{\lambda_{Fmax}} \int_{\lambda_{Imin}}^{\lambda_F} \Phi_{FII}(L) s_{II}(\lambda_F) \beta(L, \lambda_I) \sigma(L, \lambda_I) I(L, \lambda_I) d\lambda_I d\lambda_F dL \quad (C4) \text{ (b)} \end{aligned} \right.$$

293

294

(7)

295 Here  $C_c$  is the CO<sub>2</sub> partial pressure in the stroma of chloroplast and  $\Gamma^*$  is the CO<sub>2</sub> compensation  
 296 point in the absence of day respiration. We further assume that the electron ( $e^-$ ) use efficiency of

297  $\frac{C_c - \Gamma^*}{4C_c + 8\Gamma^*}$  carboxylation,  $\frac{C_c - \Gamma^*}{4C_c + 8\Gamma^*}$  does not vary along the depth of a canopy, which requires either  $C_c$   
 298 and  $\Gamma^*$  are uniform vertically or  $C_c$  is much larger than  $\Gamma^*$  (**A9**). Assuming **A1-A9** and inserting  
 299 Eqs S24 and 27 into Eq 7, we have the  $q_{LII}$ -based GPP- $F_{\uparrow}(\lambda_F)$  relationship, Eq 10 in the main  
 300 text (also included below for completeness):

$$GPP_T = \underbrace{\frac{\left(\frac{k_{\lambda_F}}{k_{PAR}} + 1\right) [1 - e^{-(b+1)k_{PAR}LAI}]}{\varepsilon_{\uparrow 0}(\lambda_F) [1 - e^{-(k_{\lambda_F} + k_{PAR})LAI}]}}_{\text{Structure}} \times \underbrace{\frac{\Phi_{PSII m}(1 + k_{DF})}{1 - \Phi_{PSII m}}}_{\text{Constant}} \times \underbrace{\frac{\overbrace{aPAR_0^b}^{\text{Redox state}}}{b+1}}_{\text{ChlaF weighting factor}} \times F_{\uparrow}(\lambda_F)$$

301

$$\times \begin{cases} \frac{C_c - \Gamma^*}{4C_c + 8\Gamma^*} & \text{(C3) (a)} \\ \frac{1-x}{3} & \text{(C4) (b)} \end{cases}$$

302

303

304

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