

The Physiological Basis for Estimating Photosynthesis from Chlorophyll a Fluorescence

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Summary

- The availability of Solar-Induced chlorophyll Fluorescence (SIF) offers potential to curb large uncertainties in estimating photosynthesis across biomes, climates, and scales. However, it remains unclear how SIF should be used to mechanistically estimate photosynthesis.
- This study built a quantitative framework to estimate photosynthesis, based on a mechanistic light reaction model with chlorophyll *a* fluorescence from PSII (SIF_{PSII}) as an input (MLR-SIF). Utilizing 29 C_3 and C_4 plant species representative of major plant biomes across the globe, we verified such a framework at the leaf level.
- MLR-SIF is capable of accurately reproducing photosynthesis for all C_3 and C_4 species under diverse light, temperature, and CO_2 conditions. We further tested the robustness of MLR-SIF using Monte Carlo simulations, and found that the estimated photosynthesis is much less sensitive to parameter uncertainties relative to the conventional Farquhar, von Caemmerer, Berry (FvCB) model because of additional independent information contained in SIF_{PSII} .
- SIF_{PSII} , once inferred from direct observables of SIF, provides “parameter savings” to the MLR-SIF as compared to the mechanistically equivalent FvCB and thus shortcuts the uncertainties propagated from imperfect model parameterization. Our findings set the stage for future efforts employing SIF mechanistically to improve photosynthesis estimation across scales, functional groups, and environmental conditions.

Key words: photosynthesis model; Solar-induced chlorophyll Fluorescence (SIF); Non-Photochemical Quenching (NPQ); parameter uncertainty; redox state of PSII reaction centers

One Sentence Summary: Utilizing joint chlorophyll *a* fluorescence and gas exchange measurements across diverse plant biomes, we build the physiological foundation for employing SIF to mechanistically estimate photosynthesis.

Introduction

Accurate quantification of terrestrial photosynthesis at different spatiotemporal scales is a long-sought goal in carbon cycle science (Schimel, 1995; Beer *et al.*, 2010; Ciais *et al.*, 2014). The rapidly growing, cross-scale observational capability of Solar-Induced chlorophyll Fluorescence (SIF), the only optically detectable signal that probes the whole photosynthetic process (Porcar-Castell *et al.*, 2014), offers a promising opportunity to achieving the goal of quantifying photosynthesis across different spatiotemporal scales (Mohammed *et al.*, 2019; Porcar-Castell *et al.*, 2021). This has been evident by the dramatic growth of SIF research and efforts to transform SIF observations to terrestrial photosynthesis estimation over the last few decades (Mohammed *et al.*, 2019). However, how exactly SIF should be used to estimate photosynthetic carbon assimilation in natural environments remains elusive.

Initial findings have identified encouraging linkages between SIF and photosynthesis from both observational and modeling aspects. From the observational side, existing studies have empirically linked remotely sensed SIF with photosynthesis inferred from eddy covariance (EC) measurements of net ecosystem exchange (NEE) of CO₂ (*e.g.*, Guanter *et al.*, 2014; Joiner *et al.*, 2014; Yang *et al.*, 2015; Verma *et al.*, 2017; Sun *et al.*, 2017; Wood *et al.*, 2017; Liu *et al.*, 2017; Li *et al.*, 2018; Miao *et al.*, 2018; Yang *et al.*, 2018). However, photosynthesis inferred from NEE at EC towers, although often assumed as the observational “truth”, is not directly measured but indirectly and imprecisely derived with approaches known to contain errors or even biases (Wohlfahrt & Gu, 2015; Wehr *et al.*, 2016; Keenan *et al.*, 2019). Using potentially and likely biased estimates of photosynthesis as truth to infer SIF-photosynthesis relationships essentially contradicts the original motivation of applying SIF to constrain photosynthesis (or reduce uncertainties in photosynthesis estimates). Furthermore, it is circular to apply such SIF-photosynthesis relationships to back-calculate photosynthesis; this circular estimation does not fully take advantage of the mechanistic, independent information carried in SIF.

Existing modelling studies (*e.g.*, Zhang *et al.*, 2014; Koffi *et al.*, 2015; Verrelst *et al.*, 2016; Parazoo *et al.*, 2020) primarily adopt the leaf-level formulation of the SIF-photosynthesis relationship from the SCOPE (Soil Canopy Observation Photosynthesis Energy) model (van der Tol *et al.*, 2014). Specifically, this approach utilized the Farquhar, von Caemmerer, Berry (FvCB) biochemical model to compute photosynthesis (and photochemical quantum yield, Φ_P) (Farquhar *et al.*, 1980; Sharkey, 1985). The modeled photosynthesis in turn is used to calculate fluorescence

yield (Φ_F) and therefore SIF by empirically modeling non-photochemical quenching (NPQ) as an exclusive function of Φ_P . Terrestrial biosphere models (TBMs) that explicitly incorporate SIF and data assimilation systems that have adopted such formulations to ingest satellite SIF to improve photosynthesis (and net carbon budgets) estimates (*e.g.*, Thum *et al.*, 2017; Bacour *et al.*, 2019; Norton *et al.*, 2019). While useful for simulating SIF-photosynthesis relationships and their sensitivity to different environmental conditions, the SCOPE-based strategy cannot escape from the usual, well-known problems of parameter and scaling uncertainty in applying FvCB to estimate photosynthesis at scales beyond a leaf (*e.g.*, Rogers *et al.*, 2017; Schaefer *et al.*, 2012; Anav *et al.*, 2015). Indeed, Parazoo *et al.* (2020) reported wide discrepancies in modeled SIF and photosynthesis across TBMs and large disagreement with ground observations.

Moving forward, with emerging interest in taking advantage of the information contained in remotely sensed SIF observations to improve photosynthesis estimates, it is critical to develop a mechanistic approach that enables direct and independent estimation of photosynthesis from SIF. Photosynthesis consists of light and carbon (also known as dark, light-independent, or Calvin-Benson cycle) reactions in sequence, which collaborate via multiple feedforward and feedback mechanisms to ensure the safety and smooth operations of the photosynthetic machinery in dynamic environments (Rochaix, 2011; Roach & Krieger-Liszkay, 2014). SIF is emitted during the light reactions. The mechanistic light reaction (MLR) equations derived by Gu *et al.* (2019) established the theoretical relationship between SIF_{PSII} (*i.e.*, the true total chlorophyll *a* fluorescence - ChlF emitted from PSII, prior to signal attenuation due to leaf self-absorption) and the actual electron transport rate (J_a) from photosystem II (PSII) to photosystem I (PSI). Thus, if SIF is observed, J_a can be calculated, provided that the followings are known: 1) the escape probability, *i.e.*, the ratio of the physiologically determined SIF_{PSII} to the sensor-observed SIF, which can be determined via leaf/canopy/atmosphere radiative transfer modeling (*e.g.*, Yang & van der Tol, 2018; Liu *et al.*, 2019; Zeng *et al.*, 2019), and 2) either the fraction of open PSII reaction centers (q_L) or NPQ (only one is needed as the other can be resolved with SIF_{PSII} ; Gu *et al.*, 2019). Photosynthesis can then be determined from the rates of carboxylation and photorespiration that the SIF-informed J_a supports (Farquhar *et al.*, 1980; Sharkey, 1985; Blankenship, 2002; von Caemmerer, 2000). Photosynthesis estimated from observed SIF is based upon theory and has a clear separation between input and output, which avoids the undesirable circularity discussed above.

At present, it remains unexplored the degree to which MLR-SIF is scalable across biomes and environmental conditions, and whether it has any practical advantages for photosynthesis estimation relative to existing approaches, *e.g.*, the conventional FvCB or a simple linear scaling from SIF reported by previous studies (Sun *et al.*, 2017; Li *et al.*, 2018). Mechanistically, the MLR-SIF model and the FvCB model are equivalent, given that the light and carbon reactions are balanced (Blankenship, 2002). However, these two models differ in the number and complexity of parameters required (See Notes S1 in Gu *et al.*, 2019). The FvCB model minimally represents the light reactions via an empirical electron transport equation to focus on the mechanistic representation of the carbon reactions. No light reaction mechanisms (*e.g.*, light harvesting, photochemical and non-photochemical quenching) are represented. The carbon reactions belong to the downstream processes in photosynthesis and are highly complex. As a result, a large number of biochemical and kinetic parameters are needed to run the FvCB model and these parameters can be highly variable across biomes and environments. Consequently, different TBMs that employ the same FvCB model show considerable disagreements in simulated photosynthesis and its response to environmental drivers; and much of the disagreements can be attributed to model parameter uncertainties (*e.g.*, Schaefer *et al.*, 2012; Anav *et al.*, 2015; Rogers *et al.*, 2017; Walker *et al.*, 2021). The MLR-SIF model requires fewer input parameters than FvCB, because SIF_{PSII} as an input together with q_L implicitly contains environmental and physiological information represented by the FvCB model for estimating photosynthesis (Gu *et al.*, 2019). We thus predict that the parsimony of the MLR-SIF model can reduce the impact of parameter uncertainties for photosynthesis estimation when the extra independent information (both environmental and physiological) contained in SIF is available.

This study has two objectives. The first objective is to demonstrate and validate the effectiveness of the mechanistic MLR-SIF model that uses SIF_{PSII} as an input to compute photosynthesis. The second objective is to demonstrate the practical advantages of the parameter parsimoniousness of the MLR-SIF approach when facing parameter uncertainties, *i.e.*, to test the above hypothesis across a broad range of Plant Functional Types (PFTs) and dynamic environments. To our knowledge, this is the first study to demonstrate the possibility and advantage of mechanistically estimating photosynthesis from the perspective of light reactions using SIF_{PSII} as an input across a wide range of PFTs and climates. We focus on the leaf level so that fundamental processes can be more fully investigated. To achieve our objectives, we collected

concurrent measurements of leaf gas exchange and pulse amplitude modulated (PAM) ChlF for 29 species of 11 representative PFTs native to Temperate, Boreal, and Tropical climates (Table S1). Using this dataset, we unraveled the regulation of environmental and physiological variations on the dynamic relationship between SIF_{PSII} and photosynthesis across PFTs, and assessed the advantages of MLR-SIF for estimating photosynthesis in terms of the capability, scalability, and uncertainty across PFTs and environments. We demonstrate that the key value of SIF lies in the process information it contains, which reduces the number of hard-to-measure parameters and the associated uncertainties for estimating photosynthesis. Our findings should pave the way for future investigations to apply SIF as an observational input to mechanistically estimate photosynthesis at the canopy scale and beyond.

Materials and Methods

Derivation of the MLR-SIF model

SIF_{PSII} is emitted during the photosynthetic light reactions, and can be used to directly quantify the actual electron transport rate (J_a) balanced by carboxylation and photorespiration in the carbon reactions (Blankenship, 2002), following the principle of energy conservation (Gu *et al.*, 2019). Once J_a is determined, net photosynthesis (A_n) can be calculated based on the electron requirements of carboxylation and oxygenation (Farquhar *et al.*, 1980; Sharkey, 1985; von Caemmerer, 2000):

$$A_n = A_g - R_d = \begin{cases} \frac{C_i - \Gamma^*}{4C_i + 8\Gamma^*} J_a - R_d, & \text{for } C_3 \text{ species} \\ \frac{1-x}{3} J_a - R_d, & \text{for } C_4 \text{ species} \end{cases} \quad \text{Eq. 1a}$$

$$J_a = \frac{\Phi_{PSII_{max}} \times (1 + k_{DF})}{1 - \Phi_{PSII_{max}}} \times q_L \times SIF_{PSII} \quad \text{Eq. 1c}$$

Here A_g refers to gross photosynthesis; SIF_{PSII} represents the true total ChlF emitted from PSII, which in principle should be utilized to establish the mechanistic relationship with photosynthesis; C_i the intercellular CO_2 concentration; Γ^* the CO_2 compensation point in the absence of mitochondrial respiration in the light for C_3 plants; x the fraction of total electron transport of mesophyll and bundle sheath allocated to the CO_2 -concentrating mechanism for C_4 plants; R_d the day respiration; $\Phi_{PSII_{max}}$ the maximum photochemical quantum efficiency of PSII in dark-adapted leaves; $k_{DF} = k_D/k_F$, with k_D and k_F representing the rate constants of constitutive thermal dissipation and fluorescence, respectively; q_L is derived under the assumption of lake model for photosynthetic unit connectivity. Note that MLR-SIF applies to all carboxylation limitation states, regardless of whether the carboxylation is limited by Ribulose 1,5-bisphosphate (RuBP) regeneration, RuBP carboxylase/oxygenase (Rubisco), or triose phosphate use (TPU), because it directly models the “actual” electron transport rate J_a from SIF_{PSII} (as opposed to the “potential” electron transport rate employed in FvCB) (Gu *et al.*, 2019). As in most applications of the FvCB model, Eq. 1a assumes that the supply of NADPH, rather than ATP, from the light reactions limits carboxylation.

J_a can also be derived alternatively from SIF_{PSII} via NPQ (Gu *et al.*, 2019):

$$J_a = PAR \times \alpha \times \beta - (1 + NPQ) \times (1 + k_{DF}) \times SIF_{PSII} \quad \text{Eq. 2}$$

where α is leaf absorptance; β the fraction of absorbed light allocated to PSII.

Eq. 2 and Eq. 1c are theoretically equivalent (Gu *et al.*, 2019), but practically have different complexity and thus applicability. Eq. 2 shows more clearly the principle of energy conservation among different dissipation pathways of absorbed photons. For actual applications, it requires PAR, NPQ, and SIF_{PSII} as inputs. Eq. 1c requires only SIF_{PSII} and q_L . q_L reflects the redox state of PSII and provides a good steady-state approximation of the state of Cytochrome b6f (Cyt b6f) which plays a central role in the control of steady-state photosynthesis (Johnson & Berry, 2021). NPQ involves both energetic and enzymatic reactions. Although the heat dissipation from NPQ is predominantly localized in the light-harvesting complexes of PSII, the activation and regulations of this release occur in the lumen, thylakoid membrane, and stroma. NPQ has a delayed response to light variations (Kromdijk *et al.*, 2016), a property that is exploited in PAM fluorometry to transiently decouple the photochemical and non-photochemical quenching to calculate various fluorescence variables (*e.g.*, Φ_P , NPQ, and q_L). Furthermore, NPQ has multiple components (*e.g.*, the energy-dependent qE, the irreversible components qI and qZ, and state transitions qT) and each operates at different time scales (Ruban, 2016, Nilkens *et al.*, 2010, Demmig-Adams *et al.*, 2014). The complex activation and regulations, delayed time response, and involvement of multiple time scales in the dynamics of NPQ components greatly increase the complexity in modeling NPQ as compared to q_L . Thus, we choose the q_L -based approach for calculating J_a from SIF_{PSII} which simplifies the mechanistic modeling of photosynthesis as advocated in Gu *et al.* (2019). As PAM only measures ChlF parameters but not SIF_{PSII} itself, we had to derive SIF_{PSII} from the following theoretical equations (Gu *et al.*, 2019):

$$SIF_{PSII} = \Phi_F \times PAR \times \alpha \times \beta \quad \text{Eq. 3}$$

$$\Phi_F = \frac{1 - \Phi_{PSII\max}}{(1 + k_{DF}) \times [(1 + NPQ) \times (1 - \Phi_{PSII\max}) + q_L \times \Phi_{PSII\max}]} \quad \text{Eq. 4}$$

Here, we used $\Phi_{PSII\max}$, NPQ and q_L inferred from PAM measurements to derive SIF_{PSII} (full list of symbols/variables defined in Table S2). Note that if SIF_{PSII} is available as an observational input

(*i.e.*, inferred from direct observables), we do not need to model SIF_{PSII} , but simply use Eq. 1c (in this case, NPQ is not needed) to compute J_a and therefore photosynthesis. Even though it is indeed now possible to measure leaf-level ChlF emission spectra (in absolute radiometric units, *e.g.*, Magney *et al.*, 2019b; Meeker *et al.*, 2021), such measurements always contain contributions from PSII and PSI, while in theory SIF_{PSII} is required to estimate photosynthesis (Eq. 1). Also, such measurements cannot resolve the issue of leaf re-absorption of fluorescence. Together these factors mean that direct fluorescence emission measurements in the absolute radiometric units unavoidably contain uncertainties. Furthermore, spectral fluorescence measurements have yet to be widely collected for diverse biomes under dynamic natural environments, as utilized in this study. Balancing consideration of these factors, we first used direct leaf-level ChlF emission spectra measurements as a qualitative check for the realism of the theoretically-derived SIF_{PSII} (see supporting information in Notes S1 and Fig. S1 for the validation of SIF_{PSII}). Subsequently, the theoretically-derived SIF_{PSII} (Eq. 3) was used to estimate photosynthesis (Eq. 1) across all plant species in our main analyses.

Note that SIF_{PSII} (Eq. 3) is the physiologically determined, spectrally and hemispherically integrated fluorescence emission in quantum unit, whereas in the remote sensing community, SIF is often given as radiance at a specific wavelength given in power unit per solid angle. From the point of view of probing photosynthesis, only the physiologically determined, spectrally and hemispherically integrated fluorescence emission in quantum unit is meaningful.

In this study, the parameters α and β are assumed constant at 0.84 (Björkman & Demmig, 1987, Schreiber, 2004) and 0.5 (von Caemmerer, 2000), respectively. Gu *et al.* (2019) set k_{DF} to 19 using the normalized values of k_D and k_F used in van der Tol *et al.* (2014). This study utilized a k_{DF} value of 10, as inferred from Pfündel (1998). This value was further corroborated by Tesa *et al.* (2018) with actual measurements (see their Fig. 6).

Plant species and their growth environment

We collected concurrent measurements of leaf gas exchange and ChlF parameters using PAM fluorometry for 29 species (25 C_3 and 4 C_4) that are representative of major PFTs (commonly adopted by TBMs) across the globe (Table S1). Measurements were taken at four locations:

Cornell Botanic Gardens (CBG), Cornell Musgrave Research Farm (CMRF), Oak Ridge National Lab (ORNL), and Xishuangbanna Tropical Botanical Garden (XTBG) (Table S1). The meteorological data and other growth environmental information at these four locations were described in Notes S2. This dataset was utilized to demonstrate the possibility and advantage in mechanistically estimating photosynthesis from the perspective of light reactions using SIF_{PSII} as an input (Eq. 1) across a wide range of PFTs and climates at the leaf scale.

Measurements of concurrent leaf gas exchanges and ChlF parameters with PAM

Nineteen among all the 29 species were measured with both light and CO₂ response curves, while only light response curves were collected for the remaining species (Table S1). For each light or CO₂ response curve, we selected 3-4 healthy and fully expanded sunlit leaves as replicates of each species. The specific procedures for measuring light and CO₂ response curves are described in Notes S3. Gas-exchange variables (A_n and C_i), steady-state and maximum ChlF under light (F_s and F_m') were obtained from light and CO₂ response curves. After sequentially collecting light and CO₂ response curves for the same leaves, we subsequently measured the maximum and minimum ChlF under fully dark-adapted conditions (F_m and F_o) for each leaf replicate (see procedure in Notes S3). These measured ChlF parameters were in turn used to calculate $\Phi_{PSII_{max}}$ ($\Phi_{PSII_{max}} = \frac{F_m - F_o}{F_m}$), the minimum ChlF under light ($F_o' = \frac{F_o}{\Phi_{PSII_{max}} + \frac{F_o'}{F_m}}$, Oxborough & Baker, 1997), q_L ($q_L = \frac{F_m' - F_s}{F_m' - F_o'} \times \frac{F_o'}{F_s}$), NPQ ($NPQ = \frac{F_m - F_m'}{F_m'}$), Φ_F (Eq. 4), and SIF_{PSII} (Eq. 3).

Data processing and analysis

Parameter fitting and aggregation: The MLR-SIF model (Eq. 1) requires the following parameters and driving variables as input: four parameters ($\Phi_{PSII_{max}}$, k_{DF} , I^* , R_d) and three variables (C_i , q_L , and SIF_{PSII}) for C_3 , four parameters ($\Phi_{PSII_{max}}$, k_{DF} , x , R_d) and two variables (q_L and SIF_{PSII}) for C_4 . At the leaf level, these variables and $\Phi_{PSII_{max}}$ can either be directly measured (e.g., C_i) or inferred from measurements (e.g., SIF_{PSII} , $\Phi_{PSII_{max}}$ and q_L), and thus can be readily incorporated into Eq. 1. Specifically, the set of parameters (I^* , R_d , x) were derived by fitting the MLR-SIF model with data that met the quality control criteria (see Notes S4) using

scipy.optimize.curve_fit script in Spyder 3.8. This fitting procedure was performed separately for each leaf replicate of all species.

We designed a parsimonious function to explicitly model q_L as a function of PAR instead of treating it as an input variable. The rationale here is that, although SIF observations can be readily available from remotely sensed measurements, q_L is usually not available at regional/global scale. We used an exponential equation with two parameters (a_{q_L} and b_{q_L}) to represent the relationship between q_L and PAR, a parsimonious formulation that can take advantage of available PAR:

$$q_L = a_{q_L} e^{-b_{q_L} PAR} \quad \text{Eq. 5}$$

Here a_{q_L} and b_{q_L} were derived by fitting this exponential equation with q_L inferred from ChlF and PAR measured by Li-6800 and/or GFS3000 for each leaf of all species. The means of the fitted a_{q_L} and b_{q_L} were then calculated across all leaves for each PFT, which were used to calculate q_L for each leaf in the corresponding PFT. The fitted and observed q_L agree well with each other for different PFTs (Fig. S2). Although this parsimonious model does not account for the impact of variation in C_i on q_L , it is adequate to capture the first-order variations in q_L in natural conditions. This is because that C_i covaries with PAR in order to keep the balance between light and carbon reactions of photosynthesis, thus the parsimonious q_L model as function of PAR is not independent of the changes in C_i . Moreover, if we deliberately force the model to “fail” in experiments by holding PAR at a high constant value and changing C_i , there would be two scenarios: 1) q_L would vary with C_i but only within a narrow range, unless C_i is made close to zero; 2) when C_i is close to zero, q_L will have to be close to zero too because the Calvin-Benson cycle cannot support any electron transport. Neither of these scenarios occurs in nature.

For MLR-SIF, once its parameters were fitted (I^* , R_d , x , a_{q_L} and b_{q_L}) or derived ($\Phi_{PSII\max}$) for each leaf replicate under 25 °C, we obtained “PFT-specific” parameter values by averaging fitted parameters across all species within the same PFT, and “PFT-universal” parameter values by averaging fitted parameters across all species of all PFTs respectively (Table S3). Details of parameter fitting and aggregation to PFT levels can be found in Fig. S3. Note that the motivation of PFT-level parameter aggregation is to avoid the needs for acquiring plant traits for individual

species which are challenging to obtain for global applications, the eventual goal of the MLR-SIF application. On the other hand, considering only 29 plant species were employed in this study and in some cases a PFT is characterized by only one or two species, we reported our statistical assessment (in Results) using datasets from all plant species instead of that aggregated to PFT.

To enable comparison with the conventional FvCB model, we further derived key relevant parameters required by FvCB (including the maximum carboxylation rate- V_{cmax} , maximum electron transport rate- J_{max} , I^* , and R_d) through parameter fitting utilizing measured CO_2 response curves in conjunction with the corresponding light response curves (see Notes S5 for detailed procedures) for the same leaf replicate across all species of a subset of six C_3 PFTs. These six PFTs used here are BDT-Temperate, BDS-Temperate, BDT-Boreal, NET-Boreal, C_3 Crop and C_3 grass. For a fair comparison of the performance between MLR-SIF and FvCB models in estimating photosynthesis, only the six C_3 PFTs with both CO_2 and light response curves available were used to obtain “PFT-specific” and “PFT-universal” parameters for both models. The parameters required by FvCB are $\Phi_{\text{PSII}_{\text{max}}}$, I^* , R_d , V_{cmax} , J_{max} , the fraction of absorbed light allocated to PSII β , the curvature parameter θ , and the Michaelis-Menten coefficients of Rubisco – K_{co} , where $K_{\text{co}}=K_c(1+O/K_o)$. $\Phi_{\text{PSII}_{\text{max}}}$ was inferred from PAM. K_c , K_o , θ , and β were assumed as constants. Specifically, we adopted *in vivo* values for K_c (*i.e.*, $404.9 \mu\text{mol mol}^{-1}$) and K_o (*i.e.*, $278.4 \mu\text{mol mol}^{-1}$) provided by Bernacchi *et al.*, (2001); θ was assumed to be 0.9 (Medlyn *et al.*, 2002) and β assumed to be 0.5 (von Caemmerer, 2000). The remaining parameters, *i.e.*, V_{cmax} , J_{max} , I^* , and R_d , were fitted by using the python optimization Scipy in Spyder 3.8. Note that we decided to fit only the four parameters here but pre-set others (to standard literature values), due to the consideration of balancing the degree of freedom (that represents the most variability in A_n) and the goodness of model-data fitting.

Validation of the MLR-SIF model: We first assessed the fitted parameters using the leave-one-out cross-validation for each species. Specifically, MLR-SIF is trained on all samples except for one replicate and a validation is made for that replicate, and we repeat this process N times for each species (N = the replicate number of each species). The parameters under assessment included a_{q_L} , b_{q_L} , $\Phi_{\text{PSII}_{\text{max}}}$, I^* (for C_3), x (for C_4), and R_d . Fig. S4 shows that the RMSE between the modeled A_n computed with parameters obtained from the training group and the actual observed

A_n is $2.42 \mu\text{mol m}^{-2} \text{s}^{-1}$ for the validation group, suggesting that the parameters fitted from the training group well captures that of the validation group.

Next, we refitted the parameters for each leaf replicate for demonstrating the performance of the MLR-SIF model across PFTs, light levels, and temperatures. Here the PFT-specific parameters (a_{q_L} , b_{q_L} , R_d , I^* , x , and $\Phi_{\text{PSII}_{\text{max}}}$) were used to estimate photosynthesis by combining measured C_i and SIF_{PSII} of each leaf replicate in the corresponding PFT (Fig. S3). We further validated the robustness of the MLR-SIF under different temperatures (20, 25, 30, 35, 40 °C) using a subset of species (for which measurements under different temperatures were made) for illustrative purpose, including C_3 (*Cornus racemosa* ‘Cuyzam’) and C_4 (*Andropogon gerardii*). This test is similar to the above demonstration of MLR-SIF performance across PFTs, except that the averages of the parameters of all the replicates within the same species at the reference temperature (25 °C), rather than PFT-specific parameters were used to estimate photosynthesis of each leaf replicate under different temperatures.

Assessment of parameter sensitivity and the propagated estimation uncertainty (PEU) in estimated A_n : We performed two independent analyses to assess the parameter sensitivity of MLR-SIF and PEU in A_n resulted from model parameter uncertainties. In the first analysis, we utilized the PFT-universal parameters to estimate photosynthesis of each leaf replicate. To examine which input parameter the MLR-SIF model is most sensitive to, we altered each parameter one at a time to be the corresponding PFT-universal value while keeping the remaining parameter values to be PFT-specific. Parameters examined here are: I^* (C_3 only), x (C_4 only), as well as those shared by C_3 and C_4 , including $\Phi_{\text{PSII}_{\text{max}}}$, R_d , a_{q_L} and b_{q_L} .

In the second analysis, we assessed the uncertainty on the estimated A_n propagated from model parameter uncertainties utilizing Monte Carlo simulations for both MLR-SIF and FvCB models under different light levels (100, 300, 500, 800, 1000, and 1200 $\mu\text{mol photon m}^{-2} \text{s}^{-1}$) at CO_2 concentration of 400 $\mu\text{mol CO}_2 \text{mol}^{-1}$ and 25 °C. The uncertainty assessment here was exemplified by a single PFT, *i.e.*, BDT Temperate, for illustrative purposes. Specifically, for each model, we perturbed its parameters by randomly drawing values from their corresponding parameter distribution. For each parameter, we assumed that their values follow a Gaussian distribution, with the fitted values and the standard errors directly returned by the Scipy

optimization package for each individual leaf replicate. Here, we focus on perturbing parameters that were fitted (most influential), *i.e.*, a_{q_L} , b_{q_L} , I^* , and R_d for MLR-SIF, V_{cmax} , J_{max} , I^* , and R_d for FvCB. For each model, we randomly drew 50,000 combinations of these parameters, calculated the corresponding A_n , and derived the standard deviation (SD) of the resulting A_n , which is denoted as the PEU. Note that, the randomly drawn 50,000 V_{cmax} and J_{max} were highly linearly correlated (Wullschleger, 1993; Walker *et al.*, 2014). Also, we constrained the randomly generated parameters to their physically meaningful ranges, *i.e.* $0 < a_{q_L} < 1$, $b_{q_L} < 0$, and V_{cmax} , J_{max} , I^* , and R_d were all positive.

Results

The dynamic relationship between photosynthesis and SIF_{PSII}

We first employed direct leaf-level ChlF emission spectra measurements ($SIF_{abaxial}$) to verify the realism of the modeled theoretical SIF_{PSII} (Notes S1). Our results (Fig. S1) show that SIF_{PSII} is highly correlated with $SIF_{abaxial}$ with R^2 ranging from 0.75 to 0.95 for three crop species (almond, grape, and walnut) under well-watered, mild, and moderate drought conditions (Table S4). With confidence gained in cross-checking the theoretically modeled SIF_{PSII} with measured $SIF_{abaxial}$, we subsequently evaluated the relationships between measured A_n and theoretical SIF_{PSII} for all plant species (Table S1) that cover a much broader PFTs and environments. We found a nonlinear relationship between A_n and SIF_{PSII} across all C_3 and C_4 plant species (Fig. 1a; Fig. S5) and temperatures (Fig. 1b-c). This relationship is characterized by an initial increase of A_n and then leveling-off when SIF_{PSII} is high, because the former saturates while the latter can keep increasing under high light as predicted by Gu *et al.* (2019). However, the saturation level of A_n and the rate approaching saturation differ considerably among species (especially between C_3 and C_4 plants) and temperatures. For instance, C_4 plants overall exhibit a higher light saturation level and slower rate towards saturation than C_3 plants, resulting in a lower degree of nonlinearity for the former, consistent with patterns observed at the canopy scale (*e.g.*, Liu *et al.*, 2017; He *et al.*, 2020). Notably, different species within the same PFT also show disparate A_n - SIF_{PSII} relationships (Fig. S5). Temperatures further impact the degree of A_n - SIF_{PSII} nonlinearity even for the same species and have distinct influences for C_3 and C_4 plants (Fig. 1b,c).

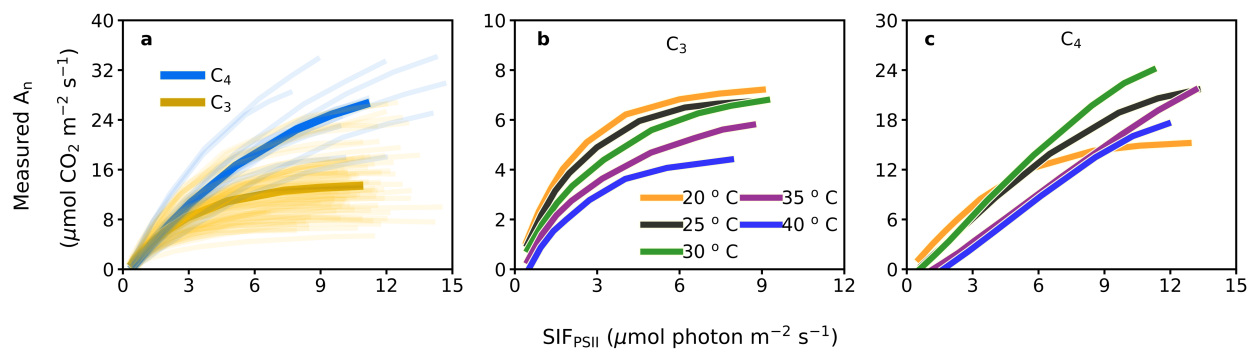


Fig. 1. The dynamic relationships between net photosynthesis (A_n) and chlorophyll a fluorescence from PSII (SIF_{PSII}) across Plant Functional Types (PFTs) and environments. (a) the A_n - SIF_{PSII} relationships across all C_3 and C_4 species; the thin and bold curves represent

individual leaf replicates and the mean of all species under the same photosynthetic pathways, respectively; **(b and c)** the impact of temperatures on the A_n - SIF_{PSII} relationship for a subset of species for C_3 (*Cornus racemosa* 'Cuyzam') and C_4 (*Andropogon gerardii*) respectively; curves represent the mean of leaf replicates under the same temperatures.

We found relatively higher inter-species variability in NPQ than in q_L (Fig. S6), resulting in more complex relationships among NPQ, SIF_{PSII} and A_n (Fig. 2a, b). Temperature had greater impact on NPQ than on q_L (Fig. 2c, d). Across light levels, NPQ achieves a local minimum at the optimal temperature for photosynthesis (Fig. 2d). In contrast, PAR dominates the variation of q_L , with temperature playing a minor role, supporting the use of PAR as a primary predictor to capture the first order variation in q_L (Fig. 2c).

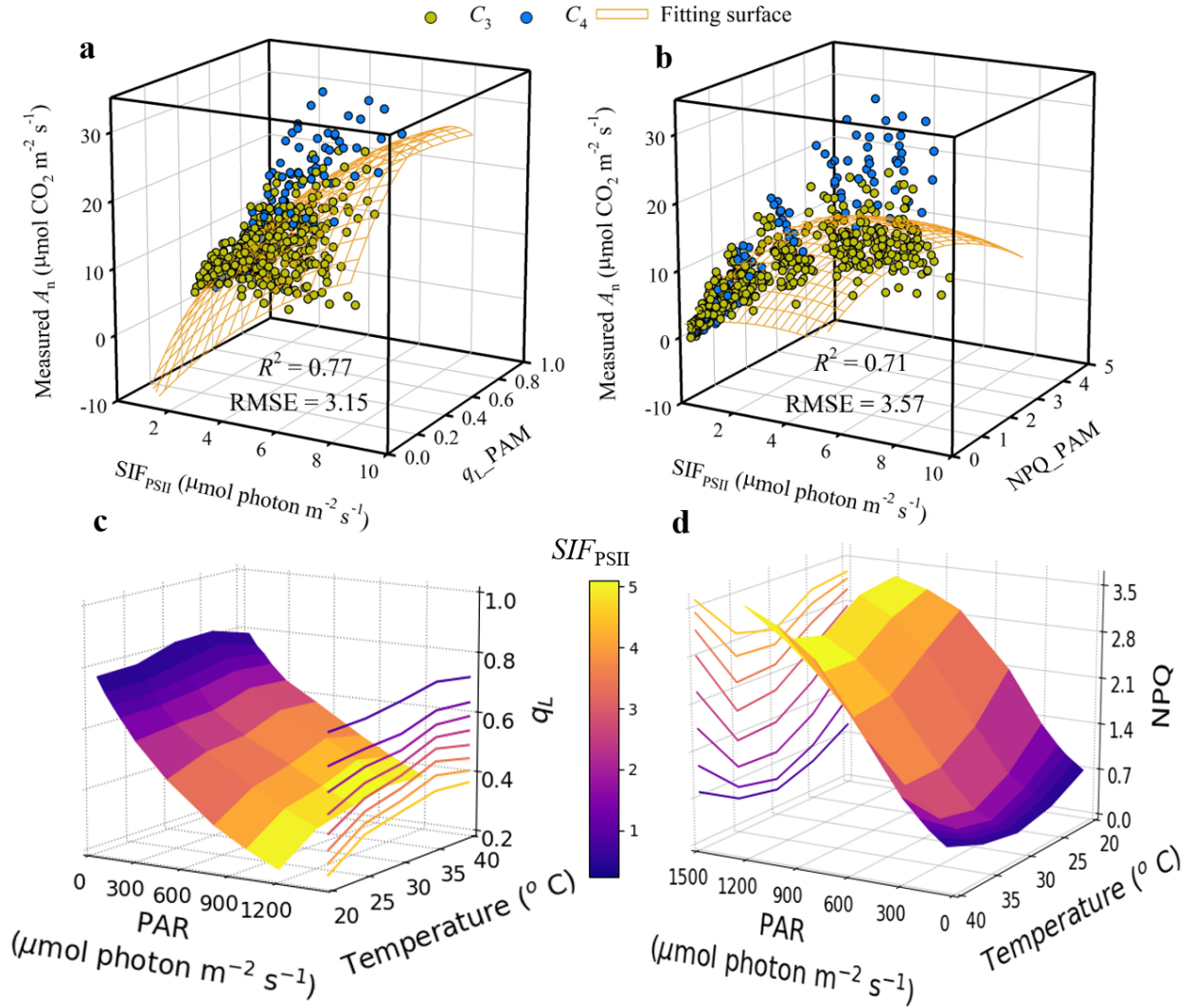


Fig. 2. The dynamic net photosynthesis (A_n) - chlorophyll a fluorescence from PSII (SIF_{PSII}) relationships modulated by the fraction of open PSII reaction centers (q_L) and non-photochemical quenching (NPQ) across Plant Functional Types (PFTs) and environments. (a and b) the relationships among q_L , NPQ, A_n , and SIF_{PSII} in 3D space across all species, the corresponding 2D figures are shown in Fig. S7; statistics (R^2 and RMSE) were obtained by fitting the 3D data with polynomial regression. (c and d) the impact of PAR and temperatures on q_L and NPQ, using a single C_3 species (*Cornus racemosa* 'Cuyzam') for illustrative purposes.

The capability, scalability, and uncertainty of MLR-SIF in estimating photosynthesis

The MLR-SIF model requires knowledge of q_L and C_i , which are dynamic. Using a minimalistic approach, we modeled q_L as a decreasing function of PAR with only two parameters a_{q_L} and

b_{q_L} (Eq. 5), since PAR captures the first-order effect in q_L variations (Fig. 2c, Fig. S6a). This parsimonious q_L model works reasonably well for a wide range of species (Fig. S2), which enables examining the potential of applying MLR-SIF across climates and biomes, a necessary step towards global applications.

With the use of PFT-specific parameter values, a common practice in TBMs, MLR-SIF successfully reproduces the variation of measured A_n with changing light ($R^2 = 0.83$, regression slope = 0.92) across all major PFTs (Fig. 3a). Moreover, MLR-SIF is capable of simulating A_n dynamics under different temperatures for both C_3 and C_4 (Fig. 3c-d), even though parameters were obtained solely at the reference temperature.

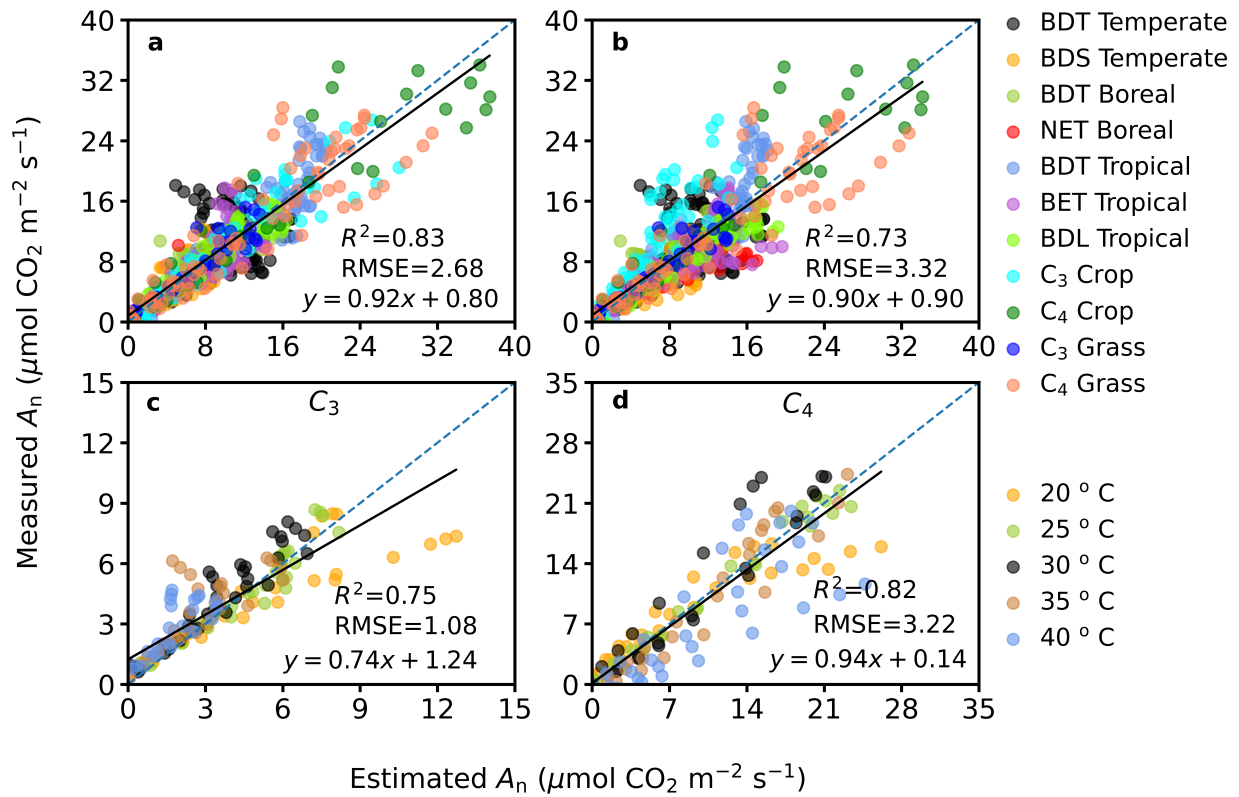


Fig. 3. Assessment of the estimated net photosynthesis (A_n) based on MLR-SIF (*i.e.*, mechanistic light reaction model with chlorophyll a fluorescence from PSII as an input, Eq. 1) against measurements across (a and b) Plant Functional Types (PFTs) and (c and d) temperatures. (a and b) estimated A_n using PFT-specific and PFT-universal parameters (Table S3) respectively under variable light conditions at 25 °C for all species (Table S1); parameters required are: I^* (C_3 only), x (C_4 only), and Φ_{PSIImax} , R_d , as well as a_{q_L} and b_{q_L} for calculating q_L

(shared by C_3 and C_4); **(c and d)** estimated A_n under five temperatures for C_3 (*Cornus racemosa* 'Cuyzam ') and C_4 (*Andropogon gerardii*) respectively. I^* and R_d are adjusted with a temperature response function (Bernacchi *et al.*, 2002); remaining parameters were set to values at 25 °C. Colored scatters represent individual leaf replicates (**a and b**, color-coded by different PFTs; **c and d**, color-coded by different temperatures). The regression coefficients (R^2 , RMSE, regression slope and intercept) were obtained by combining all species across PFTs (**a-b**) and temperatures (**c-d**). Solid lines represent the ordinary least square regression of all colored points; the dashed line represents 1:1.

To further demonstrate the advantages of MLR-SIF, we performed two independent analyses. First, we removed the PFT-specific parameters in MLR-SIF and evaluated how much the estimated A_n degrades if a constant value is used across all PFTs for each parameter. We found that, if using PFT-universal parameters (refer to Fig. S3 for details), the estimated A_n could still explain 73% of the variation in the measured A_n under changing light, and the estimation bias was minimal with a regression slope of 0.90 (Fig. 3b). The loss of explanation power (relative to PFT-specific values) comes from the combination of parameters uncertainty (Fig. S8a), *i.e.*, a_{qL} , b_{qL} , I^* (C_3) or x (C_4), R_d and $\Phi_{PSII\max}$. In addition, we used the same PFT dataset to compare the performance of MLR-SIF and FvCB models. FvCB had an overall weaker capability in estimating photosynthesis than MLR-SIF for both PFT-specific and PFT-universal parameters (Fig. 4a-d). Specifically, relative to MLR-SIF, FvCB showed a larger bias (underestimation) with a regression slope of 0.80 as compared to 0.86 for MLR-SIF for PFT-specific (Fig. 4a-b), 0.71 vs 0.81 for PFT-universal (Fig. 4c-d), albeit both models exhibited similar R^2 and RMSE. This performance difference is not due to difference in models' theoretical rigor (both MLR-SIF and FvCB are mechanistically equivalent) but due to differences in the level of parameter requirements and the associated impacts of the parameter uncertainties in model applications. All the differences between MLR-SIF and FvCB shown below should be interpreted this way.

In the second analysis, we used Monte Carlo simulations to explicitly quantify the uncertainty in A_n propagated from model parameter errors. We compared PEU between MLR-SIF and FvCB using Temperate Broadleaf Deciduous Tree (BDT Temperate) as an example (Fig. 4e, f). Our results showed that MLR-SIF consistently exhibits lower PEU than FvCB under all light

conditions (Fig. 4e). Correspondingly, A_n estimated with MLR-SIF tends to have a narrower statistical distribution relative to FvCB (Fig. 4f).

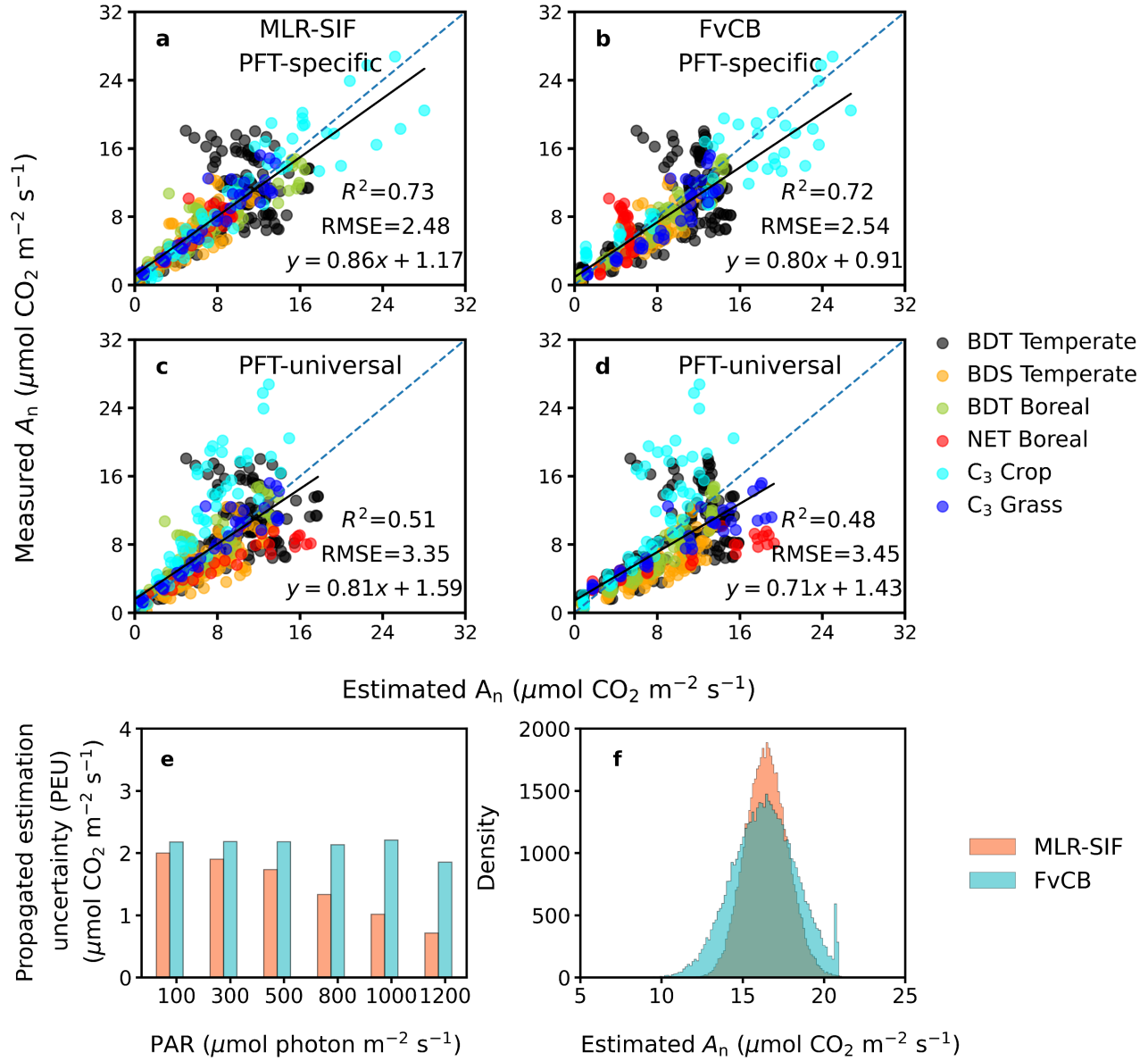


Fig. 4. Comparison of MLR-SIF (*i.e.*, mechanistic light reaction model with chlorophyll a fluorescence from PSII as an input) and FvCB (*i.e.*, Farquhar, von Caemmerer, Berry model) in estimating net photosynthesis (A_n) (a to d) and the propagated estimation uncertainty (PEU) in A_n from parameter perturbation using Monte Carlo simulations (e and f). (a and c) are similar to Fig. 3 a and b, except that only six C₃ Plant Functional Types (PFTs)

(for which both CO₂ and light response curves are available) were used, to ensure fair comparison of MLR-SIF and FvCB. **(b and d)** parameters required for FvCB are: the maximum photochemical quantum efficiency of PSII in dark-adapted leaves (Φ_{PSIImax}), the CO₂ compensation point in the absence of mitochondrial respiration in the light (I^*), day respiration (R_d), the maximum carboxylation rate (V_{cmax}), and maximum electron transport rate (J_{max}). **(a to d)** the regression coefficients (R^2 , RMSE, regression slope and intercept) were obtained by combining all species of six C₃ PFTs. **(e)** PEU, quantified as the standard deviation in A_n estimated with randomly perturbed parameters under different light levels. For illustration purposes, only Temperate Broadleaf Deciduous Tree (BDT Temperate) was used in this analysis. **(f)** histograms of estimated A_n for MLR-SIF and FvCB at PAR = 1200 $\mu\text{mol photon m}^{-2} \text{s}^{-1}$.

Discussion

The physiological and environmental controls on the photosynthesis- SIF_{PSII} relationship

The relationship between photosynthesis and SIF_{PSII} across all plant species and temperatures is close to a linear correlation at low light, especially for C_4 plant species. But the overall shape is non-linear (Figs. 1-2), which reveals that the variations in q_L and C_i prevent an exclusive dependence of photosynthesis on SIF_{PSII} (Eq. 1). Indeed, q_L decreases with light (Fig. S6), which in turn increases the nonlinearity between photosynthesis and SIF_{PSII} under high PAR (Fig. 2a). In addition, the responses of photosynthesis and SIF_{PSII} to C_i were not synchronized due to dynamic NPQ. For example, A_n increased initially and then reached a stable value when C_i is high (Fig. S9), whereas SIF_{PSII} can have a slight decrease at the very low C_i (for some species) and then increased to a peak followed by a subsequent decrease or remaining constant at high C_i (Fig. S10). The patterns of SIF_{PSII} vs C_i shown in Fig. S10 reflect the dynamics in the impact of competitive interactions between photochemical and non-photochemical quenching on ChlF emission. At low C_i , NPQ dominates whereas the impact of photochemical quenching is limited. As C_i increases, photochemical quenching increases while NPQ weakens. This asynchrony of the responses of A_n and SIF_{PSII} to C_i , especially under the low C_i induced by constraints of stomatal conductance, explains the apparent “decoupling” of SIF and photosynthesis (*i.e.*, high SIF and low photosynthesis) following artificially induced stomatal closure observed in single-factor analyses (Marrs *et al.*, 2020). Under these conditions, low C_i inhibits photosynthetic carbon assimilation, and also induces low q_L and increases NPQ to dissipate excess energy to offset the elevated photo-oxidative stress. As a result, low C_i contributes substantially to the dynamics and complexity of the photosynthesis- SIF_{PSII} relationship.

In previous studies, the complex environmental and physiological regulations on the photosynthesis-SIF relationship are typically hidden in the simplified term of light use efficiencies, which prevents a consistent interpretation of photosynthesis-SIF relationship across time scales, phenological stages, biomes, and environmental variations. For example, previous studies reported linear and even approximately biome-independent scaling between SIF and photosynthesis at the canopy level (*e.g.*, Sun *et al.*, 2017; Li *et al.*, 2018), because they were conducted at the seasonal scale and beyond, under which scales the co-variation of SIF and photosynthesis is dominated by the temporal variability in leaf area index (LAI, and therefore fPAR) (*e.g.*, Yang *et al.*, 2015; Magney *et al.*, 2020). However, the linearity tends to break down at shorter time scales (*e.g.*, sub-

daily, Zhang *et al.*, 2016; Damm *et al.*, 2015) as analogous to the typical light response curves in this study and/or under stress (Marrs *et al.*, 2020). In the former case, LAI remains relatively stable diurnally or within a few days, the relationship between SIF and photosynthesis can deviate from being linear due to the strong physiological regulation of variables such as q_L , and/or C_i . Further, these physiological regulations can vary among phenological stages, resulting in disparate phenology-dependent photosynthesis-SIF relationships (Yang *et al.*, 2018; Miao *et al.*, 2018, 2020). On the other hand, at sub-daily timescales, decoupling of photosynthesis and SIF could occur also due to variations in APAR and escape probability arising from canopy structure and illumination-viewing geometry (Chang *et al.*, 2021). In the latter case, *e.g.*, under cases of extreme photo-oxidative stress, it is crucial to incorporate q_L and/or C_i in order to accurately interpret the coupling/decoupling of photosynthesis-SIF relationships (as explained above).

SIF as an optical ‘shortcut’ reduces uncertainty from parameters in MLR-SIF

Currently, TBMs and some remote sensing products (*e.g.*, BESS, Ryu *et al.*, 2011; PR model, Keenan *et al.*, 2016) have almost exclusively adopted the FvCB biochemical model to calculate leaf photosynthesis (Farquhar *et al.*, 1980; Sharkey, 1985; von Caemmerer, 2020), with considerably variable implementation across TBMs, resulting in largely different responses of simulated photosynthesis to environmental drivers (*i.e.*, light, temperature, CO₂, VPD, and soil moisture, Rogers *et al.*, 2017). Notably, the fundamental biochemical and kinetic parameters required by FvCB constitute major sources of uncertainty in simulated photosynthesis (Bonan *et al.*, 2011, 2012). For example, V_{cmax} and J_{max} vary widely across PFTs, and are sensitive to leaf nitrogen contents, leaf ontology, and environmental changes (Field & Mooney, 1986; Kattge *et al.*, 2009, 2020; Detto & Xu, 2020), which in turn lead to significant model output uncertainty (Walker *et al.*, 2017; Rogers *et al.*, 2017; Bonan *et al.*, 2011).

We demonstrated the capability, scalability, and effectiveness of MLR-SIF across PFTs and environments, which stems from the fact that SIF_{PSII} , once inferred from direct observations (after appropriately accounting for factors such as spectral integration and escape probability), carries information on instantaneous plant functional responses to atmospheric forcings and integrates over the dynamic physiological complexities of photosynthesis. This means that MLR-SIF can circumvent estimation uncertainty propagated from model parameter errors/deficiency. For example, unlike FvCB, MLR-SIF does not rely on highly sensitive biochemical and kinetic

parameters such as V_{cmax} , J_{max} , and K_{co} , or selection of limitation stage of carboxylation (Walker *et al.*, 2021). Note that FvCB has larger PEU than MLR-SIF does, not because the former has a structural weakness but because the latter takes advantage of an observable photosynthetic functional ‘shortcut’ (SIF) (Gu *et al.*, 2019), *i.e.*, at least in theory, SIF makes estimating photosynthesis simpler although there are still difficult aspects that need to be resolved through continuing research. MLR-SIF effectively utilizes the mechanistic information in observed SIF to estimate photosynthesis in a forward way, independent from other existing photosynthesis estimation approaches that are known to have different levels of uncertainties (Kira *et al.*, 2021; Wehr *et al.*, 2016; Keenan *et al.*, 2019). Independent estimates are essential for confidence building as photosynthesis cannot be measured directly beyond a single leaf.

A recent new photosynthesis model based on Cytochrome b6f (Johnson & Berry, 2021) also established from light reaction perspective, but there are numerous differences with MLR-SIF. First of all, the model from Johnson & Berry (2021) does not use SIF_{PSII} (or SIF) as an input and focuses on PSI, rather than PSII. In contrast, MLR-SIF use SIF_{PSII} as input, and its goal is to build a physiological foundation that can mechanistically and accurately utilize SIF_{PSII} to directly and independently estimate photosynthesis. In addition, MLR-SIF applies to all carboxylation limited states, regardless of whether the carboxylation is limited by RuBP regeneration, Rubisco, or TPU, while the model developed by Johnson & Berry (2021) aims to establish a mechanistic light reaction model that can replace the empirical light-reactions sub-model of FvCB when photosynthetic assimilation is RuBP-regeneration limited.

Prospects of future work for facilitating MLR-SIF applications to large scales

As the first effort for building the physiological foundation towards utilizing SIF_{PSII} to mechanistically and independently estimate photosynthesis, this study starts from and focuses on the leaf level, the same as the introduction of the original FvCB model. Building the physiological foundation and gaining confidence on MLR-SIF at the leaf level is a necessary step, as existing leaf-level simulations of Φ_{F} , NPQ, Φ_{PSII} as well as their functional relationships exhibit strong discrepancy with observations and across different TBMs (Yang *et al.*, 2021; Parazoo *et al.*, 2020). Moving forward, to fully unleash the power of MLR-SIF to infer photosynthesis at large scales that are independent from currently existing photosynthesis estimates (with well-documented uncertainties), future work in the following aspects are needed.

- a) Parameterization of q_L or NPQ: In principle, modeling J_a requires either q_L or NPQ (but not both) if SIF_{PSII} could be inferred from direct observational input (Gu *et al.*, 2019). To facilitate large-scale applications (without the needs of PAM measured q_L or NPQ), q_L or NPQ must be modeled independently. To achieve this, the present application of MLR-SIF empirically models q_L as a function of PAR. Our results confirm that this parsimonious approach can capture the first-order effect of the SIF_{PSII} -photosynthesis relationship, as q_L reflects the redox poise of PSII reaction centers and is far more sensitive to variations in light than to other environmental variations such as temperature or CO_2 . Nevertheless, other environmental factors can also influence q_L . For example, temperature can play an increasing role in regulating q_L under high PAR (Fig. 2c). This will require more controlled experiments and/or synthesis of existing measurements across biomes and environmental conditions to refine our current parsimonious parameterization of q_L . Conceivably, it may be possible to mechanistically model the dynamic responses of q_L to environmental variations based on the redox relationships between reaction centers and electron carriers along the electron transport chain. Using a mechanistic q_L model will considerably improve the applicability of the MLR-SIF model. Although this study does not pursue a NPQ route for the application of the MLR-SIF model, this alternative route also has values. For example, it will promote field research in the dynamics of NPQ, which has important implications for land surface energy balance (Raczka *et al.*, 2019), at different time scales. It will also lead to estimates of photosynthesis that are independent from those of the q_L -based MLR-SIF model when SIF is available as a direct observable input. Empirical models of NPQ that consider the memory effect of past illumination history such as that used in Zhu *et al.* (2004) will have some capacity to deal with the multiplicity of NPQ at different time scales and can be used as a starting point for an NPQ-based MLR-SIF. Mechanistically modeling NPQ (Zaks *et al.*, 2012) for broad applicability will be a huge challenge but will be necessary to enabling the general use of the NPQ-based MLR-SIF model at different scales.
- b) Dynamic calculation of C_i : This study utilized measured C_i as input to MLR-SIF, with the intention to eliminate uncertainties not specifically related to SIF_{PSII} , which is our major focus here. Similarly, FvCB in this study also utilized measured C_i as an input. This way ensures a fair comparison between them in the context of leaf-level application. Moving

toward an eventual application of MLR-SIF to large scales would necessitate coupling the MLR-SIF model with stomatal conductance and energy balance models. In order to dynamically determine C_i by closing the system of equations of MLR-SIF, stomatal conductance, Fick's law of CO₂ diffusion from atmosphere to leaf interior, and energy balance are required, much like how FvCB is applied in TBMs.

c) Parameter $\Phi_{PSII_{max}}$: We employed the measured $\Phi_{PSII_{max}}$ values to MLR-SIF, which range from 0.74 to 0.81 (Table S3). The slight variability in $\Phi_{PSII_{max}}$ across PFTs is likely a consequence of the different leaf ages resulted from the longtime span of our measurements and perhaps also environmental stress. Fortunately, utilizing a fixed $\Phi_{PSII_{max}}$ value across plant species has only very minor impacts on our results (comparing Fig. 3a with Fig. S8d), giving us confidence that it is reasonable to apply a constant $\Phi_{PSII_{max}}$ for large-scale applications.

d) Parameter k_{DF} : In MLR-SIF, estimation of J_a requires k_{DF} as a parameter input. Yet, the precise value of k_{DF} and the degree to which it varies across plant species are presently unknown, as it is impossible to isolate k_{DF} with the current PAM fluorometry (Gu *et al.*, 2019). We note that the uncertainty in the precise value of k_{DF} does not affect our conclusion, as it is the product term $(1+k_{DF}) \times SIF_{PSII}$, instead of k_{DF} itself, matters for J_a estimation at the leaf level. Specifically, SIF_{PSII} and k_{DF} always appear together as a product term $(1 + k_{DF}) \times SIF_{PSII}$ in the J_a calculations (Eq. 1c and Eq. 2). If k_{DF} increases, the modeled SIF_{PSII} must decrease in order to keep the modeled J_a meaningful (*i.e.*, in agreement with PAM J_a measurements). On the other hand, the precise determination of k_{DF} is a critical step to scale up MLR-SIF to larger-scale applications, at which, SIF can be directly observed but not its product with k_{DF} . It is possible that the value of k_{DF} can be constant across species, as both k_F and k_D are physical properties of chlorophyll molecules whose structures (*e.g.*, electron orbitals) are highly conserved for higher plants. This argument can be implicitly supported by the highly conservative $\Phi_{PSII_{max}}$ value across plant species when they are not under stress, even though there are more processes involved in determining it than k_F or k_D . In terms of potential dependence of k_{DF} on temperature, earlier work (van der Tol *et al.*, 2014) hypothesized that k_D varies with temperature. This hypothesis will need to be verified and its physical mechanisms will

need to be identified. In the future, the value of k_{DF} can be precisely determined by measuring both adaxial and abaxial fluorescence emissions, as well as leaf absorptions. This way can lead to direct measurements of the true total SIF emission from the photosystems, which together with measured q_L and NPQ can be used to determine k_{DF} (Gu *et al.*, 2019). This additionally will require the development of a leaf-level full spectral fluorescence system that is capable of separating PSII and PSI contributions.

e) PSI and alternative electron flow: The functional stability of PSII and PSI differs under stress (Ivanov *et al.*, 2001), which might change their relative contributions to fluorescence emission. Thus, fluorescence emission from both PSII and PSI should be considered when SIF_{PSII} is inferred from at-sensor SIF for the broad application of MLR-SIF. Meanwhile, when plants are under stress, alternative electron sinks other than carboxylation oxygenation may be large. These issues may affect SIF – photosynthesis relationships and should be explored in the future. An integration of the PSII-focused (*i.e.*, Gu *et al.* 2019) and PSI-focused (*i.e.*, Johnson & Berry, 2021) light reaction modeling approaches may lead to new insights in this direction.

f) Coupling MLR-SIF with leaf and canopy radiative transfer: This study starts from and focuses on the leaf level, assuming that SIF_{PSII} can be inferred from at-sensor SIF observations. Currently, SIF_{PSII} is built upon PAM fluorometry (as used in this study), not a directly observable. However, in theory, SIF_{PSII} can be derived from the directly observable at-sensor SIF, and once this is achieved, we do not need PAM anymore. In reality, from SIF_{PSII} to at-sensor SIF, multiple radiative transfer processes within the leaf and across the canopy, *i.e.*, re-absorption and scattering (their relative strength depends on wavelength), can largely attenuate the observed signal. Therefore, large-scale applications of MLR-SIF would require a coupling with leaf/canopy radiative transfer scheme (as commonly done in TMBs) or invoking an escape probability factor determined from other means to infer SIF_{PSII} from at-sensor SIF, a currently key research topic in SIF remote sensing (*e.g.*, Yang *et al.*, 2018; Liu *et al.*, 2019; Zeng *et al.*, 2019).

Conclusions

Here we demonstrate the possibility and advantage in mechanistically estimating photosynthesis using SIF_{PSII} as an input across a wide range of PFTs and climates. The fidelity, scalability, and lower uncertainty compared with the traditional FvCB model suggests that MLR-SIF has great

potential in applying the rapidly increasing volumes of satellite SIF monitoring to estimate global photosynthesis. This model framework has similar mechanistic rigor as the conventional FvCB model but requires fewer parameters. It enables a truly independent estimate of photosynthesis based on SIF observations. The importance of SIF lies in the fact that it is a functional signal of photosynthesis and reflects collective responses of plants to environmental variations. Therefore, the availability of SIF observations can greatly ease the efforts for modeling photosynthesis by avoiding the need to explicitly and accurately represent individual environmental/physiological controls on photosynthesis (*i.e.*, which carboxylation limitation occurs under what conditions) and by reducing parameterization burdens and associated uncertainties.

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Author contributions

JH and YS planned and designed the research. JH, CY-YC, YZ, EWM, TSM, JW, OK, and SM performed experiments. JH analyzed data. JH, LG and YS wrote the manuscript. CY-YC and APW edited the manuscript.

Data Availability

Data are available from the Cornell University eCommons Repository at <https://doi.org/10.7298/q3hb-zq56>.

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Supporting Information

Fig. S1 The relationships between the theoretical SIF_{PSII} and the $SIF_{abaxial}$ measured with a modified LI-6800 coupled with a VIS-NIR FLAME Spectrometer.

Fig. S2 Comparison of q_L inferred from ChlF parameters vs estimated values using Eq. 5 for different PFTs.

Fig. S3 Diagram of the parameter fitting and performance of MLR-SIF and FvCB.

Fig. S4 The assessment of the performance of MLR-SIF model using leave-one-out cross-validation for each species.

Fig. S5 The observed relationship of measured A_n with SIF_{PSII} for different plant species grouped by PFTs.

Fig. S6 The responses of q_L and NPQ to PAR for each PFT.

Fig. S7 The relationships between measured A_n and q_L and NPQ, and between the modeled SIF_{PSII} and q_L and NPQ for C_3 and C_4 species.

Fig. S8 The impact of PFT-specificity of parameter values on the estimated A_n for different PFTs at the reference temperature 25 °C.

Fig. S9 The responses of measured A_n to C_i for different plant species grouped by PFTs.

Fig. S10 The responses of SIF_{PSII} to C_i for different plant species grouped by PFTs.

Table S1 Description of plant species, the corresponding PFTs, their growth conditions, and specific measurement curves.

Table S2 List of symbols and their definitions.

Table S3 The fitted parameter values and statistics for each PFT in the MLR-SIF and FvCB models.

Table S4 Description of plant species that used to concurrently measure PAM ChlF parameters and active ChlF spectral emission, and their growth and measurement conditions.

Notes S1 Verification of the validity of the computed SIF_{PSII} using the directly measured ChlF emission spectra

Notes S2 Plant growth environment

Notes S3 Procedures for measuring light and CO_2 response curves, and F_m and F_o

Notes S4 Data quality control

Notes S5 Details of parameters fitting with FvCB