Supporting Information for ”Representation of leaf-to-canopy radiative transfer processes improves simulation of far-red solar-induced chlorophyll fluorescence in the Community Land Model version 5”

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Introduction

The supporting information includes: 1) details and/or derivation of some equations related to CLM SIF simulation (text S1–S7, Table S1, and Figure S1); 2) comparisons between escape probability at the near-infrared band and at 740 nm (text S8 and Figure S2); 3) supplementary evaluation of the escape probability method (Figure S3); 4) SCOPE inputs for evaluation of the escape probability method and for site-level simulations (Tables S2 and S3); 5) additional information about the evaluation CLM simulation at the site-level (Figures S4–S9 and S13) and at the global scale (Figures S10–S12, S14, and S15).

Text S1. Calculation of the actual photochemical yield $\Phi_p$ Based on previous work (Lee et al., 2015; CLM5.0 Technical Description, 2020), the actual photochemical yield $\phi_p$ for C3 and C4 plants are calculated by Eq. S1 and Eq. S2, respectively.

$$\phi_p = \phi_{po} \frac{J_e}{J_o}$$

(S1)

$$\phi_p = \phi_{po} \frac{A}{A_j}$$

(S2)

where $\phi_{po}$ is the dark adapted maximum photochemical yield calculated by Eq. 7 in the main text. $J_e$ is the actual electron transport rate calculated as Eq. S3, $J_o$ is the maximum possible electron transport rate calculated as Eq. S4, $A$ is the leaf gross photosynthesis rate, and $A_j$ is the light-limited rate of carboxylation.

$$J_e = 0.5(1 - fnps)APAR$$

(S3)

$$J_o = 4A \frac{C_i + 2C_p}{C_i - C_p}$$

(S4)
where \( fnps = 0.15 \) is the fraction of PAR absorbed by nonphotosynthetic materials, \( C_i \) is the leaf intercellular \( CO_2 \) concentration, \( C_p \) is the \( CO_2 \) compensation point. \( C_i, C_p, A \) and \( A_j \) are simulated by the original CLM model.

**Text S2. Derivation of the bi-directional scattering coefficient**

The bi-directional scattering coefficient \( w \) in Eq. 10 in the main text converts incident direct solar radiation to scattered radiation at the nadir direction. \( w \) is related to leaf angle distribution, solar direction, viewing direction, and leaf reflectance and transmittance. From the information available in CLM5, the mean leaf zenith angle \( (\bar{\theta}_l) \) can be derived, but other information on leaf angle distribution is not available. Thus, we derive the formula for \( w \) with leaf zenith angle fixed at \( \bar{\theta}_l \), viewing direction set as nadir, and random leaf azimuth angle based on the method described in (Verhoef, 1984) as follows:

When the sum of leaf zenith angle \( (\bar{\theta}_l) \) and solar zenith angle \( (\theta_s) \) is less than \( \frac{\pi}{2} \) (i.e., \( \bar{\theta}_l \leq \frac{\pi}{2} - \theta_s \)), the Sun and the sensor are always on the same side of the leaf. \( w(\bar{\theta}_l) \) can be calculated as:

\[
w(\bar{\theta}_l) = \frac{1}{2\pi} \int_0^{2\pi} f_s f_o d\phi = \frac{1}{2\pi} \int_0^{2\pi} \frac{\cos \theta_s \cos \bar{\theta}_l + \sin \theta_s \sin \bar{\theta}_l \cos \phi}{\cos \theta_s} \rho \cos \bar{\theta}_l d\phi = \rho \cos^2 \bar{\theta}_l (S5)
\]

where \( f_s \) and \( f_o \) are conversion factors associated with the projection of solar radiation and radiation at nadir viewing direction on leaf, respectively. And \( f_s \) and \( f_o \) are calculated as \( \frac{\cos \theta_s \cos \bar{\theta}_l + \sin \theta_s \sin \bar{\theta}_l \cos \phi}{\cos \theta_s} \) and \( \cos \bar{\theta}_l \), respectively (see Verhoef, 1984).

If \( \bar{\theta}_l > \frac{\pi}{2} - \theta_s \), the Sun and the sensor are on different sides of the leaf when the relative azimuth angle between leaf normal and solar direction exceeds a threshold \( \gamma \). In this case, \( w(\bar{\theta}_l) \) is calculated as:
\[ w(\bar{\theta}_l) = \frac{1}{2\pi} \left[ \int_{-\gamma}^{\gamma} f_s \rho f_o d\phi - \int_{-\gamma}^{2\pi-\gamma} f_s \tau f_o d\phi \right] \]
\[ = \frac{1}{2\pi} \cos \bar{\theta}_l \left[ \int_{-\gamma}^{\gamma} (\cos \theta_s \cos \bar{\theta}_l + \sin \theta_s \sin \bar{\theta}_l \cos \phi) d\phi - \tau \int_{-\gamma}^{2\pi-\gamma} (\cos \theta_s \cos \bar{\theta}_l + \sin \theta_s \sin \bar{\theta}_l \cos \phi) d\phi \right] \]
\[ = \frac{1}{\pi} \left[ \cos^2 \bar{\theta}_l \left( \gamma (\rho + \tau) - \pi \tau \right) + \sin \gamma \tan \theta_s \sin \bar{\theta}_l \cos \bar{\theta}_l (\rho + \tau) \right] \]

(S6)

where

\[ \gamma = \arccos \left( -\frac{\cos \theta_s \cos \bar{\theta}_l}{\sin \theta_s \sin \bar{\theta}_l} \right) \]

(S7)

**Text S3. Calculation of the upscatter parameter for the observing direction**

As is shown in (Verhoef, 1984), scattering coefficients that converts direct solar radiation to upward or downward diffuse radiation is the same as the scattering coefficients that convert upward or downward diffuse radiation to the viewing direction, if the viewing zenith angle equals the solar zenith angle. Therefore, calculation of \( \beta'_o \) is similar to the calculation of \( \beta_0 \) in CLM5 (see CLM5.0 Technical Description, 2020), and the only modification needed is to replace solar angle with viewing angle (i.e., nadir in this study):

\[ \omega \beta'_o = \frac{1 + \bar{\mu} K_o}{\bar{\mu} K_o} a_s(\mu_o) \]

(S8)

where

\[ a_s(\mu_o) = \frac{\omega}{2} \int_0^1 \frac{\mu' G(\mu_o)}{\mu_o G(\mu') + \mu' G(\mu_o)} d\mu' \]

(S9)

definitions of the variables can be found in the main text.

**Text S4. Solution of the radiative transfer equations**
The only difference between Eqs. 10a and 10b and the radiative transfer equations in the original CLM5 (Eqs. 3.1 and
3.2 in *CLM5.0 Technical Description*, 2020) is the inclusion of clumping index (CI). The solution of Eqs. 10a and 10b (i.e., $I_\uparrow$ and $I_\downarrow$) is similar to the solution of the radiative transfer equations in original CLM5 (see *CLM5.0 Technical Description*, 2020; Sellers, 1985), the only change needed is to scale leaf area index and stem area index with CI and is not provided here. Here we provided the solution for the radiation flux at the observing direction ($I_o$, the third line of Eq. 10). Following the method used by (Verhoef, 1998) and integrating the solutions of $I_\uparrow$ and $I_\downarrow$, Eq. 10c (i.e., $I_o$) is solved as follows. Definitions of variables that have been provided in the main text are not repeated here.

Gap probability at the viewing direction is introduced as Eq. S10. The hotspot effect is not considered as most current satellite SIF products are not likely affected by the hotspot effect according to the orbits and overpass time of the satellites. While a small fraction of TROPOMI observations are affected by the hotspot effect (Köhler et al., 2018), only the measurements with phase angle (angle between the directions of the Sun and the sensor) larger than 20° from TROPOMI was used for comparisons with CLM SIF in the study. Thus, the impact of the hotspot effect on our comparison between CLM simulated SIF and TROPOMI observed SIF is minimal.

$$P_o = \exp[-K_o \cdot CI(L + S)]$$  \hspace{1cm} (S10)

The differential equation for $I_o P_o$ can be derived as:

$$\frac{dI_o P_o}{d(L + S) CI} = \frac{d(I_o \exp[-K_o \cdot CI(L + S)])}{d(L + S) CI} = P_o \frac{dI_o}{d(L + S) CI} - K_o I_o P_o$$  \hspace{1cm} (S11)

Thus,

$$-\frac{dI_o P_o}{d(L + S) CI} = P_o \left(we^{-K \cdot CI(L+S)} + v I_\uparrow + v'I_\downarrow\right)$$  \hspace{1cm} (S12)
Contribution of vegetation (i.e., excluding soil) to $I_o$ at top-of-canopy (TOC) can be calculated as:

$$I_{o,v}(0) = I_{o,v}(0)P_o(0) = \int_{0}^{L_T+S_T} -e^{-K_oCI(L+S)} [we^{-K_oCI(L+S)} + vI^\uparrow + v' I^\downarrow] \, CId(L+S)$$

where $L_T$ and $S_T$ are total leaf area index and total stem area index, respectively.

By combining Eq. S13 with solutions of Eqs. 10a and 10b, contribution of vegetation to $I_o$ at TOC for direct incident radiation and diffuse incident radiation can be derived as Eqs. S14 and S15, respectively.

$$I_{o,v}^{\text{dir}}(0) = h_{11} \frac{1 - s_2s_3}{K + K_o} + h_{12} \frac{1 - s_1s_3}{h + K_o} + h_{13} \frac{1 - s_3/s_1}{K_o - h}$$  \hspace{1cm} (S14)

$$I_{o,v}^{\text{dif}}(0) = h_{14} \frac{1 - s_1s_3}{h + K_o} + h_{15} \frac{1 - s_3/s_1}{K_o - h}$$  \hspace{1cm} (S15)

where

$$s_3 = e^{-K_oCI(L+S)}$$  \hspace{1cm} (S16)

$$h_{11} = w + \frac{vh_1}{\sigma} + \frac{v'h_4}{\sigma}$$  \hspace{1cm} (S17)

$$h_{12} = vh_2 + v'h_5$$  \hspace{1cm} (S18)

$$h_{13} = vh_3 + v'h_6$$  \hspace{1cm} (S19)

$$h_{14} = vh_7 + v'h_9$$  \hspace{1cm} (S20)

$$h_{15} = vh_8 + v'h_{10}$$  \hspace{1cm} (S21)

Definitions of other variables are the same as in (CLM5.0 Technical Description, 2020), except that $L$ and $S$ are scaled by $CI$. For cases where $K_o - h$ is close to zero ($|K_o - h| < 10^{-6}$), the first two terms of Taylor series are used for Eqs. S14 and S15, and the possible singularity when $\sigma = 0$ is taken care of with an approach similar to that presented by (Dai et al., 2004).

Contribution of soil to $I_o$ at TOC can be calculated as Eqs. S22 and S23 for direct incident radiation and diffuse incident radiation, respectively.
where $I_{\text{dir} o,s}$ and $I_{\text{diff} o,s}$ are downward diffuse radiation at the bottom of canopy per direct incident radiation and diffuse incident radiation, respectively. And they are solutions of Eqs. 10a and 10b.

Finally, $I_o$ at TOC per direct and diffuse incident radiation are calculated as Eqs. S24 and S25, respectively. TOC nadir reflectance and hemispherically integrated reflectance can be calculated as Eq. S26 and Eq. S27, respectively.

$$R_c,\text{nadir} = \left[ S_{\text{dir}} \mu I_{\text{dir} o} + S_{\text{diff} o} \right] / (S_{\text{dir} o} + S_{\text{diff} o})$$

$$R_c,\text{hem} = \left[ S_{\text{dir} o} \mu I_{\text{dir} o} + S_{\text{diff} o} \right] / (S_{\text{dir} o} + S_{\text{diff} o})$$

where $I_{\text{dir} o}$ and $I_{\text{diff} o}$ are upward diffuse radiation at TOC per direct incident radiation and diffuse incident radiation, respectively.

**Text S5. Calculation of transmittance coefficients**

Here, we provide both an intuitive explanation and a proof based on radiative transfer for Eqs. S28 and S29 that link upward transmittance coefficients with downward transmittance coefficients (i.e., Eq. 23 in the main text). Note that while Eq. S29 is for nadir direction in this study, the relationship is valid for any direction.
\[
T_{sh} = T_{ii}
\]
\[
T_{sn} = T_{in} + T_{nn}
\]

where \(T_{sh}\) and \(T_{sn}\) are the transmittance coefficients that represent the probabilities for radiation from soil to escape the top of canopy (directly or after scattering) from any direction in the upper hemisphere and at the nadir direction, respectively. \(T_{ii}\) is the downward diffuse flux below canopy per unit incident diffuse flux, \(T_{in}\) is the downward diffuse flux below canopy per unit nadir incident radiation, and \(T_{nn}\) is the probability that downward nadir flux reaches soil without interception by the canopy.

As canopy is vertically homogeneous (there is no vertical variation of canopy structural and optical properties) in CLM, downward and upward radiative transfer processes are similar. Transmittance of upward diffuse radiation from soil to upward diffuse radiation at TOC can be considered as the sum of three components (Fig. S1): 1) transmittance of diffuse radiation from soil to TOC without interaction with canopy (\(t_1\)); 2) transmittance of diffuse radiation from soil to TOC after scattering within canopy (without interaction with soil, \(t_2\)); 3) transmittance of diffuse radiation from soil to TOC with multiple scattering that involves soil (\(t_3\)). Similarly, transmittance of downward diffuse radiation from TOC to soil consists of three components: \(t'_1\), \(t'_2\), and \(t'_3\). Their definitions are the same as \(t_1\), \(t_2\), and \(t_3\), except that the fluxes are downward from TOC to soil. As the canopy is vertically homogeneous, upward and downward fluxes are identical. Therefore, we have \(t_1 = t'_1\), \(t_2 = t'_2\), and \(t_3 = t'_3\). Thus,

\[
T_{sh} = t_1 + t_2 + t_3 = t'_1 + t'_2 + t'_3 = T_{ii}
\]

The explanation for Eq. S29 is similar. Transmittance of upward diffuse radiation from soil to upward nadir radiation at TOC can be considered as the sum of three components
(Fig. S1): 1) transmittance of nadir radiation from soil to TOC without interaction with the canopy ($t_4$); 2) transmittance of diffuse radiation from soil to nadir radiation at TOC after scattering within canopy (without interaction with soil), which can in turn be considered as the product of the transmittance of diffuse radiation from soil to the last point of interaction with vegetation ($t_6$) and the transmittance of nadir radiation from the last point of interaction with vegetation to TOC ($t_5$); 3) transmittance of diffuse radiation from soil to nadir radiation at TOC with multiple scattering that involves soil, which can in turn be considered as the product of the transmittance of diffuse radiation from soil to the last point of interaction (the last point may be at soil surface or within canopy, $t_8$) and the transmittance of nadir radiation from the last point of interaction to TOC ($t_7$). Similarly, $t'_4$, $t'_5$, $t'_6$, $t'_7$, and $t'_8$ can be identified as components of the transmittance of downward nadir radiation at TOC to downward radiation at the bottom of canopy, whose definitions are the same as $t_4$–$t_8$, except that the fluxes are downward. As upward and downward fluxes are identical for vertically homogeneous canopy, we have $t_4 = t'_4$, $\cdots t_8 = t'_8$. Thus,

$$T_{sn} = t_4 + t_6 t_5 + t_8 t_7 = t'_4 + t'_5 t'_6 + t'_7 t'_8 = T_{nn} + T_{in} \quad (S31)$$

Eqs. S28 and S29 can also be derived from radiative transfer equations. $T_{ii}$ and $T_{in}$ have been derived in previous literature as Eq. S32 and Eq. S33 (CLM5.0 Technical Description, 2020). $T_{nn}$ is $P_o$ calculated by Eq. S10. $T_{sh}$ and $T_{sn}$ are $I_{\uparrow}$ and $I_o$ at TOC (i.e., $L + S = 0$) solved from Eq. S34 under the boundary condition defined in Eq. S35, respectively. By comparing Eq. S36a when $L + S = 0$ with Eq. S32 and comparing Eq. S36c when $L + S = 0$ with Eqs. S10 and S33, Eqs. S28 and S29 can be derived.
\[ T_{ii} = h_9 s_1 + h_{10} s_1 = \frac{u_2 + \tilde{\mu} h}{d_2} - \frac{(u_2 - \tilde{\mu} h)}{d_2} = \frac{2 \tilde{\mu} h}{d_2} \]  
(S32)

\[ T_{in} = \frac{h_4}{\sigma} e^{-K_o C_l (L_T + S_T)} + h_5 s_1 + \frac{h_6}{s_1} \]  
(S33)

\[
\begin{aligned}
  -\frac{\mu}{d(L + S) C_l} \frac{dI_{\uparrow}}{dt} + [1 - (1 - \beta)\omega]I_{\uparrow} - \omega I_{\downarrow} &= 0 \\
  \frac{\mu}{d(L + S) C_l} \frac{dI_{\downarrow}}{dt} + [1 - (1 - \beta)\omega]I_{\downarrow} - \omega I_{\uparrow} &= 0 \\
  -\frac{dI_o}{d(L + S) C_l} &= vI_{\uparrow} + v'I_{\downarrow} - K_o I_o
\end{aligned}
(S34a)

\[
\begin{aligned}
  I_{\downarrow}(0) &= 0 \\
  I_{\uparrow}(L_T + S_T) &= 1 + \alpha g I_{\downarrow}(L_T + S_T)
\end{aligned}
(S35a)

where \( I_{\downarrow}(0) \) is downward diffuse radiation at TOC, \( I_{\uparrow}(L_T + S_T) \) and \( I_{\downarrow}(L_T + S_T) \) are upward and downward diffuse radiation at bottom of canopy (cumulative plant area index of \( L_T + S_T \)), respectively. See (CLM5.0 Technical Description, 2020) for the definition of other variables. Solution of Eq. S34 under the boundary condition of Eq. S35 is:

\[
\begin{aligned}
  I_{\uparrow} &= \frac{b + \tilde{\mu} h}{d_2} e^{h \cdot C_l (L + S)} - \frac{b - \tilde{\mu} h}{d_2} e^{-h \cdot C_l (L + S)} \\
  I_{\downarrow} &= \frac{c}{d_2} \left[ e^{h \cdot C_l (L + S)} - e^{-h \cdot C_l (L + S)} \right] \\
  I_o &= \frac{v(b + \tilde{\mu} h) + v' c}{d_2(K_o - h)} \left( e^{(h-K_o) C_l (L + S)} - e^{[(h-K_o) C_l (L_T + S_T)]} \right) \\
  &\quad - \frac{v(b - \tilde{\mu} h) + v' c}{d_2(K_o + h)} \left( e^{[-(K_o+h) C_l (L + S)]} - e^{[-(K_o+h) C_l (L_T + S_T)]} \right) \\
  &\quad + e^{-K_o C_l (L_T + S_T - L - S)} \left[ 1 + \alpha g \frac{c}{d_2} e^{h \cdot C_l (L_T + S_T)} - \alpha g \left( \frac{c}{d_2} \right) e^{-h \cdot C_l (L_T + S_T)} \right]
\end{aligned}
(S36a)

(S36b)

(S36c)

Text S6. Correction of incident PAR

When not coupled with the Community Atmosphere Model (CAM), the original CLM estimates incident PAR by assuming a fixed ratio of 0.5 between incident PAR and short-
wave radiation (SR) (CLM5.0 Technical Description, 2020). However, the ratio (0.5) is too high according to literature, especially when PAR is defined as 400-700 nm as in CLM (Tsubo & Walker, 2005). Based on measurements at 31 Ameriflux sites (Table S1), we set the ratio between incident PAR and SR to 0.435 for simulation of photosynthesis and fluorescence (except for CLM5SP-exp4). Radiation for other parts of CLM was not changed.

Text S7. Modifications for the calculation of APAR

In the original CLM5, absorbed photosynthetically active radiation (APAR) per leaf area was calculated using Eq. S37. Thus, stem and snow affect APAR per leaf area. We remove the impact of stem and snow on APAR per leaf area by introducing correction factors as shown in Eq. S38.

\[
APAR = \frac{APAR_{\text{tot}}}{eLAI + eSAI} \tag{S37}
\]

where \(APAR\) is APAR per leaf area, \(APAR_{\text{tot}}\) is total PAR absorbed by leaf, stem, and snow. \(eLAI\) and \(eSAI\) are leaf area index and stem area index not buried by snow, respectively.

\[
APAR = \frac{APAR_{\text{leaf}}}{eLAI} \tag{S38}
\]

where

\[
APAR_{\text{leaf}} = PAR_{\text{leaf}}(1 - \omega_{\text{leaf}}) = PAR_{\text{veg}} \frac{eLAI}{eLAI + eSAI}(1 - \omega_{\text{leaf}}) = APAR_{\text{veg}} \frac{eLAI}{1 - \omega_{\text{veg}} eLAI + eSAI}(1 - \omega_{\text{leaf}}) \tag{S39}
\]
\[ APAR_{\text{veg}} = PAR_{\text{veg}} (1 - \omega_{\text{veg}}) = PAR_{\text{tot}} (1 - f_{\text{snow}})(1 - \omega_{\text{veg}}) = \frac{APAR_{\text{tot}}}{1 - \omega_{\text{tot}}}(1 - f_{\text{snow}})(1 - \omega_{\text{veg}}) \] (S40)

where \( APAR_{\text{leaf}} \) and \( APAR_{\text{veg}} \) are total PAR absorbed by leaf and by vegetation (leaf and stem), respectively; \( PAR_{\text{tot}}, PAR_{\text{leaf}}, \) and \( PAR_{\text{veg}} \) are total PAR intercepted by the whole canopy (leaf, stem, and snow), by leaf, and by vegetation, respectively; \( f_{\text{snow}} \) is the fraction of canopy that is snow-covered; \( \omega_{\text{leaf}}, \omega_{\text{veg}}, \) and \( \omega_{\text{tot}} \) are single scattering albedo for leaf, vegetation, and the total canopy, respectively.

**Text S8. Escape probability at the near-infrared band and at 740 nm**

As there is only one visible band (0.4–0.7 \( \mu \)m) and one near-infrared (NIR) band (0.7–4.0 \( \mu \)m) in CLM5, we used the escape probability calculated with NIR reflectance and transmittance to approximate the escape probability at 740 nm. Here we test the difference between leaf reflectance, leaf transmittance, and fluorescence escape probability at 740 nm and in the near-infrared (NIR) band with the LOPEX93 dataset (Hosgood et al., 1993) and the SCOPE model. NIR reflectance and transmittance were calculated by weighting leaf reflectance and transmittance spectra by white-sky solar radiation spectrum over the spectral range of 700–2500 nm according to (Majasalmi & Bright, 2019) (Eqs. S41 and S42). The white-sky solar radiation spectrum was obtained by the SCOPE model with default inputs. Leaf biophysical and biochemical parameters from the LOPEX93 dataset were then used as inputs for SCOPE simulations. Fluorescence escape probability at 740 nm was simulated with both true leaf reflectance and transmittance at 740 nm and with NIR leaf reflectance and transmittance. For the 315 samples in the LOPEX93 dataset (samples that do not provide all parameters and those with leaf chlorophyll content less than 2 \( \mu \text{g} \cdot \text{m}^{-2} \) were excluded), the relative error between leaf reflectance, leaf transmitt-
tance, and fluorescence escape probability at 740 nm and at the NIR band was always less than 11% and was less than 5% for most cases (Fig. S2). Besides, there were both overestimation and underestimation. Therefore, the escape probability at the NIR band can serve as a good approximation of the escape probability at 740 nm.

\[
\rho_{\text{nir}} = \frac{\int_{700}^{2500} \rho(\lambda) E_{\text{sky}}(\lambda) d\lambda}{\int_{700}^{2500} E_{\text{sky}}(\lambda) d\lambda}
\]

\[
\tau_{\text{nir}} = \frac{\int_{700}^{2500} \tau(\lambda) E_{\text{sky}}(\lambda) d\lambda}{\int_{700}^{2500} E_{\text{sky}}(\lambda) d\lambda}
\]

where \(\rho_{\text{nir}}\) and \(\tau_{\text{nir}}\) are NIR leaf reflectance and transmittance, respectively; \(\rho(\lambda)\), \(\tau(\lambda)\), and \(E_{\text{sky}}(\lambda)\) are the spectra of leaf reflectance, leaf transmittance and white-sky solar radiation, respectively.

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**Figure S1.** Intuitive explanation of Eqs. S28 and S29. a) transmittance of upward diffuse radiation from soil to upward diffuse radiation at TOC. b) transmittance of upward radiation from soil to upward nadir radiation at TOC. c) transmittance of downward diffuse radiation at TOC to downward diffuse radiation at the bottom of canopy. d) transmittance of downward nadir radiation at TOC to downward radiation at the bottom of canopy. Black represents diffuse radiation, blue represent nadir radiation.

**Figure S2.** a) Relative difference between leaf reflectance (blue) and transmittance (red) at 740 nm and in the NIR band. b) Relative difference between escape probability at 740 nm and in the NIR band.
**Figure S3.** Evaluation of the escape probability method that we have incorporated in CLM5 with SCOPE for a) hemispherically integrated SIF at TOC \((SIF_{\text{hem}})\) and b) TOC SIF at the nadir direction \((SIF_{\text{nadir}})\). TOC SIF was limited to the realistic range of \(0–10 \text{ W} \cdot \text{m}^{-2} \cdot \text{sr}^{-1} \cdot \text{µm}^{-1}\).

**Figure S4.** Comparison between APAR simulated by CLM5SP-exp1 and SCOPE at a) Pace Forest, b) Harvard Forest, c) US-NR1, d) US-NE3, and e) BR-Sa1.
Figure S5. Comparison between Φ_f simulated by CLM5SP-exp1 and SCOPE at a) Pace Forest, b) Harvard Forest, c) US-NR1, d) US-NE3, and e) BR-Sa1.
Figure S6. Comparison between $f_{SIF}^{esc, nadir}$ simulated by CLM5SP-exp1 and SCOPE at a) Pace Forest, b) Harvard Forest, c) US-NR1, d) US-NE3, and e) BR-Sa1.
Figure S7. Comparison between nadir reflectance simulated by CLM5SP-exp1 and SCOPE at a) Pace Forest, b) Harvard Forest, c) US-NR1, d) US-NE3, and e) BR-Sa1.
Figure S8. Comparisons between nadir SIF simulated by SCOPE (blue solid lines), simulated by CLM5SP-exp1 (red dash-dotted dotted lines), simulated by CLM5SP-exp9 (with sustained NPQ, grey dotted line), observed from tower (green dashed lines) and observed from GOME-2 (asterisks) at US-NR1

Figure S9. Comparisons between nadir SIF simulated by CLM5SP-exp9 (with sustained NPQ) and observed at tower at US-NR1
Figure S10. Global maps of the difference between multi-year average CLM5SP-exp2 SIF and GOME-2 SIF (a); CLM5SP-exp3 SIF and GOME-2 SIF (b), CLM5SP-exp4 SIF and GOME-2 SIF (c). And the improvements of the comparison to GOME-2 SIF by considering bidirectional effect (d, $|\text{CLM5SP-exp2 - GOME-2}| - |\text{CLM5SP-exp1 - GOME-2}|$), clumping (e, $|\text{CLM5SP-exp3 - GOME-2}| - |\text{CLM5SP-exp1 - GOME-2}|$), and correction of PAR (f, $|\text{CLM5SP-exp4 - GOME-2}| - |\text{CLM5SP-exp1 - GOME-2}|$).
Figure S11. Comparison between seasonal variations of SIF observed by OCO-2 (blue solid lines), simulated by CLM5SP-exp1 (orange dashed lines), and simulated by CLM5BGC-exp1 (green dash-dotted lines) for a) broadleaf deciduous temperate tree, b) needleleaf evergreen boreal tree, c) broadleaf evergreen tropical tree, d) crop, and e) C3 non-arctic grass. All pixels dominated (> 70% land unit) by the corresponding PFT were used for comparison, locations of the pixels are the same for CLM5SP-exp1 and CLM5BGC-exp1 and are shown in f): blue: broadleaf deciduous temperate tree, cyan: needleleaf evergreen boreal tree, green: broadleaf evergreen tropical tree, yellow: crop, and red: C3 non-arctic grass. Pace SIF values are averages from 2008 to 2014, OCO-2 SIF values are from September 2014 to April 2018.
Figure S12. Comparison between seasonal variations of SIF observed by TROPOMI (blue solid lines), simulated by CLM5SP-exp1 (orange dashed lines), and simulated by CLM5BGC-exp1 (green dash-dotted lines) for a) broadleaf deciduous temperate tree, b) needleleaf evergreen boreal tree, c) broadleaf evergreen tropical tree, d) crop, and e) C3 non-arctic grass. All pixels dominated (> 70% land unit) by the corresponding PFT were used for comparison, locations of the pixels are the same for CLM5SP-exp1 and CLM5BGC-exp1 and are shown in f): blue: broadleaf deciduous temperate tree, cyan: needleleaf evergreen boreal tree, green: broadleaf evergreen tropical tree, yellow: crop, and red: C3 non-arctic grass. CLM SIF values are averages from 2008 to 2014, TROPOMI SIF values are from April 2018 to March 2020.
Figure S13. Comparisons between nadir SIF simulated by SCOPE with the new spectral distribution function for SIF emission (blue solid lines), simulated by SCOPE with the old spectral distribution function for SIF emission (grey dotted lines), simulated by CLM5SP-exp1 (red dash-dotted line), observed from tower (green dashed lines) and observed from satellites (asterisks) at a) Pace Forest, b) Harvard Forest, c) US-NR1, d) US-NE3, and e) BR-Sa1.
Figure S14. Seasonal variations (average of 2008–2014) of SIF observed by GOME-2 (blue solid line), simulated by CLM5SP-exp1 (orange dashed line), simulated by CLM5BGC-exp1 SIF (green dash-dotted line), and simulated by CLM5SP-exp5 (purple dotted line) for boreal needleleaf evergreen tree (location indicated in Fig. 6f).

Figure S15. Seasonal variations (average of 2008–2014) of LAI from MODIS product (blue solid line), prescribed for CLM5SP-exp1 (red dashed line), and simulated by CLM5BGC-exp1 (green dash-dotted line) for a) needleleaf evergreen boreal, and b) crop in the United States.
| Site name | Latitude | Longitude | Start year | End year | mean PAR/SR | DOI          |
|-----------|----------|-----------|------------|----------|-------------|--------------|
| AR-TF1    | -54.9733 | -66.7335  | 2016       | 2018     | 0.469656    | 10.17190/AMF/1543389 |
| CA-CF2    | 58.6658  | -93.83    | 2008       | 2011     | 0.505076    | 10.17190/AMF/1634879 |
| CA-Ca1    | 49.8673  | -125.334  | 1996       | 2010     | 0.422588    | 10.17190/AMF/1480300 |
| CA-Ca3    | 49.8705  | -125.291  | 1999       | 2010     | 0.418955    | 10.17190/AMF/1480302 |
| CA-LP1    | 55.11194 | -122.841  | 2007       | 2016     | 0.423894    | 10.17190/AMF/1660337 |
| CA-Obs    | 53.98717 | -105.118  | 1997       | 2010     | 0.440207    | 10.17190/AMF/1375198 |
| MX-Aog    | 26.99683 | -108.789  | 2015       | 2018     | 0.437952    | 10.17190/AMF/1756414 |
| MX-PMm    | 20.84617 | -86.8992  | 2017       | 2018     | 0.420761    | 10.17190/AMF/1756415 |
| PE-QFR    | -3.83444 | -73.319   | 2013       | 2016     | 0.426774    | 10.17190/AMF/1756433 |
| US-A10    | 71.3242  | -156.615  | 2011       | 2019     | 0.472556    | 10.17190/AMF/1498753 |
| US-An1    | 68.99    | -150.28   | 2008       | 2019     | 0.394907    | 10.17190/AMF/1246142 |
| US-BZF    | 64.70373 | -148.313  | 2013       | 2016     | 0.426774    | 10.17190/AMF/1756433 |
| US-Bo1    | 40.0062  | -88.2904  | 1996       | 2008     | 0.407699    | 10.17190/AMF/1246036 |
| US-Hn2    | 46.68866 | -119.464  | 2015       | 2018     | 0.433935    | 10.17190/AMF/1562389 |
| US-Ho1    | 45.2041  | -68.7402  | 1996       | 2018     | 0.459791    | 10.17190/AMF/1246061 |
| US-Mpj    | 34.4385  | -106.238  | 2008       | 2019     | 0.412291    | 10.17190/AMF/1246123 |
| US-NR1    | 40.0329  | -105.546  | 1998       | 2020     | 0.407762    | 10.17190/AMF/1246088 |
| US-Ne2    | 41.16487 | -96.4701  | 2001       | 2019     | 0.428731    | 10.17190/AMF/1246085 |
| US-Ro1    | 44.7143  | -93.0898  | 2004       | 2016     | 0.439374    | 10.17190/AMF/1246092 |
| US-SR1    | 31.78938 | -110.828  | 2008       | 2020     | 0.411883    | 10.17190/AMF/1246154 |
| US-Tw1    | 38.1074  | -121.647  | 2011       | 2020     | 0.420457    | 10.17190/AMF/1246147 |
| US-Vcs    | 35.9193  | -106.614  | 2016       | 2019     | 0.443394    | 10.17190/AMF/1416861 |
| US-xBN    | 65.15401 | -147.503  | 2017       | 2020     | 0.452766    | 10.17190/AMF/1617727 |
| US-xDJ    | 63.88112 | -145.751  | 2017       | 2020     | 0.446562    | 10.17190/AMF/1634884 |
| US-xML    | 37.37828 | -80.5248  | 2017       | 2020     | 0.438178    | 10.17190/AMF/1671897 |
| US-xNQ    | 40.17759 | -112.452  | 2017       | 2020     | 0.424364    | 10.17190/AMF/1617733 |
| US-xSB    | 29.68927 | -81.9934  | 2017       | 2020     | 0.441938    | 10.17190/AMF/1671899 |
| US-xTR    | 45.49369 | -89.5857  | 2017       | 2020     | 0.439434    | 10.17190/AMF/1634886 |
| US-xUK    | 39.04043 | -95.1922  | 2017       | 2020     | 0.443933    | 10.17190/AMF/1617740 |
| US-xUN    | 46.23388 | -89.5373  | 2017       | 2020     | 0.449242    | 10.17190/AMF/1617741 |
| US-xWD    | 47.12823 | -99.2414  | 2017       | 2020     | 0.446499    | 10.17190/AMF/1579724 |
Table S2. Variation ranges of SCOPE input parameters for evaluation of the escape probability method. The parameters were selected based on sensitivity analysis (Verrelst et al., 2015), and the variation range of the parameters are determined based on published datasets and expert knowledge (Féret et al., 2008).

| Input       | Interpretation                                      | Unit     | Range               |
|-------------|-----------------------------------------------------|----------|---------------------|
| N           | Leaf mesophyll structural parameter                 | –        | 1–3                 |
| Cw          | Leaf water equivalent layer                          | cm       | 0–0.0713            |
| Cdm         | Leaf dry matter content g·cm⁻²                       | g·cm⁻²   | 0–0.0331            |
| Cab         | Leaf chlorophyll content µg·cm⁻²                     | µg·cm⁻²  | 5–100               |
| LIDFa, LIDFb| Leaf inclination distribution function parameters    | –        | -1–1 with constrain of | [LIDFa]+[LIDFb] ≤1 |
| LAI         | Leaf area index m²·m⁻²                               | m²·m⁻²   | 0.2–7               |
| hc          | Canopy height m                                      | m        | 0.1–30              |
| SZA         | Solar zenith angle degree                            | degree   | 0–70                |
| Vcmo        | Maximum carboxylation capacity (at optimum temperature) fluorescence quantum | µmol·m⁻²·s⁻¹ | 0–200 |
| fqe         | fluorescence quantum yield efficiency at photosystem level | –     | 0–0.04              |
| Type        | Photochemical Pathway                                | –        | 0, 1                |
| Rin         | Broadband incoming shortwave radiation (0.4-2.5 um)  | W·m⁻²    | 0–1200              |
| spectrum    | Type of soil reflectance spectrum                    | –        | 1, 2, 3             |
| Atmos_file  | File defining atmospheric radiation conditions       | –        | FLEX-S3.Std.atm, FLEX-S3.V05.atm, FLEX-S3.V80.atm, FLEX-S3.Dry.atm, FLEX-S3.Wet.atm, FLEX-S3.H0000.atm, FLEX-S3.H1200.atm, FLEX-S3.Mar.atm, FLEX-S3.Urb.atm, FLEX-S3.Trop.atm, FLEX-S3.Wint.atm |
Table S3. Parameters used for site-level SCOPE simulations

| Site                               | Chlorophyll content (µg·cm\(^{-2}\)) | Vcmo (µmol·m\(^{-2}·s\(^{-1}\)) | LIDFa   | Clumping index |
|------------------------------------|---------------------------------------|---------------------------------|---------|----------------|
| Virginia Forest Research Facility (Pace Forest) | 40                                    | 58                             | -0.1732 | 0.71           |
| Harvard Forest (Barn)              | 40                                    | 58                             | -0.1732 | 0.71           |
| US-NR1                             | 25                                    | 30                             | -0.4021 | 0.53           |
| US-NE3                             | 40                                    | 100                            | -0.672  | 0.75           |
| BR-Sa1                             | 40                                    | 41                             | -0.3189 | 0.70           |