

Supplement to:  
PhotoSpec: A New Instrument to Measure Spatially  
Distributed Red and Far-Red Solar-Induced Chlorophyll  
Fluorescence

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1 **S1. Theory**

2 This section explains the derivation of Equation 2 from Section 2 (*Theory*),  
 3 Equation 6 from Section 2.1.1 (*Linearized retrieval in an ideal case*), and Equa-  
 4 tion 9 and 10 from Section 2.2.1 (*Detector nonlinearity*).

5 *S1.1. Derivation of Equation 2*

6 The change in optical density due to the additive emission by SIF can be de-  
 7 rived as follows:

$$\begin{aligned}
 \ln\left(\frac{I^C}{I_0^C}\right) &= \ln\left(\frac{a^C \cdot I + I_{\text{SIF}}}{a^C \cdot I_0 + I_{\text{SIF}}}\right) \\
 &= \ln(a^C \cdot I) + \ln\left(1 + \frac{I_{\text{SIF}}}{a^C \cdot I}\right) - \ln(a^C \cdot I_0) \\
 &\quad - \ln\left(1 + \frac{I_{\text{SIF}}}{a^C \cdot I_0}\right), \quad \text{with } \ln(1+x) \approx x \\
 &\approx \ln\left(\frac{I}{I_0}\right) + \frac{I_{\text{SIF}}}{a^C \cdot I} - \frac{I_{\text{SIF}}}{a^C \cdot I_0} \\
 &= \ln\left(\frac{I}{I_0}\right) + \frac{I_{\text{SIF}}}{a^C \cdot I_0} \cdot \left(\frac{I_0}{I} - 1\right) \\
 &\quad \text{with } \ln(1+x) \approx x \quad \text{and} \quad x = I_0/I - 1 \\
 &\approx \ln\left(\frac{I}{I_0}\right) + \frac{I_{\text{SIF}}}{a^C \cdot I_0} \cdot \ln\left(\frac{I_0}{I}\right) \\
 &= \ln\left(\frac{I}{I_0}\right) \cdot \left(1 - \frac{I_{\text{SIF}}}{a^C \cdot I_0}\right).
 \end{aligned} \tag{S1}$$

8 *S1.2. Derivation of Equation 6*

9 The linearization follows the general approach common for trace gas retrievals  
 10 in solar spectra, i.e., it is performed on the natural logarithm of the intensities  
 11 using a Taylor series of the logarithm with  $O(x^2)$  representing higher orders of

12 this approximation:

$$\begin{aligned}
\ln(I^C(\lambda)) &= \ln(a^C(\lambda) \cdot I(\lambda) + I_{\text{SIF}}(\lambda)) \\
&= \ln(a^C(\lambda) \cdot I(\lambda)) + \ln\left(1 + \frac{I_{\text{SIF}}(\lambda)}{a^C(\lambda) \cdot I(\lambda)}\right) \\
&\quad \text{with } \ln(1 + x) \approx x + \mathcal{O}(x^2) \\
&\approx \ln(a^C(\lambda) \cdot I(\lambda)) + \frac{I_{\text{SIF}}(\lambda)}{a^C(\lambda) \cdot I(\lambda)} \quad \text{with } I^C(\lambda) \approx a^C(\lambda) \cdot I(\lambda) \\
&\approx \ln(I^D(\lambda)) + \ln\left(\frac{a^C(\lambda)}{a^D(\lambda)}\right) + \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}.
\end{aligned} \tag{S2}$$

13 Equation S2 includes two approximations which need to be discussed in more  
14 detail. The first is the approximation of the logarithm. We can use the second  
15 term of the Taylor expansion of  $\ln(1 + x) = x - x^2/2 + \mathcal{O}(x^3)$  as the error of  
16 this approximation. Typical values of  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$  in the far-red wavelength range are  
17 0 - 0.03. Consequently, this approximation leads to a positive bias in  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$  of  
18 0 -  $4.5 \cdot 10^{-4}$  or, expressed in relative terms, it imposes a positive relative bias  
19 of 0 - 1.5% on  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$ . The situation is, however, different in the red wavelength  
20 range where  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$  can be 0 - 0.3, due to the much lower canopy reflectivity in this  
21 wavelength range. The positive bias can thus be up to 10 times higher, introducing  
22 considerable errors in the retrieval. We will present a solution to this problem in  
23 Section 2.1.2 in the manuscript.

24 The second approximation is  $I^C(\lambda) \approx a^C \cdot I(\lambda)$ . We can rewrite the following  
25 term of this approximation using a Taylor expansion to quantify this error:

$$\begin{aligned}
\frac{I_{\text{SIF}}(\lambda)}{a^C \cdot I(\lambda)} &= \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda) - I_{\text{SIF}}(\lambda)} \\
&= \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)} \cdot \left( \frac{1}{1 - \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}} \right) \quad \text{with} \quad \frac{1}{1 - x} = 1 + x + x^2 + \dots \tag{S3} \\
&= \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)} \cdot \left( 1 + \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)} + \left( \frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)} \right)^2 + \dots \right).
\end{aligned}$$

26 The error is thus approximately  $\left(\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}\right)^2$ . For typical values of  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$  of 0 - 3%,  
27 this approximation leads to a negative bias in  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$  of 0 -  $9 \cdot 10^{-4}$ , i.e., it imposes  
28 a negative bias of 0 - 3% on  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$ . As in the first approximation, the larger  $\frac{I_{\text{SIF}}(\lambda)}{I^C(\lambda)}$   
29 in the red wavelength range again leads to a much higher bias. It is interesting

30 to note that the two approximations are of opposite sign and thus partly cancel  
 31 each other. Combining both approximations leads to a negative bias in  $\frac{I_{\text{SIF}}(\lambda)}{I^{\text{D}}(\lambda)}$  of 0 -  
 32  $4.5 \cdot 10^{-4}$  or, expressed in relative terms, it imposes a positive bias of 0 - 1.5% on  
 33  $\frac{I_{\text{SIF}}(\lambda)}{I^{\text{D}}(\lambda)}$ , in the far-red wavelength range. As with the first approximation, the bias in  
 34 the red wavelength range is considerably higher, i.e. 0 - 15% on  $\frac{I_{\text{SIF}}(\lambda)}{I^{\text{D}}(\lambda)}$ .

### 35 S1.3. Derivation of Equation 9

36 Using the definitions introduced in Equation 8 of the manuscript, we can de-  
 37 fine the optical depth of the Fraunhofer band as:

$$\begin{aligned}
 \ln\left(\frac{I}{I_0}\right) &= \ln\left(\frac{d_1 \cdot F \cdot L_0 + d_2 \cdot F^2 \cdot L_0^2}{d_1 \cdot L_0 + d_2 \cdot L_0^2}\right) \quad \text{with } F = \frac{L}{L_0} \\
 &= \ln(d_1 \cdot F \cdot L_0) + \ln\left(1 + \frac{d_2 \cdot F^2 \cdot L_0^2}{d_1 \cdot F \cdot L_0}\right) - \ln(d_1 \cdot L_0) \\
 &\quad + \ln\left(1 + \frac{d_2 \cdot L_0^2}{d_1 \cdot L_0}\right) \quad \text{with } \frac{d_2}{d_1} \text{ small} \\
 &\approx \ln(F) + \frac{d_2}{d_1} \cdot F \cdot L_0 - \frac{d_2}{d_1} \cdot L_0 \\
 &= \ln(F) + \frac{d_2}{d_1} \cdot L_0 \cdot (F - 1) \quad \text{with } \text{NL} = \frac{d_2 \cdot L_0^2}{d_1 \cdot L_0} = \frac{d_2}{d_1} \cdot L_0 \\
 &= \ln(F) - \text{NL} \cdot (1 - F).
 \end{aligned} \tag{S4}$$

38 NL is the relative nonlinearity which determines the deviation based on the lin-  
 39 earity from the ratio of the quadratic and linear terms.

### 40 S1.4. Derivation of Equation 10

$$\begin{aligned}
 \ln\left(\frac{I + I_{\text{SIF}}}{I_0 + I_{\text{SIF}}}\right) &= \ln\left(\frac{I}{I_0}\right) \left(1 - \frac{I_{\text{SIF}}}{I_0}\right) \\
 &= \ln(F) - \ln(F) \cdot \frac{I_{\text{SIF}}}{I_0} \\
 &\approx \ln(F) - (1 - F) \cdot \frac{I_{\text{SIF}}}{I_0}.
 \end{aligned} \tag{S5}$$

41 **S2. Radiometric calibration**

42 The radiometric calibration is different for each PhotoSpec system and for  
43 each field site. Thus, the radiometric calibration has to be performed for each  
44 instrument and at each field site. The radiometric calibration measurements are  
45 preferably made around noon and when it is cloud-free for at least 15-30 minutes.  
46 The calibrated spectrometer and the PhotoSpec system are temporally synced and  
47 record spectra simultaneously. Figure S1 shows an example of the calibration  
48 results for the field site at Niwot Ridge, Colorado on 10/17/2017. The SIF calibration  
49 factor is the average value of this calibration factor in the SIF retrieval  
50 wavelength range for the red (680 - 686 nm) and far-red (745 - 758 nm) wave-  
51 length range.

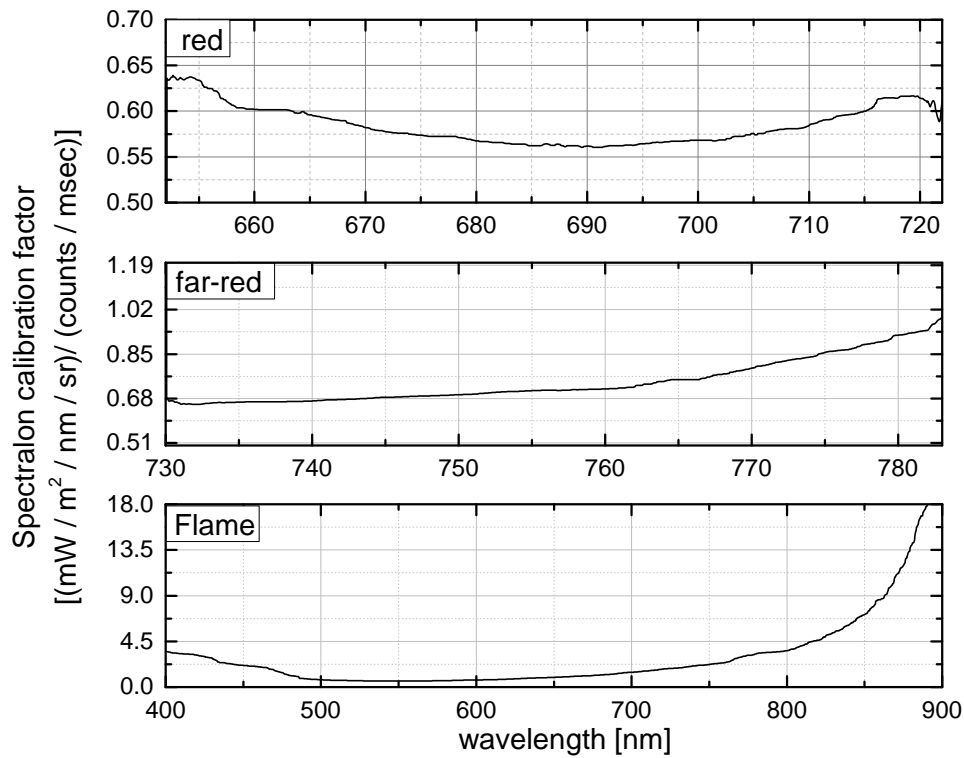


Figure S1: Spectralon calibration factors for the three PhotoSpec spectrometers for the field site at Niwot Ridge, Colorado recorded on 10/17/2017.

52 Figure S2 shows the radiances of a soil and pine tree spectrum recorded with

53 the PhotoSpec Flame spectrometer and calibrated with the calibration factor from  
54 Figure S1.

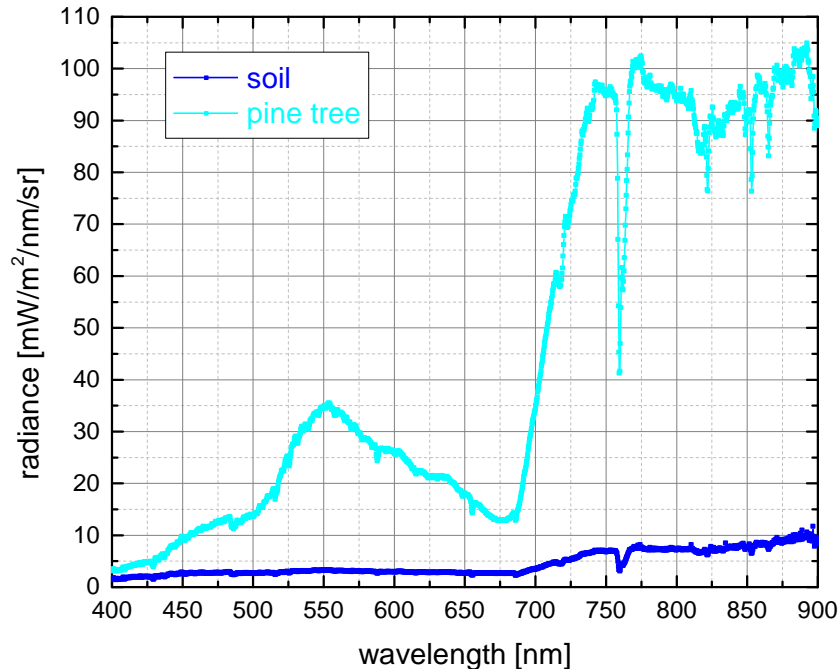


Figure S2: Flame radiances of a soil and pine tree target at Niwot Ridge, Colorado on 6/26/2017 calculated using the calibration factors from Figure S1.

### 55 S3. PAM measurements

56 The SIF measurements on the roof of the UCLA Math Sciences building were  
57 compared to field observations using a portable chlorophyll fluorometer (PAM-  
58 2500, Heinz Walz GmbH, Effeltrich, Germany) to link the SIF signal to fluores-  
59 cence yields ( $F_t$  and  $F_m$  from PAM). Leaf scale measurements of fluorescence  
60 have been carried out for decades using pulse amplitude modulation (PAM) fluo-  
61 rometers (e.g., Genty et al., 1989; Krause and Weis, 1991; Pfündel, 1998; Baker,  
62 2008; Porcar-Castell et al., 2014) to simultaneously measure chlorophyll fluores-  
63 cence and photosynthetic  $\text{CO}_2$  uptake of individual leaves (e.g., Flexas et al., 1999;  
64 Rascher et al., 2000; Magney et al., 2017). The pulse amplitude-modulated (PAM)

65 technique is an active technique that involves the use of a measuring light and a  
66 saturating light pulse with a leaf clip holder (Schreiber et al., 1986; Bilger et al.,  
67 1995; Schreiber, 2004). The PAM-2500 fluorometer (<http://www.walz.com>) is  
68 mainly used for measurements of the effective quantum yield ( $dF/F'_m$ ) of pho-  
69 tosystem II (PS II) under ambient light conditions and for measurements of the  
70 potential quantum yield ( $F_V/F_m$ ) of dark-adapted samples (Rascher et al., 2000).  
71 The PAM technique is restricted to the leaf level and cannot be applied to the  
72 canopy and landscape levels. The sample leaf was attached to a mount to avoid  
73 movements of the leaf, for example due to wind. The leaf was oriented in the  
74 horizontal direction in order to minimize shading. The PAM-2500 leaf clip was  
75 attached to one side of the leaf, next to, but outside, of the spot covered by the  
76 FOV of the PhotoSpec telescope. In order to measure the effective quantum yield  
77 of PSII, saturating light pulses were triggered every five minutes. The effective  
78 quantum yield of PSII was measured by the PAM-2500 fluorometer and is deter-  
79 mined according to:

$$\frac{dF}{F'_m} = \frac{F'_m - F}{F'_m}, \quad (\text{S6})$$

80 with  $F$  being the fluorescence yield of the light-adapted sample and  $F'_m$  being  
81 the maximum light-adapted fluorescence yield when a saturating light pulse is  
82 superimposed on the ambient light levels.

#### 83 **S4. Non-fluorescence targets**

84 Figure S3 shows the diurnal cycle of the SIF signal of soil as an example for  
85 a non-fluorescence target compared to a pine tree at Niwot Ridge, Colorado. The  
86 soil SIF signal varies around  $0 \text{ mW m}^{-2}\text{sr}^{-1}\text{nm}^{-1}$  with approximately  $\pm 0.03 \text{ mW}$   
87  $\text{m}^{-2}\text{sr}^{-1}\text{nm}^{-1}$ .



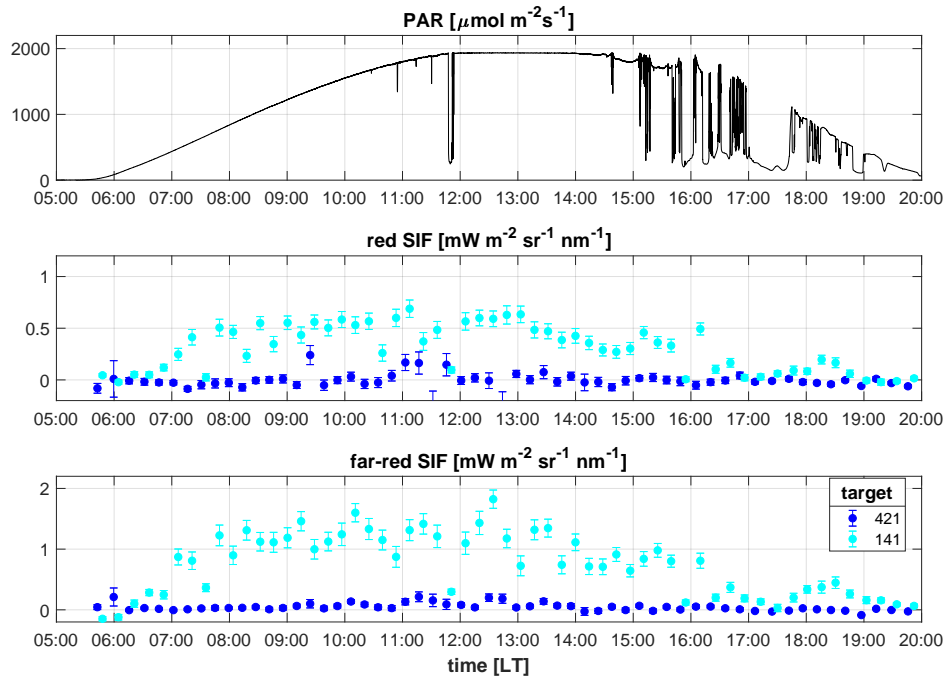


Figure S3: Diurnal cycle of (a) PAR, (b) red SIF, and (c) far-red SIF for soil (blue) and a pine tree (turquoise) observed from a 26 m tower at Niwot Ridge, Colorado on 6/26/2017.

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