

Interactive comment on “Decomposing reflectance spectra to track gross primary production in a subalpine evergreen forest” by Rui Cheng et al.

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This paper presents an exploratory study of a very nice data set studying 400-900 nm reflectance, fluorescence, and GPP along with other ancillary measurements including carotenoid composition at leaf scale at the Niwot Ridge, Colorado, USA site in a subalpine evergreen forest. As I don't believe this complement of data has been presented at such a site, the data analysis is appropriate for publication in Biogeoscience. However, there are several details that must be addressed before the paper is acceptable for publication. As the first reviewer provided a number of suggestions, this reviewer will try to present a few points not already covered there. The paper contained many small

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errors that, while minor, led to making the paper a difficult read. Hopefully this will be fixed in a revision. Otherwise I found the paper to be very informative and interesting.

Thank you very much for your generous comments. We appreciate you recognized the novelties in our work. We apologize for the confusion from mislabeled plots and complex phrases. We will answer your questions point-by-point. The corrected plots, as well as responses, will be reflected in an updated version of our manuscript.

General comments: I have two main issues with the paper. The first is that SIF contains a component of PAR while reflectance does not. This makes it a bit unfair to compare any of the reflectance- based quantities directly with GPPmax (similarly affected by PAR as is SIF) and also to derive the PLSR reconstruction of GPPmax without consideration of PAR. It may be fine to do the reconstruction of other quantities (related to pigments) without account of PAR, but generally not GPPmax. A much better result may come from normalizing GPPmax with respect to PAR (or daily averaged PAR or daily averaged potential PAR) and performing the reconstruction on this quantity. This is particularly important in Fig. 9. Some statements may need to be modified after taking into account PAR (e.g., paragraph starting on L. 320).

Thank you for pointing this out, we did not properly introduce relative SIF in the introduction. In Fig. 5(d) and Fig. 9, we accounted for the PAR impact on SIF by using relative SIF, which is SIF normalized by the reflected near-infrared radiance. In this way, relative SIF is more analogous to the SIF yield, which accounts for the incident irradiance on needles within our field of view. We will rewrite the introduction as well as methods on relative SIF to clarify this.

We agree with you that normalization is necessary. We used equation 1 to derive light use efficiency (LUE), which is conditioned on both PAR and fPAR. Benefiting from the available APAR measurements, we can use in situ APAR as the normalization

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factor instead of PAR and presumed fPAR in previous studies. According to the light response curve of photosynthesis (Fig. 2), we summarized three different scenarios LUE: 1) light-limited (low light, LUE_{lightL}); 2) carboxylation rate-limited (high light, GPP_{max}); and 3) daily average (LUE_{total}).

LUE_{lightL} is the fitted slope of GPP and APAR when PAR is between 100-500 $\mu\text{molm}^{-2}\text{s}^{-1}$. The fit was forced to go through the origin as the equation has no intercept.

LUE_{total} is the daily average of $\frac{GPP}{APAR}$ during the day.

Theoretically, we could calculate GPP_{max} similar to what we did for LUE_{lightL}, i.e. regressing GPP against APAR when PAR is saturated. Unfortunately, there is a 26-day gap in APAR measurement in the beginning of our study period. We could also normalize GPP by PAR, as you suggested. Yet, it requires assumptions about fPAR, which adds further uncertainties.

Considering GPP often asymptotes when PAR is greater than 1000 $\mu\text{molm}^{-2}\text{s}^{-1}$, the fitted slope could be biased by the spread of data points. Thus, we defined GPP_{max}, the average GPP within a moderately narrow window of PAR (1000-1500 $\mu\text{molm}^{-2}\text{s}^{-1}$), to represent the LUE when the carboxylation rate is limited. In this way, we achieved normalizing GPP without missing more data because of APAR.

Those two different definitions of GPP_{max} are significantly linearly correlated (in figure 1 in this response document). If GPP_{max} is defined as the average of normalized GPP by PAR (y-axis), the analyses on the seasonal cycle will differ little from GPP_{max} defined as mean GPP at high PAR (x-axis). Although GPP normalized PAR results

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in the correct unit of LUE, it is easily mistaken as fPAR has been considered. To avoid this confusion, we chose to use mean GPP at PAR between 1000 and 1500 $\mu\text{molm}^{-2}\text{s}^{-1}$.

We also tested the LUE defined in three scenarios: LUElightL, GPPmax, and LUEtotal for all the analyses in the manuscript. They behave similarly, and these results are included in the supplementary information. We considered that needles spent more time at highlight intensity in the daytime. Hence, we decided to use GPPmax as the only proxy of LUE in the main text. We kept the other two matrices to the supplementary. The labels were misleading in the main text. We will clean them up in the updated draft.

The second comment relates to the terminology around the component analysis. It would be helpful if the reflectance can be written in the form of equations explaining the decomposition. Then it may be more clear to express what is being plotted. In my understanding of the terminology, a coefficient should be a number multiplied by a particular spectral component to reconstruct a given spectrum. The term temporal component is confusing to me as this is not what has been decomposed, but rather it is the coefficient of a given spectral component to reconstruct a spectrum observed at a particular time if I have understood correctly. The labeling of Fig. 6 is particularly difficult to understand since panel (a) shows much more than PLSR coefficients. The line labeled GPPmax would be more clear if it had PLSR coefficient in the label.

Thank you for the advice. We will change “temporal components” to “temporal loadings”. We will add the following expression to the draft when it is updated: ICA:

$$-\log(R_{\lambda,DOY}) = \sum_i (\text{spectral component}_\lambda^i \cdot \text{temporal loading}_{DOY}^i)$$

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PLSR:

$$GPP_{max,DOY} = -\log(R_{\lambda,DOY}) \cdot PLSR \text{ coefficient}_{\lambda}$$

Specific comments: L. 118. VI's are normalized such that at least some of the solar geometry effects are removed. This may not be the case for reflectance in general.

Thank you for pointing this out. We agree the experiment related to this sentence is not enough to clarify the sun-sensor geometry impact on reflectance. Thus, we did a PLSR analysis on individual measurements of phase angle and reflectance for three summer days (2017-7-1 to 2017-7-3), such as figure 2 in this response document. The results are similar using the measurements from other days.

Indeed, the reflectance has different sensitivities not just related to phase angle. However, the poor correlation of PLSR reconstructed phase angle and the measurement suggests the variations in phase angle are not critical to account for change in reflectance. In our manuscript, we primarily removed the bi-directional impact by averaging all the individual reflectance measurements at different solar and viewing geometries over the course of a day.

L. 142. Normalized at which wavelength(s) exactly? I'm not sure I agree that normalizing by reflected radiation is going to properly "account for the complexity of signal due to canopy structure" at this particular site. Please provide more justification of this statement.

Thanks for pointing out this misleading sentence. SIF was normalized by reflected near-infrared radiation in the retrieval window (745-756nm) to account for the sunlit/shaded fraction within our FOV. Benefiting from the small FOV (0.7°) of PhotoSpec, we think the complexity of canopy structure has minimal impact on our signal.

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Since it is mentioned on L. 183 that 3 components explain more than 99.99% of variance, can you state how much variance is explained by each of the components shown.

Because ICA minimizes the dependencies of the second-order moment (variance) and higher, the randomness during the minimization makes the explained variance and order of individual components unclear (Hyvärinen and Oja, 2000). In our calculation, the ICA algorithm reduced the dimension of the input matrix by eigenvalue decomposition first, from which the first three second-order independent/orthogonal components yielded 99.99% of the variance. Then, the algorithm extracted the independent components of high-order moments from these orthogonal components.

Hyvärinen, A., Oja, E. (2000). Independent component analysis: algorithms and applications. *Neural networks*, 13(4-5), 411-430.

L. 261, it is mentioned that Tair and VPD covary with GPPmax. Please provide some numbers here such as correlations.

We will cross reference the figures in supplementary in the draft while also include the following the Pearson- r^2 value of correlations.

During the growing season:

GPPmax and VPD = 0.34,

GPPmax and Tair = 0.24,

PRI and VPD = 0.04,

PRI and Tair = 0.02,

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Tair and VPD = 0.77.

The similar Pearson- r^2 values from the correlations with VPD and Tair are due to the dependence of VPD on Tair in the growing season.

I am confused as to what is meant by “short-term” on line 262 as a few lines above it is said to be the smoothest. Some may take short-term to mean daily. In that case, we wouldn’t expect it to be smooth.

Thanks for the feedback. We meant to use “short-term” and smoothness to refer to day-to-day or sub-seasonal variations. We will revise the paragraph with a consistent description in the updated manuscript.

Have you definitively shown here that the green band captures variations in LUE? Isn’t this only inferred?

Yes, we inferred the green band captured LUE (due to changes in carotenoid pigments which change absorption in the green band) by the strong performance of GCC. We will change the word “show” to “suggest”.

Fig. 5, something appears incorrect with the r^2 value shown in panel (f).

We found a bug in the calculation and corrected it. The correct r^2 values of GPPmax with CCI, PRI, GCC, relative SIF, NDVI, and NIRv are 0.85, 0.81, 0.73, 0.87, 0.06, and 0.40, respectively.

L. 319, What exactly is meant by diurnal? The most common use of this word in my field pertains to “of or during the day” which is commonly taken to mean sub-daily.

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Yes, it means day-to-day/subseasonal variations here, similar to the previous comment. We will replace "diurnal" with "sub-seasonal" and make sure the wording is accurate and consistent.

Same paragraph: In this work, it is not definitively shown that SIF tracks seasonal or diurnal variations better than reflectance. While SIF shows slightly higher r^2 , the differences were not shown to be statistically significant. It is curious that CCI gives a higher r^2 value with respect to GPPmax than the PLSR analysis and the PRI gives the same value as PLSR. Also the sample of points looks different in Figs. 5 and 6.

Thanks for the suggestion. The phrase appears to make readers think we are competing with existing methods, which is misleading. Our goal focuses on mechanistically explaining where, when, and why certain wavelength regions are sensitive to canopy LUE seasonality. Thus, a similar performance from CCI and PLSR is expected as CCI uses the most sensitive band. Although SIF represents a different process from the reflectance-based methods the good performance of relative SIF has been discussed in Magney et al., 2019, which makes Niwot Ridge an interesting site to study.

After we corrected the calculation, relative SIF and PLSR ($r^2 = 0.87$) have the highest r^2 compared to other indices, although not significantly. The difference in figs. 5 and 6 was because we only plotted the observed GPPmax when the reflectance is also available in fig 6, while all the observed GPPmax was plotted in fig 5. In the revised draft, these two plots will only have the scatter plotted when both GPPmax and reflectance are available.

Fig. 9: There is no goodness of fit metric here relative to measurement uncertainties. To make it more clear the fits should be shown with the observations and the residuals and fit properly evaluated with standard metrics. Otherwise the differences are not convincing.

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Thank you for the suggestion. We attached a plot of individual fittings and their evaluations (figure 3 in this response document). The fitted curve has been expressed as the derivation in Appendix D. The pearson- r^2 and p values listed in each subplot were calculated from the correlation of observed and fitted variables. The residual was calculated as the average L2 norm of the difference between observed and fitted variables normalized by the observation, such as $\frac{1}{n} \sum_i (\frac{x-\hat{x}}{x})^2$. Because the ICA component lacks a clear sigmoid shape due, ICA has a larger residual.

L. 334, I may have missed something but I didn't see how this feature was shown to be directly related to LUE in the paper. This may be inferred but it wasn't directly shown.

We will be more precise in phrasing. The sentence will be changed to “The main spectral feature centered around 530 nm is most important for *infering* the seasonal cycle of reflectance (400 – 900 nm) and GPPmax, which corresponds to changes in carotenoid content.”

Detailed comments: There are a number of typos that need to be fixed, for example subscripts (L. 1, L. 226, L. 234, Fig. 3, Fig. 6 panel (b)).

Thanks a lot for pointing out the errors. We will correct the typos and make sure all the subscripts are coded correctly.

There are a number of statements that need to be clarified or corrected for language (see L. 2, for example, “Estimating . . . is a primary uncertainty” would be better phrased as “Estimation of...corresponds to a primary source of uncertainty” or similar). See also lines 11-12 (unclear sentence, L. 14, etc.).

We will rephrase those unclear sentences and be more precise.

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Line 21: Satellites do not measure GPP, rather GPP can be inferred and usually make use of other data.

We will be more precise in the updated draft.

It's a little confusing in L. 159 to start with "To implement Eq. (1), then define a particular case for Eq. 1. Please rephrase.

We are going to rephrase the sentence as "We followed the format of Eq. (1) to define light-limited LUE (LUE_{lightL}) as..." This paragraph will also be rephrased to make it more clear that LUE_{lightL} and LUE_{total} will be presented in supplementary instead of main text.

L. 164-166. It's not clear at this point what the meteorological data are included for. L. 165 would be more clear to say that daily mean . . . were computed from . . .

We will replace "meteorological variables" with "Air Temperature (T_{air}) and Vapor Pressure Deficit (VPD)" in L148. And, rephrase L164-166 as daily T_{air} and VPD were computed from averaging half-hourly T_{air} and VPD when..."

The first reviewer was unclear about what LUEs/GPP_{max} is. I think I figured it out but it took a lot of time and was very unclear.

Thanks for taking the time to sort it out. We apologize for the confusion. In the updated draft, we will clarify the usage of acronym LUE and be consistent with GPP_{max} as the only proxy for LUE in the main text. We did this to avoid confusion by presenting too many 'proxies' for canopy photosynthesis. The results for LUE_{lightL} and LUE_{total} will be put in the supplementary.

Line 217. Is LUE_{light} the same as LUE_{lightL} defined above?

Yes. Sorry about the typo.

L. 226: Confusion regarding Fig. 3 (not S3) but also most of which is repeated in Fig. S2 but with the lines that are referred to in Fig. 3. Suggest to include only one figure with all the lines (in the main manuscript). A similar thing happens with Fig. 9 and D1. Suggest to include only one of these.

We will only include Fig. 3 and Fig. 9 in the main draft, and eliminate Fig. S2 and Fig. D1.

Fig. 3: Specify that these are daily-averaged quantities?

We will specify them in both the text and captions.

Fig. 4 caption: Only the 2nd component shows the carotenoid Jacobian.

Yes, because we want to emphasize the similarity of component 1 with the chlorophyll jacobian only. We will correct the caption in Fig. 4 and make sure it is consistent with the plot.

Sect. 3.2, first par. There is a lot of information in this paragraph. It might be more effective if it was split up.

Yes, we agree with you that is too tedious to read. We will split it into paragraphs and rephrase with the equations of ICA so that it is more clear.

L. 268, the word “thus” here is confusing.

We will remove “thus” from the sentence.

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Fig. 6: Panel (a) labeling is very confusing. First, the title of panel (a) as well as the label on right side is confusing as these are not really coefficients are they, they are either components of combinations of components (caption is also unclear)? The caption states that the overlaid solid line is the 2nd ICA component, but there are two solid lines. The blue line in the legend is labeled as GPPmax, but it isn't really GPPmax as labeled in the bottom. Would suggest to just remove the titles of both panels.

Thank you for pointing this out. In Fig. 6(a), we will change the label of "GPPmax" to "PLSR coefficient of GPPmax". The blue curve indeed is the coefficient when the PLSR is written in a fashion of linear model, such as:

$$GPP_{max,DOY} = -\log(R_{\lambda,DOY}) \cdot PLSR\ coefficient_{\lambda}$$

However, the y-axis on the right is only for PLSR coefficient not for ICA. We will clarify that both Jacobians and ICA component were scaled in this plot.

The solid blue line is the PLSR coefficient. The solid orange line is the 2nd ICA component. We will clarify them in the revised draft. The titles will also be removed.

L. 297 should be "support".

We will correct it.

It would be better to subscript the small letters in Cchl, Ccar, and Cant.

We will subscript them in the revision

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Fig. B1 caption should say theoretical maximum (or clear sky)

We will change it to “theoretical maximum” in the revision.

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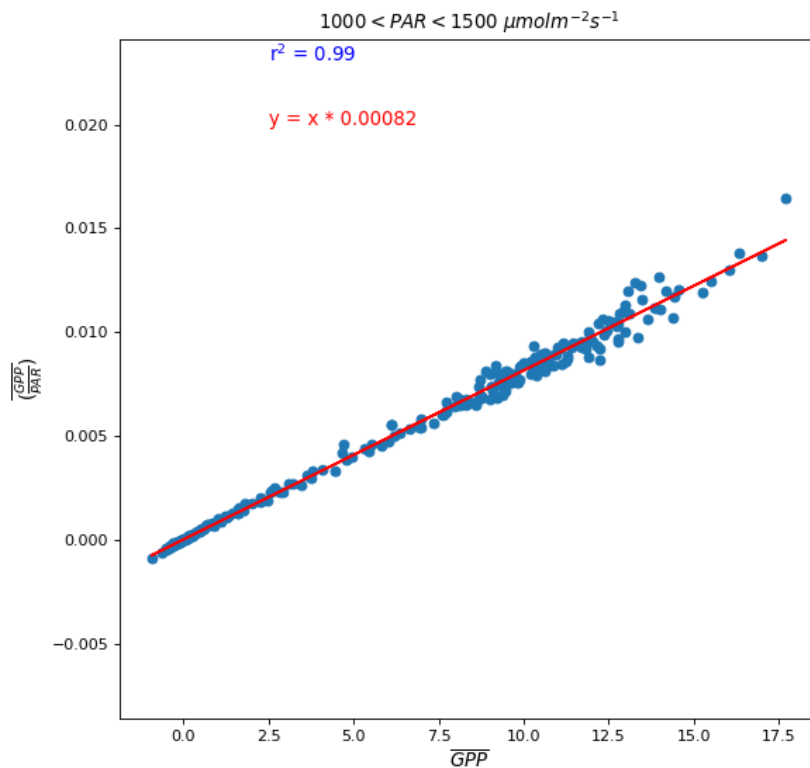


Fig. 1. Two ways to calculate GPPmax.

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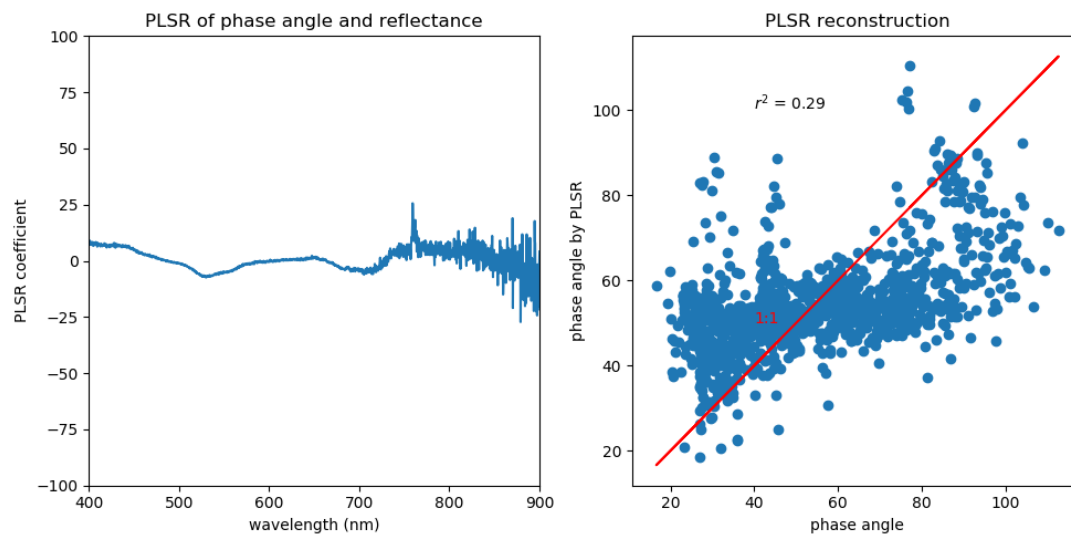


Fig. 2. PLSR analysis on phase angle and reflectance.

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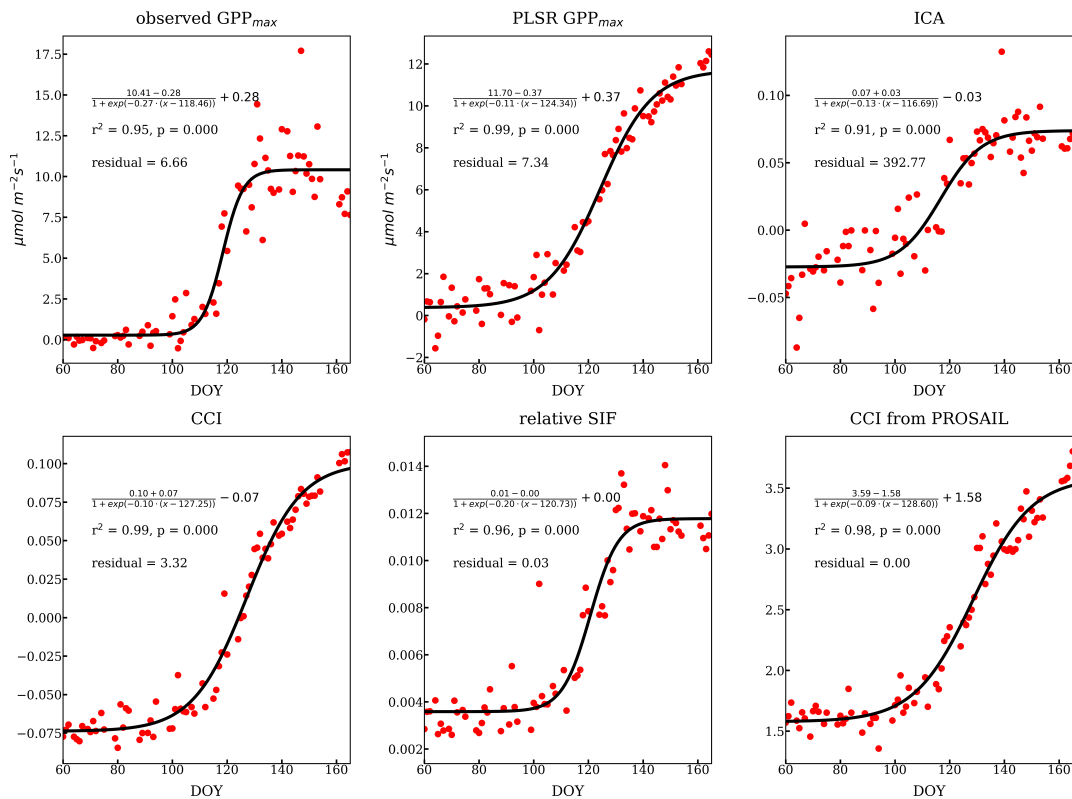


Fig. 3. Individual sigmoid fits of timeseries of interest. The fitted curve are expressed in the format as appendix D. The pearson- r^2 and p values are for the observed and fitted variables.