Response to Reviewer and Short Comments:

We thank Professor Luis Guanter, the Anonymous Reviewer, and Mr. Paolo Tasseron for their time and constructive comments on our manuscript.

Reviewer #1 (Professor Luis Guanter) Comments:

The manuscript is very well written and presented, methods and data are innovative and the results are interesting, so I recommend it for publication in Biogeosciences. Before that, however, I would appreciate if the authors could address the following two points in their revision of the manuscript:

We thank Professor Guanter for his feedback and comments on the work.

General Comments

1.) Double peak, PAR and/or physiology? The authors acknowledge that the different seasonality in SIF and vegetation indices may be due to a clear-sky bias in the vegetation indices, but also claim that *"SIF can detect the downregulation of photosynthesis even when plants appear green"*, which seems to hint that it is not only the reaction to solar irradiance which makes SIF to show the double-peaked seasonality. To substantiate this claim, it would be interesting to see a plot of $NIR_v \times PAR_{ground}$ (with PAR_{ground} the at-surface PAR for all-sky conditions), and evaluate to what extent its seasonality resembles that of SIF. The difference between SIF and $NIR_v \times PAR$ could be attributed to physiological effects captured by SIF.

The line *"SIF can detect the downregulation of photosynthesis even when plants appear green"* was based on inferences from previous work, not inferred here. The abstract has been amended to highlight this.

Page 1, Line 9: *"The different seasonality in the vegetation indices may be due to a clear-sky bias in the vegetation indices, whereas previous work has shown SIF to have a low sensitivity to clouds and to detect the downregulation of photosynthesis even when plants appear green."*

We appreciate the suggestion from Professor Guanter to show $NIR_v \times PAR$, however there are some caveats with the available PAR data that make such a comparison unreliable. Specifically, there are known issues with the all-sky PAR data from ERA Interim: "https://confluence.ecmwf.int/display/CKB/ERA-Interim+known+issues" (see known issue number 2). The clear sky PAR from ERA Interim is reliable and we have applied a correction to the statewide PAR based on the reliable clear sky PAR but we are hesitant to draw any conclusions using this scaling at finer scales. In a similar vein, the Badgely *et al.*, GBC (2019) paper found that $NIR_v \times PAR$ worked well for predicting GPP at FLUXNET sites if they used measured PAR, but using global PAR datasets actually yielded worse estimates than if they did not include PAR as a predictor (personal communication with co-first author Lee Anderegg, UC Berkeley). This is because the global PAR datasets are poor. All this is to say, the PAR presented in Figure 6 is illustrative of potential reductions in PAR during May, but we are wary of using it to directly scale NIR_v and/or compare with SIF. Further study of SIF and NIR_v in other regions is obviously needed.

2.) GPP scaling - The authors scale SIF to GPP as GPP*=18.5×SIF. However, I think we know better. There have been a number of papers in the last years showing that factors such as a canopy structure, photosynthetic pathway or observation geometry affect the SIF-GPP relationship making the use of a global scaling factor to be questionable. On the other hand, this study is based on the analysis of time series and no quantification of GPP is performed, so I don't see why the authors need to scale SIF to GPP values. I would therefore recommend the authors to simply use SIF rather than both SIF and GPP* in the analysis (Figs. 6 to 8).

Our reasoning for showing GPP* is to remind the reader of the major motivation for the use of SIF: to study carbon uptake. We acknowledge the shortcomings of our SIF-GPP relationship (i.e., the lack of eddy flux sites in important ecosystems) and put an asterisk on our GPP variable to emphasize that. We feel that his is a fair representation of the caveats while also highlighting the ultimate aim of work using SIF.

Page 13, Line 23: *"To reiterate, there is a clear correspondence between the observed SIF and GPP estimated for the different AmeriFlux sites (see Fig. 5) but we have a limited number of AmeriFlux sites in California that do not cover all ecosystems. As such, we do not report GPP here and have included an asterisk to highlight the caveats with the relationship presented here. Future work to obtain a more robust SIF-GPP relationship covering more ecosystems is warranted."*

Specific Comments

1.) p1, L3: "oversampling and downscaling" –> simply "downscaling" would probably be more clear for most of the readers.

We agree, updated.

2.) p2, L3: "more direct methods" than what methods?

Thanks for catching this. Updated to the following:

Page 2, Line 3: *"As such, methods of inferring..."*

3.) p2, L24: Several SIF downscaling methods have been published in the last years which are actually not based on machine learning nor intended to produce spatially-continuous SIF data sets from OCO-2 SIF retrievals. In particular, the method by Duveiller et al. to downscale GOME-2 SIF to 0.05° (last implementation here https://www.earth-syst-sci-data-discuss.net/essd-2019-121/) could also be adapted to TROPOMI. Please, discuss pros and cons of the oversampling/downscaling method presented in this manuscript with respect to that by Duveiller et al. and any other comparable downscaling method.

We appreciate Professor Guanter pointing out the Duveiller paper, however it is still under review at ESSDD and we prefer to cite final published papers in case there are changes during the review process. Additionally, the next line in our manuscript points readers to the review paper from Mohammed et al. (2019), a review article that is 39 pages long.

Page 2, Line 25: *"Mohammed et al. (2019) presents a detailed review of different remote sensing techniques for retrieving SIF from space-borne measurements."*

4.) p4, L10: "near-infrared and shortwave infrared".

Thank you for catching this, updated.

5.) p4, L19: "The TROPOMI SIF retrieval uses..." I don't think the average reader will understand this sentence without any further introduction to PCA-based SIF retrievals.

This line was included based on feedback from Professor Dennis Baldocchi (UC Berkeley; he provided feedback on an earlier version of the manuscript). He requested more details on the remote sensing and retrieval this was our balance between brevity and an exhaustive description: providing a few important points to those who work on SIF retrievals with references for interested readers to follow.

6.) p4, L 25: I can't find any information on cloud filtering, so I assume that the authors are simply not applying any. Please, discuss this here, e.g. whether no cloud filtering could/should applied globally when using SIF as a proxy for GPP (which would be somewhat scary...).

We use the same cloud filtering as Köhler *et al*. (2018). We filter pixels with VIIRS cloud fractions larger than 0.8. Text is updated as follows:

Page 4, Line 17: *"Köhler et al. (2018) filtered out pixels with cloud fractions larger than 80% based on VIIRS observations; we use this same cloud filtering here."*

7.) Fig 8. Panel C?

The updated manuscript now includes a Panel C showing the difference between fall 2019 and fall 2018.

Reviewer #2 Comments:

This work is highly interesting and its the main contribution to the scientific community is twofold: a) they introduce novel methods of oversampling and downscaling to the SIF community which offers the exciting opportunity to analyse SIF data at unprecedented spatial resolution. They also raise awareness of possible prominent retrieval biases related to bright surfaces. b) The different dynamics between canopy greenness and photosynthetic activity and the resulting benefits of SIF in general, and of Tropomi SIF in particular, to track GPP dynamics.

However, I have two major concerns regarding the second point and main message of the paper which in my opinion are necessary to address before a publication in Biogeosciences:

We thank the Reviewer for their detailed feedback and comments on the work.

General Comments

1.) First, it is not fully clear from the work description if the comparison between greenness and SIF is meaningful: Have any filters been applied to either tower measurements, SIF or the MODIS data to remove low quality data? Also, the authors mention a clear-sky bias of the reflectance measurements as a possible explanation for the different dynamics. This implies to me that the data of VIs and SIF have not been matched in space and time before aggregating to the spatial averages shown in Fig.6. If this was indeed the case, the time series are representative of different places and therefore not fully comparable. I would like to ask the authors to clarify and if need be, to improve on this point to corroborate the main message of the paper.

Figure 2 (the scatterplot comparison) is a direct comparison between MODIS observations at the same location on the same day. This figure serves as a one-to-one comparison of the different products and the version in the supplement is expanded to include comparison with the downscaled SIF products.

For Figure 6, we interpolate the MODIS data in time for gap-filling purposes and then compute a state-wide mean. The same number of points go into the state-wide mean for both SIF and MODIS but there is more gap filling for MODIS. The statewide mean SIF and VIs represent our best attempt at producing a statewide mean for the different variables. The MODIS data will have gaps that need to be filled via interpolation during cloudy scenes, leaving only clear-sky conditions to build a state-wide mean. TROPOMI will observe more scenes with low-to-moderate cloud cover, thus potentially inducing a clear-sky bias in the inferred statewide seasonal cycle. So the point is that the inferred seasonal cycle is different when using SIF vs VIs and part of that difference is likely due to the lack of data in cloudy periods from MODIS.

Figure 2 Caption: *"Panels show a comparison of coincident measurements in both space and time."*

2.) Second, I see the explanation for the different dynamics in SIF and greenness as incomplete. The authors convincingly argue that the different phasing of activity between evergreen forests and grasses, chaparral, and oak savanna causes the double peak in SIF. However, a similar decomposition by land cover type (Fig.6a) is missing for the greenness indices and I strongly suggest to include this in the analysis (at least for one of the indices) in order to get an idea of where/ in which ecosystems SIF and greenness are particularly dissimilar (Fig.6c). Otherwise, a sentence like in the abstract that SIF 'can detect the downregulation of photosynthesis even when plants appear green' is not justified from the material presented in the paper. Finally, this analysis of where and when VIs and SIF disagree, could be completed by a driver analysis to understand which processes does SIF see that greenness does not and to undermine the argumentation in p.17 ll.15-28. There are features as those in May in both years, which coincide with similar dips in light and rain events, it is not clear which of these is more important for which ecosystem. There are other prominent features such as the smaller peak in September 2018 in SIF which does not seem to have an obvious relationship with either precipitation or light.

The line from the abstract was based on inferences from previous work and has been amended to indicate this. See, also, the response to Comment #1 from Professor Guanter. We have included the requested driver analysis for MODIS NIR_v as two additional supplemental figures (see below).

Page 1, Line 9: *"The different seasonality in the vegetation indices may be due to a clear-sky bias in the vegetation indices, whereas previous work has shown SIF to have a low sensitivity to clouds and to detect the downregulation of photosynthesis even when plants appear green."*

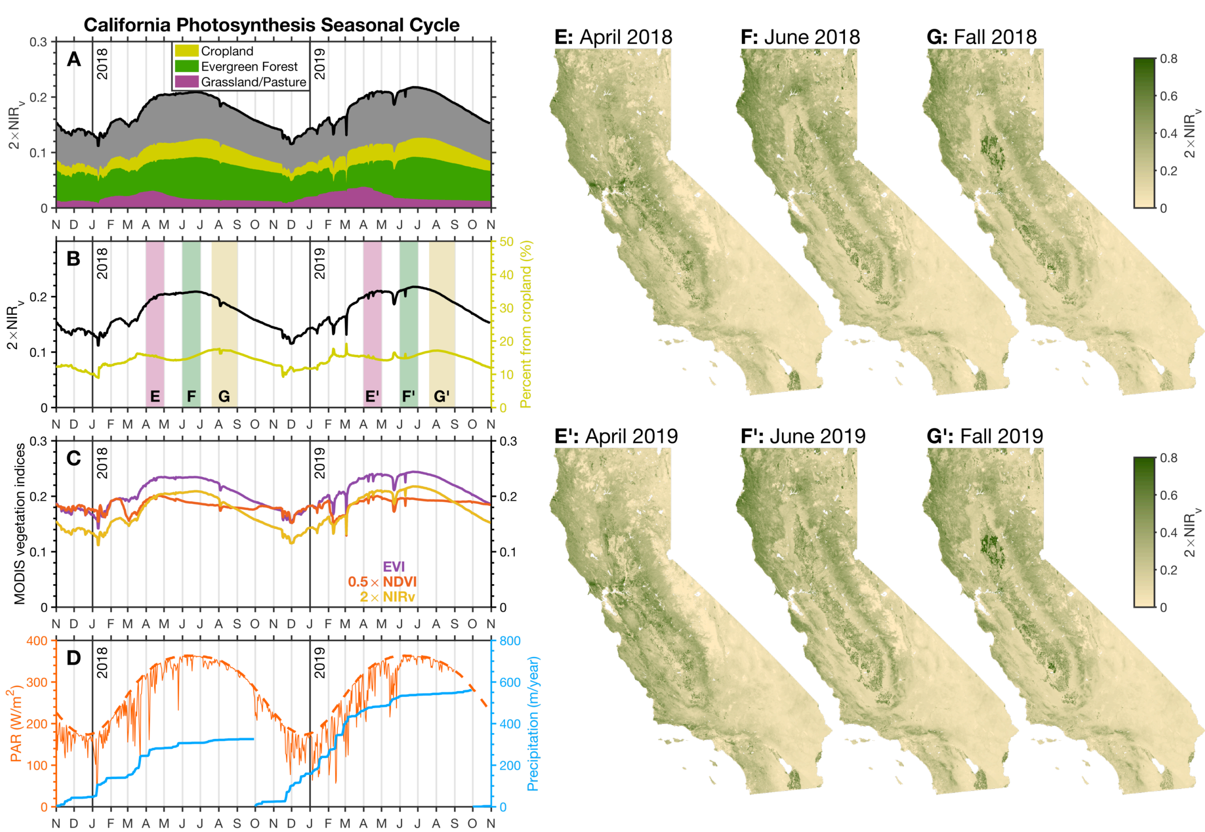


Figure S6: Same as main text Fig. 6 but for MODIS NIR_v.

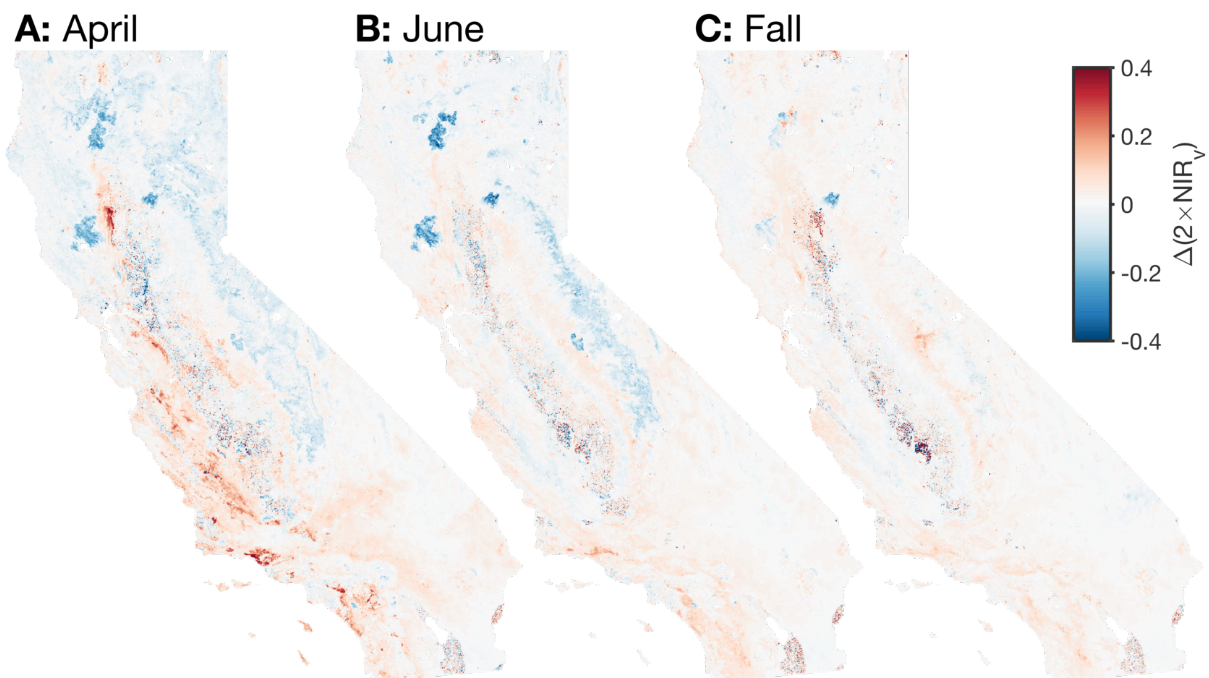


Figure S7: Same as main text Fig. 8 but for MODIS NIR_v.

Minor Comments

1.) The higher correlation between greenness and SIF at longer time scales is mentioned both in the abstract and conclusions but in the main text only in a sub-clause, and is not a main finding of your work. I see this as distracting side information as well, which does not necessarily need to be mentioned in both the abstract and the conclusions.

We disagree with the reviewer on this point. Much of the previous work comparing NIR_v and SIF was done at monthly or annual timescales and found stronger relationships (e.g., Badgely *et al.*, Science Advances 2017). As such, we do feel that it is important but there is not much additional explanation needed to understand this.

2.) Abstract: *"The different seasonality in the vegetation indices may be due to a clear- sky bias in the vegetation indices, whereas SIF has a low sensitivity to clouds and can detect the downregulation of photosynthesis even when plants appear green."* This sentence illustrates my major comment from above that the question of what drives the SIF response in the different ecosystems is not sufficiently covered by the analysis.

Updated to reflect that the latter inference was based on previous work. See response to Comment #1 from Professor Guanter and Comment #2 from Reviewer #2.

Page 1, Line 9: *"The different seasonality in the vegetation indices may be due to a clear-sky bias in the vegetation indices, whereas previous work has shown SIF to have a low sensitivity to clouds and to detect the downregulation of photosynthesis even when plants appear green."*

3.) The fact that there is a double peak in SIF but not in the VIs is mentioned twice in the conclusions.

Updated.

4.) Apart from the fact, that the scaling from SIF to GPP is not needed in this manuscript, it is rather uncommon to use the unit of mu mol/m^2/s from the tower measurements also for seasonal values as in the maps in Fig 6. gC/m^2/day is rather common.

The AmeriFlux data are provided in units of μmol/m^2/s and a number of papers use these same units. For example, the paper describing FLUXNET (Baldocchi *et al.*, 2001) uses these units for some of their figures. Magney *et al.* PNAS (2019) also used these units for some of their figures. Further, these units are useful for my own work with CO_2 flux inversions.

5.) Fig 6G' does not exist, pay attention in caption and Fig 6b.

The updated manuscript now includes Fig. 6G'.

6.) p.9 l.34: Can you really resolve daily features with an average over 14 days despite daily sampling?

We thank the review for pointing this out. We did not mean to imply that we resolve daily features, it's intended to highlight that we are **producing** our estimate every day (based on a 14-day window). Text has been updated to highlight this:

Page 9, Line 27: *"…Köhler et al. (2018) seasonal cycle is produced at weekly temporal frequency whereas we produce daily estimates using a 14-day moving window."*

7.) p.11 l.29 -p.12 l.2: To my (admittedly non-native English) ears the word 'owing' in this sentence sounds misplaced.

This is grammatically correct.

8.) Fig 6B: why is the cropland contribution stressed in this panel?

Cropland is highlighted because this is how we chose the time period for Panel G and G'.

9.) p.19 l.26: *"it seems unlikely that the grasslands and forests will exhibit opposing responses to a forcing."* It probably depends and an extended analysis as suggested above can give indications of whether this is true for California or not. There are counter examples e.g. in Flach *et al.* 2018 https://doi.org/10.5194/bg-15-6067-2018 or Walther *et al.* 2019 https://doi.org/10.1029/2018GL080535

There could certainly be a contrasting response, but it seems more likely that it falls out of the EOF requirement to compactly represent the system. From the abstract of Mohanan *et al*. (2009), a review paper on EOFs:

> "Often in the literature, EOF modes are interpreted individually, independent of other modes. In fact, it can be shown that no such attribution can generally be made. This review demonstrates that in general individual EOF modes (i) **will not correspond to individual dynamical modes**, (ii) **will not correspond to individual kinematic degrees of freedom**, (iii) **will not be statistically independent of other EOF modes**, and (iv) **will be strongly influenced by the nonlocal requirement that modes maximize variance over the entire domain**. The goal of this review is not to argue against the use of EOF analysis in meteorology and oceanography; rather, it is to demonstrate the care that must be taken in the interpretation of individual modes in order to distinguish the medium from the message."

Short Comment from Mr. Paolo Tasseron & Prof. Wouter Peters:

This review was prepared as part of graduate program course work at Wageningen University, and has been produced under supervision of Prof Wouter Peters. The review has been posted because of its good quality, and likely usefulness to the authors and editor. This review was not solicited by the journal.

…

In my opinion, the study is interesting and introduces a relevant novelty in the narrow scientific community bridging remote sensing science and photosynthesis research. However, I think three flaws are present in the current manuscript, of which I recommend some revisions before publication.

We thank Mr. Tasseron and Professor Peters for their feedback on the work. We have responded to their comments below.

General Comments

1.) To start with the first issue, on page 9 (lines 7-27) a fourteen-day moving window is used in combination with a spatial downscaling method to obtain daily estimates of SIF at a high resolution. In combination with the consequent pre-weighting of the SIF signal by the underlying vegetation fraction (MODIS NIR_v), large-scale changes in spatio-temporal patterns are conserved. On lines 20-21, the authors assume that the observed SIF from TROPOMI likely originates from more vegetated regions within that scene. However, the R^2 value of the linear correlation between SIF and NIR_v (0.52, Figure 2 on page 7) implies that a significant part of the variance in SIF cannot be explained by the underlying vegetation fraction. Besides, by using the averaged value of the 14-day moving window, a pseudo-daily average SIF value is created, rather than the actual daily value. This is fine, provided that a certain accuracy assessment is conducted. Especially because the authors mention, on page 9 lines 31-32, significant differences are found with the similar method of Köhler et al. (2018) in which a quality control and accuracy assessment are indeed present. In addition, the downscaling (from 24.5 km^2 to 0.25 km^2) is likely to introduce inaccuracies, which requires quantification.

There is an implicit physiological argument being made here. Solar induced chlorophyll fluorescence is *inherently* a signal emitted from chlorophyll. As such, one would expect that the measured SIF signal to originate from regions within a TROPOMI scene that have more vegetation and chlorophyll.

For the second part of this comment (*"the r^2 of the linear correlation between SIF and NIR_v implies a significant part of the variance in SIF cannot be explained by underlying vegetation fraction"*), the r^2 Mr. Tasseron refers to is using two years of data over the entire state. So it implies that SIF and NIR_v do observe similar (but not identical) phenomena, making it an excellent candidate for downscaling. Regarding Mr. Tasseron's criticism of our comparison with the Köhler *et al.* (2018) paper: differences are found at fine spatial scales but large-scale patterns are consistent. Finally, we point Mr. Tasseron to our response to Comment #1 from Reviewer 2 on the temporal differences.

2.) Secondly, from page 11 onwards, the authors use a method to infer GPP from SIF, based on light-use efficiency and the probability of SIF photons escaping the canopy. Interestingly, Paul-Limognes *et al.* (2018) found that SIF was more affected by environmental conditions than GPP. Midday-depressions in SIF were linked to peak VPD values following peak photosynthetic photon flux density (PPFD). Besides, Walther *et al.* (2016) state that in evergreen needle-leaf forests, the length of the photosynthetically active period indicated by SIF is up to six weeks longer and commences a month earlier than the green biomass changing period proxied by EVI. Even though the authors used NIR_v instead of EVI to downscale SIF, the different timing could significantly alter the double peak structure. Moreover, the authors state there is a lack of GPP measurements in evergreen forests, while much of California is dominated by this vegetation type (page 13, line 17-19). In combination with the a-synchronous SIF/MODIS dynamics, this will propagate into a major bias in the scaling factor of 18.5 ± 4.9 which is inferred on page 13, line 14. Therefore, I think that the equation on page 13, line 20 (*GPP* := 18.5 • *SIF*) should include a revised quantification of the error margins. In doing so, the authors should determine an alternative error margin whilst taking into account the fractional contribution of evergreen forests to GPP. The latter can best be inferred from a biosphere model or studies which used eddy-covariance measures in similar evergreen forests.

Regarding the first point that the use of MODIS vegetation indices could impact the double peak, it does not. The large-scale patterns are invariant to the choice of oversampling or downscaling. This can be clearly seen in the inset in the left column of Figure 4 where both the oversampling and downscaling result in the same 2018 seasonal cycle. The major features (i.e. the double peak) are also present in the Köhler *et al*. (2018) gridding for California. This is because the oversampling and downscaling conserve the SIF over a given TROPOMI pixel, so averaging to coarser spatial scales will yield an identical seasonal cycle. For the second point, see our response to Comment #2 from Professor Guanter.

The following text has been added:

Page 13, Line 23: *"To reiterate, there is a clear correspondence between the observed SIF and GPP estimated for the different AmeriFlux sites (see Fig. 5) but we have a limited number of AmeriFlux sites in California that do not cover all ecosystems. As such, we do not report GPP here and have included an asterisk to highlight the caveats with the relationship presented here. Future work to obtain a more robust SIF-GPP relationship covering more ecosystems is warranted."*

3.) Lastly, the authors successfully identify a double-peak in the seasonality of GPP. However, the number of (recent) references concerning underlying reasons for this double peak or other case studies in which a double peak is found, is unsatisfactory. References to Xu & Baldocchi (2003), Xu *et al.* (2004), Xu & Baldocci (2004) explain changes in carbon fluxes between ecosystems and vegetation types well, yet the link with SIF dynamics is lacking (Page 17, lines 15-22). Perhaps the following is a cause of the state-of-the-art novelty of this subject, but there are zero references made to any other recent papers discovering the double peak in GPP/SIF. Given the importance of this conclusion to the subject of the manuscript, I highly suggest investigating and mentioning recent existing literature explaining the double peak phenomenon. If the latter turns out to be infeasible because it is such a novelty, it is suggested to emphasize the scientific novelty in this paper. For instance, Li *et al.* (2014) imply that MODIS EVI is unsuitable for detecting a double peak in vegetated areas which usually manifest double peaks. This would strengthen the relevance as to why SIF needs to be used.

We do not reference other papers on this double peak because (to our knowledge) this is the first time it has been noted. This inference could have probably been made in earlier work (e.g., the papers we cite from the Baldocchi group) but, to our knowledge, it has not been investigated before. Satellite measurements of SIF are a fairly novel measurement (first global retrievals were made in 2011) and previous work using other satellites (e.g., GOME-2) has been limited to very coarse spatial resolutions. Our work is one of the first to get down to this spatial resolution that allows separating the processes driving this.

Given this, we chose the title of the paper to highlight the novelty of the finding. We also devoted two full sections of the text to discussing the processes driving this phenomenon.

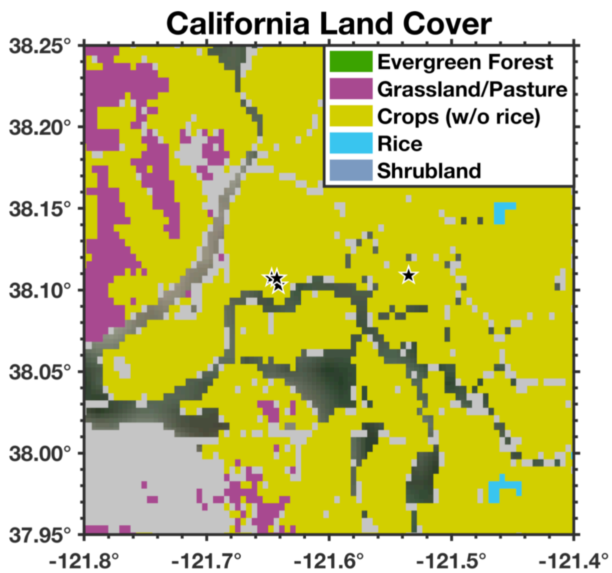
Specific Comments

1.) In Table 1, all vegetation types have two or more study sites except for the WSA (Woody Savannas). I would like to give the authors awareness that one study site might not be representative for the entire ecosystems, especially when all other vegetation types have multiple sites.

Agreed. However, there is not much we can do in response because there simply are not additional AmeriFlux sites in California. This is, again, why we include the asterisk on GPP. We have plans to extend this analysis globally to include more sites, but the focus of this study was on California.

2.) In Figure 1, Page 3: The description mentioned that black stars show the location of six Ameriflux sites, However I can only discern three and they seem to be closely packed at this resolution.

Many of the AmeriFlux sites are in close proximity to each other. For example, the US-Tw1 US-Tw3, US-Tw4, and US-Tw5 are located on the same island in the Sacramento Delta (their longitudes differ by less than 0.01° longitude). See below for a zoomed in view of the Sacramento Delta. So there are indeed 6 AmeriFlux sites plotted, some of the stars just lie on top of each other in the Figure. This is an important point for the comparison of the wetland sites, as there is still local heterogeneity observed at these eddy flux sites that sub-grid scale.



3.) In Figure 2 on page 7, the axes lack titles. This is relevant to include for the x-axes of the bottom row of graphs, as the range of the axes are different.

Axes cover the dynamic range for each product and units are included in the caption.

4.) In Figure 3 on page 8 the swath resolution is 4.0 km × 7.0 km, whereas in the text on Page 9, line 4 it is stated that this resolution is 3.5 km × 7.0 km. This should match.

The left panel is a schematic. The TROPOMI resolution at nadir is 3.5 × 7 km^2, but is larger at the edges. Supplemental Figure 1 from Köhler *et al.* (2018; see below) shows how the pixel size varies across the swath. Further, the TROPOMI team reduced the along-track integration time in August 2019 thus reducing the along-track pixel size from 7 km to 5 km. Again, this left panel referred to by Mr. Tasseron is a schematic meant to illustrate how differences in viewing geometry allow us to bisect subdivide pixels from the nominal resolution.

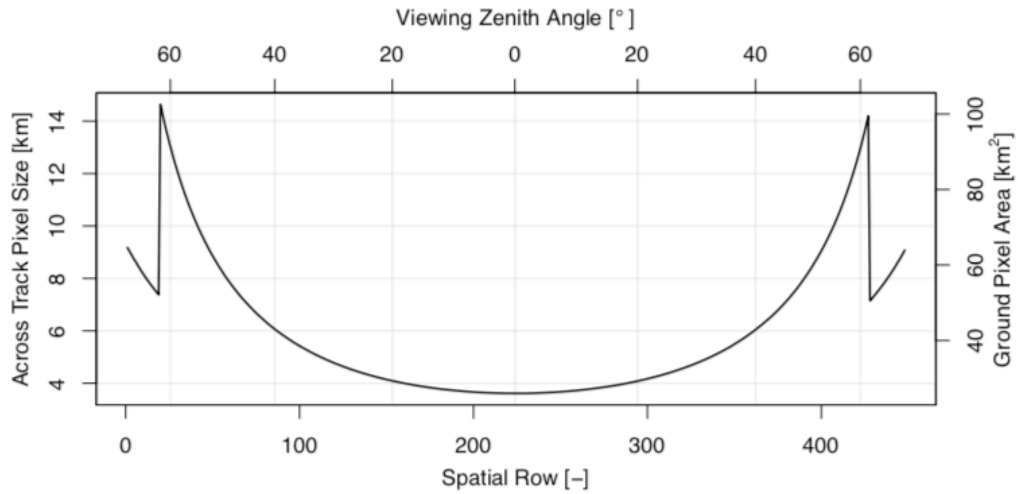


Figure S1: Across track pixel size/ground pixel area as function of spatial row/viewing zenith angle computed from soundings at the equator (same orbit as in Fig. 1).

5.) On page 9, line 19-20: perhaps it is necessary to introduce that the NIR_v was used in the pre-weighting of SIF, rather than introducing it later on Page 11, line 5.

The pre-weighting can be applied with any vegetation index, the rest of the paper simply uses NIR_v because it showed the strongest correspondence with SIF. Supplemental Figure 2 actually shows a comparison of the SIF downscaled using other MODIS vegetation indices (NDVI and EVI) as well. So we prefer to keep this expression more general here.

6.) On page 14 in the figure description, a reference to Panel G' is made, whereas this panel is not present in the accompanying figure (6).

Updated to include Panel G'.

7.) On page 16, line 8-9 it is stated that a 'reasonable consistency' is found. This should be quantified.

The figure is the quantification of the difference between the years.

8.) In the conclusion on page 20, parts of line 6-7 and line 22-23 have very similar information.

Updated.