### RC1

In the manuscript "On the impact of canopy model complexity on simulated carbon, water, and solar-induced chlorophyll fluorescence fluxes", Wang and Frankenberg examined how different representations of canopy structure in models influence the estimates of carbon, water and SIF fluxes. They used a recent version of Land model in Climate Modelling Alliance to design 5 different representations of canopies – from simple to complex, and compared their estimated fluxes at one example site. I think this work is a valuable theoretical contribution to both model and remote sensing communities. It delivers a key message that the underlying assumptions of models and remote sensing on canopy structure are often not compatible with each other, and integrating them without proper consideration canopy structural can lead to biases. I am happy to support the paper, however, there is one major concern that I hope the authors could address first.

RESPONSE: We thank reviewer 1 for the support and appreciation. We have now addressed the concerns and minor issues, and believe that the revised manuscript has been significantly improved and would benefit the land modeling community.

- I am not sure the definition of big leaf adopted by the authors is consistent with previous studies. From Sellers (Sellers et al., 1992) and De Pury and Farquhar ((De Pury and Farquhar, 1997), the big-leaf model is generally regarded as a single layer leaf without separation of sun/shaded fractions. My understanding is that once a canopy is separated into sunlit and shaded, it is regarded as a two-leaf or two-big-leaf structure.

RESPONSE: Thanks for highlighting the distinguishment among big-leaf, two-big-leaf, and two-leaf schemes, and Luo et al. (2018) provided a good overview to this. We now have these issues covered in the revision, and distinguish the models as two-leaf radiation scheme, one-big-leaf canopy model, two-big-leaf canopy model, and two-leaf canopy model throughout the main text. Changes related to this comment:

Lines 23-39 (in clean revision, hereafter): It should be noted that "big leaf model" may refer to different models within the last decades given their interchangeable uses (Luo et al., 2018). According to Luo et al. (2018), the "big leaf model" can be categorized as least as the following types given the purposes they were developed. (1) One-big-leaf canopy model that regards canopy as a single big leaf was typically used with Penman-Monteith equation (Penman, 1948; Monteith, 1965) to compute land surface evaporation in early LSMs. Sellers et al. (1992) updated the one-big-leaf model by adding an exponentially diminishing photosynthetic rate within the canopy depth to upscale photosynthesis for the carbon-water coupled LSMs. Yet, this scheme often underestimated canopy assimilation rate as the exponential function cannot properly represent the vertical light and photosynthesis profiles. (2) Two-leaf radiation scheme that separates the canopy into a group of sunlit leaves and a group of shaded leaves (Norman, 1982; De Pury and Farquhar, 1997; Campbell and Norman, 1998; Chen et al., 1999) was used to account for the horizontal and vertical light heterogeneity in the canopy. (3) Two-big-leaf canopy model combines one-big-leaf canopy model and two-leaf radiation scheme to upscale carbon and water fluxes, and treats each of the sunlit and shaded fractions as a single big leaf where leaf biochemical parameters and radiation are upscaled to canopy level (De Pury and Farquhar, 1997; Wang and Leuning, 1998). (4) Two-leaf canopy model uses two-leaf radiation scheme, and treats each of the sunlit and shaded fractions as a leaf with average traits for its representation (not integrated value as in a big leaf) (Chen et al., 1999, 2012; Sprintsin et al., 2012). Therefore, the use of term"big leaf model" needs to be cautious as it may refer to (i) two-leaf radiation scheme which is a canopy radiative transfer model or (ii) upscaling schemes which differ in the way leaf biochemical parameters are integrated (such as one-big-leaf and two-big-leaf models) or averaged (such as two-leaf canopy model).

- the author suggested that big-leaf model overestimated carbon and water fluxes, but that seems to contrast with previous studies (Sprintsin et al., 2012)(Luo et al., 2018) – sorry for self-citation - where these studies suggested that big-leaf underestimated GPP and ET. I think that's partly relevant to the different definitions of big-leaf used in the current study. One characteristic of big-leaf is that they often do not use leaf-level Vcmax. Instead they use canopy-level Vcmax (such as those introduced in Sellers and De Pury papers, or CLM4.5) – just imagine a really big-leaf with a Vcmax of up to 500 umol/m2/s (LAI X leaf-level Vcmax) and how it will never be light saturated! In this case, the Jenson's inequity is working in the opposite way that reduce GPP and ET through lower Ci/Ca and the problematic upscaling from gs to canopy conductance.

RESPONSE: We now clarify in our method section that our 1X model differs from the one-big-leaf model in that we did not integrate leaf parameters and light but used average values. So it is a one-leaf canopy model compared to the two-leaf canopy model. Because the models are different between one-leaf model and one-big leaf model, the results were not directly comparable. See the following changes made related to this comment

- Lines 145-148: Also, we note here that leaf biochemical parameters and APAR were not integrated within a canopy layer or sunlit/shaded fractions; instead, we used average APAR and leaf traits in our simulations. Thus, our "1X" model is a one-leaf model rather than a one-big-leaf model, and our "2X" model resembles the two-leaf model rather than two-big-leaf model.
  - I think the authors have done a great modelling experiment, and I agree with that multi-layer and sunlit/shaded separation is the way to go. But perhaps it is helpful to describe your different structure representations in the context of previous studies, or I concern that it may bring more confusions to the community admittedly the perceptions of big-leaf have been already quite different between scholars.

RESPONSE: We have now added a paragraph to highlight the difference among canopy models, following the naming/definition in Luo et al. (2018). Changes related to this comment:

• Lines 23-39: It should be noted that "big leaf model" may refer to different models within the last decades given their interchangeable uses (Luo et al., 2018). According to Luo et al. (2018), the "big leaf model" can be categorized as least as the following types given the purposes they were developed. (1) One-big-leaf canopy model that regards canopy as a single big leaf was typically used with Penman-Monteith equation (Penman, 1948; Monteith, 1965) to compute land

surface evaporation in early LSMs. Sellers et al. (1992) updated the one-big-leaf model by adding an exponentially diminishing photosynthetic rate within the canopy depth to upscale photosynthesis for the carbon-water coupled LSMs. Yet, this scheme often underestimated canopy assimilation rate as the exponential function cannot properly represent the vertical light and photosynthesis profiles. (2) Two-leaf radiation scheme that separates the canopy into a group of sunlit leaves and a group of shaded leaves (Norman, 1982; De Pury and Farguhar, 1997; Campbell and Norman, 1998; Chen et al., 1999) was used to account for the horizontal and vertical light heterogeneity in the canopy. (3) Two-big-leaf canopy model combines one-big-leaf canopy model and two-leaf radiation scheme to upscale carbon and water fluxes, and treats each of the sunlit and shaded fractions as a single big leaf where leaf biochemical parameters and radiation are upscaled to canopy level (De Pury and Farquhar, 1997; Wang and Leuning, 1998). (4) Two-leaf canopy model uses two-leaf radiation scheme, and treats each of the sunlit and shaded fractions as a leaf with average traits for its representation (not integrated value as in a big leaf) (Chen et al., 1999, 2012; Sprintsin et al., 2012). Therefore, the use of term"big leaf model" needs to be cautious as it may refer to (i) two-leaf radiation scheme which is a canopy radiative transfer model or (ii) upscaling schemes which differ in the way leaf biochemical parameters are integrated (such as one-big-leaf and two-big-leaf models) or averaged (such as two-leaf canopy model)."

#### Other minor comments:

1. Considering the importance IJKX in this study and how other representations of canopy are based on it, maybe there is a need to show the equations on how to separate sunlit and shaded leaves in IJKX

RESPONSE: It is a really good point. We have now included three new equations to show what we did with the sunlit/shaded partitioning. Changes related to this comment:

- Lines 115-124: (screenshot pasted below for equation display).
- the inclination angle, and "azi" is the azimuth angle). The fraction of sunlit leaves relative to total canopy leaf area in a given canopy layer is computed as

$$\sum_{\text{incl,azi}} p_{\text{sl,i}}(\text{incl,azi}) = \frac{\text{LAI(i+1)} - \text{LAI(i)}}{\text{LAI}} \cdot \int_{\text{LAI(i)}}^{\text{LAI(i+1)}} \exp(-k\Omega x) \cdot \mathrm{d}x, \tag{1}$$

where LAI is total leaf area index, LAI(i) is the leaf area index above the ith canopy layer, LAI(i) is the leaf area index in and above the ith canopy layer, k is the distinction coefficient as a function of leaf inclination angle distribution, and  $\Omega$  is the

120 clumping index. Then  $p_{sl.i}$  (incl,azi) is computed using

$$p_{\text{sl,i}}(\text{incl,azi}) = \sum_{\text{incl,azi}} p_{\text{sl,i}}(\text{incl,azi}) \cdot \frac{1}{I} \cdot \frac{1}{J}, \tag{2}$$

where I is the number of inclination angles and J is the number of azimuth angle. The fraction of shaded leaves relative to total canopy leaf area in a given canopy layer is computed as

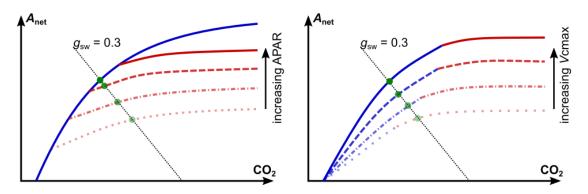
$$p_{\rm sh,i} = \frac{\rm LAI(i+1) - \rm LAI(i)}{\rm LAI} \cdot \left[ 1 - \int_{\rm LAI(i)}^{\rm LAI(i+1)} \exp(-k\Omega x) \cdot dx \right]. \tag{3}$$

2. FQE was not defined, so it was not easy to grasp the key points from the heavy discussion in L240-260. Adding a few summary statements at the beginning of these paragraphs might help readers to follow.

RESPONSE: We have defined FQE already as  $\phi F$  in the method section, to be more consistent, we changed the FQE to  $\phi F$  throughout the manuscript. To help readers know better what PSII and fluorescence quantum yields are, we have added a brief description of them along with the discussion of the two. Changes related to this comment:

- Lines 299-302: These contrasting patterns of the simpler models resulted from the different photosynthesis system II (PSII) quantum yield and fluorescence quantum yield (namely  $\phi F$ ) responses to APAR and CO2 (Figure 11a,b). PSII quantum yield measures efficiency of converting absorbed photons to electrons by PSII; and  $\phi F$  measures the efficiency of converting absorbed photons to fluorescence photons.
  - 3. Figure 2b. Just curious about the environmental conditions for leaves described in this plot. Not very clear why Anet increases with Vcmax while gs becomes saturated.

RESPONSE: We set a maximum stomatal conductance limit to the leaf, so that gsw cannot go beyond the maximum structural limit. We used an arbitrary value 0.3 in our simulations. When gsw is limited to a maximum, gsw would increase with higher APAR when APAR is low, and stay at the maximum when APAR is high. However, Anet may saturate at a different APAR depending on whether Anet is Rubisco- or electron transport limited. See our sketch below for a scenario of increasing Anet at a fixed maximum gsw. Blue curve: Rubisco limited photosynthetic rate (Ac). Red curve: electron transport limited photosynthetic rate (Aj). Black dotted line: stomatal conductance is 0.3 mol m-2 s-1. The intersection of a A-Ci curve (lower of Ac and Aj) vs the black dotted curve is the Anet at the given gsw. When APAR increases from 0, Anet increases as Anet is limited by electron transport. When APAR is high enough, Anet saturates as Anet is limited by Rubisco. Similarly, when Vcmax increases from 0 (Jmax increases accordingly), Anet increases with higher Vmax (and Jmax).



This is why gsw peaks but Anet still increases with higher APAR and Vcmax. We have clarified this in the caption of Figure 2. Changes related to this comment:

• Figure 2 caption in page 5: Environmental and leaf physiological settings for the simulations are: air and leaf temperatures at 298.15 K, atmospheric vapor pressure at 1500 Pa (relative humidity at 0.47), atmospheric CO2 partial pressure at 40 Pa, atmospheric pressure at 101325 Pa, Vcmax (for panel a) at 60 μmol

# m-2 s-1, and maximal stomatal conductance at 0.3 mol m-2 s-1. (Figure pasted below).

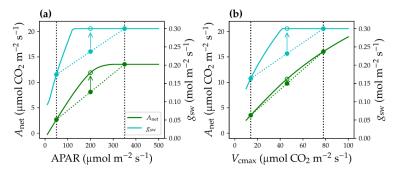


Figure 2. Non-linear leaf responses to the environmental and physiological parameters. (a) Stomatal conductance to water vapor  $(g_{sw}; \text{ cyan} \text{ solid curve})$  and net photosynthetic rate  $(A_{net})$  responses to absorbed photosynthetically active radiation (APAR). The black dotted vertical lines indicate two leaves at low and high light conditions. Mean behavior of the two leaves ought to be the closed circles on the colored dotted lines. However, use mean APAR for the leaves would result in overestimated  $g_{sw}$  and  $A_{net}$  (open circles). (b) Non-linear  $g_{sw}$  and  $A_{net}$  responses to leaf photosynthetic capacity, represented by maximum carboxylation rate  $(V_{cmax})$ . Environmental and leaf physiological settings for the simulations are: air and leaf temperatures at 298.15 K, atmospheric vapor pressure at 1500 Pa (relative humidity at 0.47), atmospheric CO<sub>2</sub> partial pressure at 40 Pa, atmospheric pressure at 101325 Pa,  $V_{cmax}$  (for panel a) at 60  $\mu$ mol m<sup>-2</sup> s<sup>-1</sup>, and maximal stomatal conductance at 0.3 mol m<sup>-2</sup> s<sup>-1</sup>.

De Pury, D.G.G., Farquhar, G.D., 1997. Simple scaling of photosynthesis from leaves to canopies without the errors of big-leaf models. Plant, Cell Environ. 20, 537–557. https://doi.org/10.1111/j.1365-3040.1997.00094.x

Luo, X., Chen, J.M., Liu, J., Black, T.A., Croft, H., Staebler, R., He, L., Arain, M.A., Chen, B., Mo, G., Gonsamo, A., McCaughey, H., 2018. Comparison of Big-Leaf, Two-Big-Leaf, and Two-Leaf Upscaling Schemes for Evapotranspiration Estimation Using Coupled Carbon-Water Modeling. J. Geophys. Res. Biogeosciences 123. https://doi.org/10.1002/2017JG003978

Sellers, P.J., Berry, J.A., Collatz, G.J., Field, C.B., Hall, F.G., 1992. Canopy reflectance, photosynthesis, and transpiration. III. A reanalysis using improved leaf models and a new canopy integration scheme. Remote Sens. Environ. 42, 187–216. https://doi.org/10.1016/0034-4257(92)90102-P

Sprintsin, M., Chen, J.M., Desai, A., Gough, C.M., 2012. Evaluation of leaf-to-canopy upscaling methodologies against carbon flux data in North America. J. Geophys. Res. Biogeosciences 117, 1–17. https://doi.org/10.1029/2010JG001407

### RC2

The authors show the impact of using radiative transfer schemes of increasing complexity on the SIF simulated by a land model. The different options include a big leaf versus a multilayer canopy, having sun and shaded leaves, considering the leaf angle distribution and a vertically varying Vcmax. The paper is very didactic with nice illustrative figures. It demonstrates in a very elegant way the consequences of using an average APAR when lots of the relationships are non-linear. The results are as expected, differences between models are quantified, and specific behaviors of the simpler models are explained in detail to the readers (e.g. Figure 10). The authors draw important conclusions, while using a simple formalism.

RESPONSE: We thank reviewer 2 for the support and valuable suggestions. We have now addressed all the main and minor comments, and believe the revision has improved significantly. Please see our point-to-point responses below for the detailed changes.

### Main comments

The authors should clarify what they consider a land surface model. Indeed, they cite models such as CLM and ORCHIDEE that can run at global scales over centuries, such models simply cannot integrate the large number of operations performed by a model such as CliMA Land.

RESPONSE: We consider land surface models as the models that can be used to simulate terrestrial biosphere processes at regional and global scales. We have now included sentences to highlight the importance of LSM in earth system modeling at the beginning of the Introduction. A major difference between existing LSMs and the CliMA Land, which we are making use of in the present study, is that the CliMA Land can simulate the hyperspectral canopy radiative transfer, whereas the traditional LSMs uses broadband radiative transfer. This new feature, in particular, allows us to evaluate not only carbon, water, and energy fluxes (which existing LSMs are capable of doing), but also canopy reflectance and fluorescence spectra simultaneously (which existing LSMs are not able to do because they use big leaf models). The ability to simulate hyperspectral canopy spectra is crucial in the new generations of LSM so as to use the increasing number of remote sensing data, such as MODIS and TROPOMI satellite retrievals.

Besides the model incompatibility with hyperspectral radiative transfer, computation resources required for the hyperspectral radiative transfer and multiple canopy layers may be another reason that existing LSMs choose not to run them. Yet, this is becoming less of a problem given the advances in hardware technology and software engineering (like we use Julia for C-like speed and script-like coding experience). Actually, we can perform the large number of operations in the CliMA Land at the global scale such as the hyperspectral radiative transfer scheme. In the CliMA Land, a single evaluation of the basic biophysics only takes a few ms. Overall, it takes less than 3 minutes to perform an hourly simulation of a site for a year (8760 values). It takes about 2 hours when we perform the global scale land surface simulations on a 1x1 degree resolution using 200 cores. Thus, running our new Land model for a century will not be overkilling in the near future. We will elaborate this part of discussion more thoroughly and show the result of the global simulation in a future publication. Changes related to this comment (clarification of what we consider a LSM):

- Lines 17-19 clean revision, hereafter): Land surface models (LSMs) simulate the
  carbon, water, and energy fluxes at the land-atmosphere interface at regional
  and global scales, and are key component for Earth system models (ESMs). The
  ability of LSMs to accurately model the carbon, water, and energy fluxes within
  vegetation canopy largely determines the predictive skills of the ESMs.
- Line 69-77: Ideally, LSMs can be constrained using raw reflection and fluorescence spectra. This, nevertheless, requires the LSMs moving from broadband canopy radiation to a hyperspectral representation, and from sunlit and shaded fractions to leaf angular distributions (such as the land model developed by Climate Modeling Alliance, CliMA Land; Wang et al., 2021b). This way, the LSM can be directly coupled to remotely sensed canopy spectra (e.g., Shiklomanov et al., 2021) rather than to reprocessed datasets using often incompatible assumptions. The increasing canopy complexity, however, comes with high costs: (a) muchmore computational resources required by increasing amount of leaves (e.g., CliMA Land canopy has a default of 6500 leaves per tree in the canopy whereas two-leaf canopy has 2 "leaves"), (b) more complicated canopy radiation and fraction (e.g., CliMA Land model calculates the radiation and fraction based on leaf angular distribution for a default of 6500 leaves), and (c) most importantly, increasing difficulty for research communities to understand or use the model.
- Lines 140-142: In comparison, radiative transfer and sunlit/shaded fractions are computed analytically in the two-leaf radiation scheme as the model is single layered and uses broadband reflectance and transmittance (Campbell and Norman, 1998; Bonan et al., 2021). Yet, the two-leaf radiation scheme that use broadband radiative transfer are not adequate for accurate fluorescence modeling.

Do the authors precise somewhere how many layers they used (K)? Same for the leaf angle distribution?

RESPONSE: We have now included the default settings for I, J, and K in the revision. Changes related to this comment:

 Lines 125-126: We used a default I = 9 inclination angles, J = 36 azimuth angles, K = 20 vertical layers for "IJKX" (K = 20 for for "2KX" and "KX" as well).

Page 4, Figure 2: "The black dotted vertical lines indicate two leaves at low and high light conditions.": Are they representative of shaded and sun leaves? Do sun and shaded leaves have different characteristics/parameter values? Or do they just differ by the level of light they receive? The authors should maybe show values/curves of APARsun, APARshaded and APAR for 1X/KX to clarify this point (e.g. Figure 6c in Bonan et al., 2021).

RESPONSE: Thanks for pointing out the points that need clarification. We did not use the term sunlit or shaded leaves here in the diagram as we classify leaves by the level of light they receive. For example, in 2KX or IJKX, APAR for sunlit and shaded fractions may be above 500 umol m-2 s-1 for the top canopy layer. In this case, averaging APAR would not result in any difference. However, averaging APAR could be problematic if two APARs are on different sides of the turning point, say 150-250 umol m-2 s-1 as in Figure 2a. For example, the two leaves can be both from shaded fraction, but one is from the upper canopy layer and one is from the lower canopy layer (such as when we move from 2KX to 2X). Changes related to this comment:

Lines 97-100: Note that averaging APAR values that are beyond the turning point, say 350 μmol m-2 s-1, may not result in any bias in modeled gsw and Anet (such as for sunlit and shaded leaves in the top canopy layer); however, averaging APAR for leaves with high APAR and low APAR, say 300 and 50 μmol m-2 s-1 would result in overestimated gsw and Anet (such as for shaded leaves in upper and lower canopy as typically done in the two-leaf radiation scheme).

Regarding the difference between sunlit and shaded leaves, as the sunlit and shaded fraction change throughout the day as a function of solar zenith angle, it is not realistic to use different characteristics for the leaves based on whether they are sunlit or shaded. Yet, it is more reasonable to use different parameters for leaves at different canopy height, for example, leaves in the top canopy layer have higher Vcmax25. And we had this mentioned along with equation 8 (old equation 5). We also have revised the text to clarify this. Changes related to this comment:

- Lines 160-163: Note that as leaves are experiencing dynamically changing light
  environment throughout the day, it is unrealistic to assume the sunlit and shaded
  leaves have different traits; thus, we only accounted for the vertical heterogeneity
  but neglected the horizontal heterogeneity in each canopy layer, namely using
  the same characteristics for leaves within the same canopy layer.
- Equation 8:  $V_{\text{cmax,i}} = V_{\text{cmax,top}} \cdot \exp\left[-0.15 \cdot \text{LAI}(i)\right],$

As to the figure, we had a similar figure as that from Bonan et al. (2021) in an earlier model description paper (Wang et al., 2021), and Figure 4b of the paper showed the magnitude of APAR for sunlit and shaded leaves. To better inform readers of the difference among APARs at different canopy complexity levels, we have included a new figure to highlight the differences. Changes related to this comment:

• Figure 3 in page 8 (pasted below).

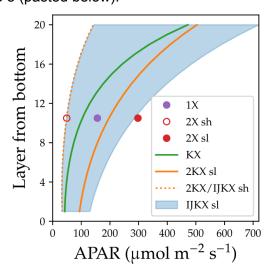


Figure 3. Comparison of mean absorbed photosynthetically active radiation (APAR) profiles for four different canopy complexity levels. "1X": single layer canopy without sunlit or shaded fractions. "2X": single layer canopy with sunlit and shaded fractions. "KX": multiple layer canopy with sunlit and shaded fractions per layer. "IJKX": multiple layer canopy with sunlit and shaded fractions per layer, and the sunlit fraction is further partitioned based on leaf inclination and azimuth angular distributions. The "sl" and "sh" stand for sunlit and shaded leaves, respectively.

Page 4, lines 86-90: It is nice to show the correspondence with other land surface models.

RESPONSE: Thanks for the suggestion. We have now classified more LSMs to each canopy complexity type in a new table. Changes related to this comment:

- Table 1 in page 6 (pasted below)
- Lines 108-110: "IJKX" further modifies "2KX" by accounting for leaf inclination and azimuth angle distributions per layer (Figure 1). See Table 1 for the canopy model complexity adopted by other vegetation models (see https://yujie-w.github.io/PAGES/dev/methods/#Vegetation-canopy-model-complex ity for a growing list).

**Table 1.** A list of vegetation models that corresponds to our tested canopy complexity schemes.

Model	Version	Reference	Complexity
CLM	4	Bonan et al. (2011)	2X
	5	Lawrence et al. (2019)	2X
	ml	Bonan et al. (2018)	2KX
ISBA	A-gs	Carrer et al. (2013)	2KX
	MEB	Boone et al. (2017)	2KX
JULES	can_rad_mod 1	Jogireddy et al. (2006)	one-big-leaf
	can_rad_mod 4	Clark et al. (2011)	IJKX
	can_rad_mod 5	Clark et al. (2011)	2KX
ORCHIDEE	CAN v1	Ryder et al. (2016)	KX
SCOPE	1	Van der Tol et al. (2009)	IJKX
	2, lite off	Yang et al. (2021)	IJKX
	2, lite on	Yang et al. (2021)	2KX

Equations page 5: The authors should precise that not all models compute the APAR and fractions this way. I understand Bonan et al. (2011) describe in their section 2.3 "Radiative Transfer" different ways to address the 2X problem for CLM, with different results shown in their Figure 1.

RESPONSE: This is a good point, and thanks for bringing it up. We have now included a paragraph to highlight the difference between the equations and why we performed the calculation differently. Changes related to this comment:

• Lines 137-148: We emphasize here that to derive canopy fluorescence spectrum and its sun-sensor geometry, we need to simulate the canopy radiative transfer using hyperspectral reflectance, transmittance, and fluorescence. Due to the high spectral resolution and multiple layers required, radiative transfer and canopy fractions in complex models such as SCOPE are computed numerically. In comparison, radiative transfer and sunlit/shaded fractions are computed analytically in the two-leaf radiation scheme as the model is single layered and uses broadband reflectance and transmittance (Campbell and Norman, 1998; Bonan et al., 2021). Yet, the two-leaf radiation scheme that use broadband radiative transfer are not adequate for accurate fluorescence modeling. Crucially, the difference in the analytic and numerical solutions could result in biases in the

simulated APAR and fraction. To avoid such bias, we computed the APAR and sunlit/shaded fractions for the simpler canopy setups numerically using the algorithm in "IJKX". See Figure 3 for the APAR profiles for "2KX", "KX", "2X", and "1X" derived from "IJKX". Also, we note here that leaf biochemical parameters and APAR were not integrated within a canopy layer or sunlit/shaded fractions; instead, we used average APAR and leaf traits in our simulations. Thus, our "1X" model is a one-leaf model rather than a one-big-leaf model, and our "2X" model resembles the two-leaf model rather than two-big-leaf model.

Page 6, equation 8: What is p? Is the summation over i? Same questions for equation 9 on Page 7.

RESPONSE: p need to be iterated through all sunlit and shaded fractions (if any) and all canopy layers. Now we have included the two suites of equations. Changes related to this comment:

- Equations 11 (pasted below)
- Equations 12 (pasted below)

At each canopy complexity level, for a given environmental condition set, we were able to obtain the steady state stomatal conductance for each APAR, from which we computed steady state  $A_{\rm net}$  using the classic C3 photosynthesis model (Farquhar et al., 1980) and E as well as leaf fluorescence quantum yield  $(\phi_{\rm F})$  using the model developed in van der Tol et al. (2014). Stand level carbon flux, namely net ecosystem exchange (NEE; normalized per ground area) was computed using NEE = LAI  $\cdot \sum (A_{\rm net} \cdot p) - R_{\rm remain}$ :

$$\begin{split} \text{IJKX} \text{NEE} &= \text{LAI} \cdot \sum_{\text{i,incl,azi}} \left[ A_{\text{net}} \left( \text{APAR}_{\text{sl,i}} (\text{incl,azi}) \right) \cdot p_{\text{sl,i}} (\text{incl,azi}) \right] + \text{LAI} \cdot \sum_{\text{i}} \left[ A_{\text{net}} \left( \text{APAR}_{\text{sh,i}} \right) \cdot p_{\text{sh,i}} \right] - R_{\text{remain}}; \\ 2^{\text{KX}} \text{NEE} &= \text{LAI} \cdot \sum_{\text{i}} \left[ A_{\text{net}} \left( ^{2\text{KX}} \text{APAR}_{\text{sl,i}} \right) \cdot ^{2\text{KX}} p_{\text{sl,i}} + A_{\text{net}} \left( ^{2\text{KX}} \text{APAR}_{\text{sh,i}} \right) \cdot ^{2\text{KX}} p_{\text{sh,i}} \right] - R_{\text{remain}}; \\ K^{\text{X}} \text{NEE} &= \text{LAI} \cdot \sum_{\text{i}} \left[ A_{\text{net}} \left( ^{\text{KX}} \text{APAR} \right) \cdot ^{\text{KX}} p_{\text{i}} \right] - R_{\text{remain}}; \\ 2^{\text{X}} \text{NEE} &= \text{LAI} \cdot A_{\text{net}} \left( ^{2\text{X}} \text{APAR}_{\text{sl}} \right) \cdot ^{2\text{X}} p_{\text{sl}} + \text{LAI} \cdot A_{\text{net}} \left( ^{2\text{X}} \text{APAR}_{\text{sh}} \right) \cdot ^{2\text{X}} p_{\text{sh}} - R_{\text{remain}}; \\ 1^{\text{X}} \text{NEE} &= \text{LAI} \cdot A_{\text{net}} \left( ^{1\text{X}} \text{APAR} \right) - R_{\text{remain}}. \end{split} \tag{11}$$

where LAI is leaf area index, and  $R_{\text{remain}}$  is the ecosystem respiration rate per ground area excluding the leaves. The transpiration rate from the canopy is computed and used as a proxy for estimating the difference in model ecosystem evapotranspiration

(ET; normalized per ground area) using  $\mathrm{ET} \approx \mathrm{LAI} \cdot \sum (E \cdot p)$ 

$$\begin{split} \text{IJKX} \text{ET} &\approx \text{LAI} \cdot \sum_{\text{i,incl,azi}} \left[ E\left( \text{APAR}_{\text{sl,i}}(\text{incl,azi}) \right) \cdot p_{\text{sl,i}}(\text{incl,azi}) \right] + \text{LAI} \cdot \sum_{\text{i}} \left[ E\left( \text{APAR}_{\text{sh,i}} \right) \cdot p_{\text{sh,i}} \right]; \\ &^{2\text{KX}} \text{ET} \approx \text{LAI} \cdot \sum_{\text{i}} \left[ E\left( ^{2\text{KX}} \text{APAR}_{\text{sl,i}} \right) \cdot ^{2\text{KX}} p_{\text{sl,i}} + E\left( ^{2\text{KX}} \text{APAR}_{\text{sh,i}} \right) \cdot ^{2\text{KX}} p_{\text{sh,i}} \right]; \\ &^{\text{KX}} \text{ET} \approx \text{LAI} \cdot \sum_{\text{i}} \left[ E\left( ^{\text{KX}} \text{APAR} \right) \cdot ^{\text{KX}} p_{\text{i}} \right]; \\ &^{2\text{X}} \text{ET} \approx \text{LAI} \cdot E\left( ^{2\text{X}} \text{APAR}_{\text{sl}} \right) \cdot ^{2\text{X}} p_{\text{sl}} + \text{LAI} \cdot E\left( ^{2\text{X}} \text{APAR}_{\text{sh}} \right) \cdot ^{2\text{X}} p_{\text{sh}}; \\ &^{1\text{X}} \text{ET} \approx \text{LAI} \cdot E\left( ^{1\text{X}} \text{APAR} \right). \end{split} \tag{12}$$

We remind here that soil evaporation is a function of soil water content, soil surface temperature, and atmospheric vapor pressure deficit, and that soil evaporation should be the same for all tested canopy complexity models. Therefore, the modeled ET difference is 100% caused by canopy transpiration, and using transpiration would not result in any biases in the relative difference of modeled ET.

Page 7, lines 138-139: "The transpiration rate from the canopy is computed and used as a proxy for ecosystem evapotranspiration": I don't understand why the authors are doing that. Does this mean they don't have information on the evaporation of the bare soil and intercepted water? Or do they consider that these terms are negligible?

RESPONSE: Thanks for pointing out the inconsistency. As the soil and intercepted water evaporations do not impact the estimation of canopy transpiration, the model predicted ET difference results only from canopy transpiration. Therefore, we did not model soil or intercepted evaporation but used transpiration as a proxy for ET, we have now revised the sentence to clarify this. Changes related to this comment:

- Lines 184-191: The transpiration rate from the canopy is computed and used as a proxy for estimating the difference in model ecosystem evapotranspiration (ET; normalized per ground area) using ET ≈ LAI·sum(E·p). We remind here that soil evaporation is a function of soil water content, soil surface temperature, and atmospheric vapor pressure deficit, and that soil evaporation should be the same for all tested canopy complexity models; so does for evaporation from intercepted water on plant surface. Therefore, the modeled ET difference is 100% caused by canopy transpiration, and using transpiration would not result in any biases in the relative difference of modeled ET.
- Equations 12 (pasted above)

Page 7, line 142: "For "2KX", we plugged the Phi\_F calculated for sunlit fraction": How is this Phi\_F computed?

RESPONSE: Thanks for pointing out the missing pieces. We have now added a brief description about what has been done. Changes related to this comment:

 Line 178-180: At each canopy complexity level, for a given environmental condition set, we were able to obtain the steady state stomatal conductance for each APAR, from which we computed steady state Anet using the classic C3 photosynthesis model (Farquhar et al., 1980) and E as well as leaf fluorescence quantum yield (φF) using the model developed in van der Tol et al. (2014).

Page 7, line 156: "held air humidity constant at 0.47": Give unit.

Page 7, line 156: "a water vapor pressure of 1500 Pa at 25 °C": This is not clear, please give the considered equations, including for the computation of VPD.

RESPONSE: This is a fraction. We have clarified this in the revision. Changes related to this comment:

- Lines 206-208: When we altered temperature, we changed the air and leaf temperature at the same time and held air relative humidity (RH) constant at 0.47 (fraction; unitless). Saturated water vapor pressure was computed using the Clapeyron–Clausius equation
- Equation 13 (pasted below)

$$P_{\text{sat}} = P_{\text{triple}} \cdot \left(\frac{T}{T_{\text{triple}}}\right)^{\frac{\Delta c_p}{R_v}} \cdot \exp\left[\frac{\text{LH}_{v0} - \Delta c_p \cdot T_{\text{triple}}}{R_v} \cdot \left(\frac{1}{T_{\text{triple}}} - \frac{1}{T}\right)\right],\tag{13}$$

where  $P_{\text{triple}}$  is the vapor pressure at the triple point in Pa, T is the temperature in K,  $T_{\text{triple}}$  is the temperature at triple point in K,  $\Delta c_{\text{p}}$  is the difference in isobaric specific heat of vapor and liquid in J Kg<sup>-1</sup> K<sup>-1</sup>,  $R_{\text{v}}$  is the gas constant of water vapor

in J Kg<sup>-1</sup> K<sup>-1</sup>, and LH<sub>v0</sub> is the latent heat of vaporization at triple point. Atmospheric vapor pressure was computed using  $P_{\text{sat}}$  · RH. For each tested environmental cue, we changed only the tested cue while holding all other environmental conditions

Page 7, line 164: "prescribed leaf temperature and soil water potential to maximally reduce uncertainty": What does that mean? How do the authors do that?

RESPONSE: We meant that (1) we used leaf temperature estimated from flux tower measurements in our model rather than leaf temperature from leaf energy balance, and (2) we used soil water potential estimated from soil water content from flux tower measurements in our model rather than running soil water budget. Doing this allowed us to have all the tested canopy complexity models on the same page; otherwise, some difference may arise from leaf temperature and soil conditions. We have now clarified this in the revision. Changes related to this comment:

• Lines 221-224: Briefly, we used outgoing long wave radiation from flux tower measurements to invert canopy temperature and used it as leaf temperature; we also used soil water content to estimate soil water potential and used it as boundary condition for the soil-plant-air continuum. Prescribing leaf temperature and soil water potential allowed us to tease apart the difference caused by canopy complexity from that caused by environmental and physiological differences.

Page 10, line 202-203: "The divergent flux responses to P\_CO2 underlined the importance of adopting a more complex canopy concerning the dynamically changing radiation in a diurnal cycle and rapidly increasing P\_CO2": How can we model a varying P\_CO2 in a land surface model?

RESPONSE: We were meaning that CO2 concentration within the canopy airspace may change dramatically in a diurnal cycle in the short term, and global mean CO2 concentration is also increasing rapidly due to human emission. Thus, we need to use more complex canopy models so as to make the modeling less biased. We have now rewritten the sentence to clarify this. Changes related to this comment:

Lines 262-264: The divergent flux responses to PCO2 underlined the importance
of adopting a more complex canopy in future land modeling given that (i) CO2
concentration within the canopy airspace may change dramatically within a
diurnal cycle due to plant carbon fixation, and (ii) atmospheric mean CO2 is
increasing rapidly due to anthropogenic emissions.

#### Minor comments

Page2, line 30: "and succeed the big-leaf model": weird formulation, is a word missing?

RESPONSE: We meant if the multi-layered model will have better predictive power than the big-leaf model at global scales. We have now clarified the sentence. Changes related to this comment:

• Lines 48-51: As a result, though it is shown that a multi-layered canopy model better resolves energy fluxes in the canopy (Bonan et al., 2021), limited is known about will the multi-layered canopy models show improved predictive skills (particularly in terms of carbon and water fluxes) compared to the big leaf models which are widely used in existing LSMs.

Page 3, Figure 1: angular distribution (b is missing)

RESPONSE: Done.

Page 7, line 143: "we re-simulate" -> we re-simulated

RESPONSE: Done.

Page 7, line 153: "how they much" -> how much they

RESPONSE: Done.

Page 16, line 243: "but decrease" -> but decreases

RESPONSE: Done.

Page 19, line 319: "as did in" -> as done in

RESPONSE: We thank reviewer 2 for pointing out the typos and grammar issues. We have now fixed all the issues.

## Literature cited

Wang, Y., Köhler, P., He, L., Doughty, R., Braghiere, R. K., Wood, J. D., and Frankenberg, C.: Testing stomatal models at stand level in deciduous angiosperm and evergreen gymnosperm forests using CliMA Land (v0.1), Geosci. Model Dev. Discuss. [preprint], https://doi.org/10.5194/gmd-2021-154, in review, 2021.