Response letter to manuscript "A Modeling Approach to Investigate Drivers, Variability and Uncertainties in  $O_2$  Fluxes and the  $O_2$ : $CO_2$  Exchange Ratios in a Temperate Forest" by Yan et al. (https://bg.copernicus.org/preprints/bg-2023-30/)

## Dear Reviewers, dear Editor,

Thank you very much for your review of the above-mentioned manuscript. We have carefully inspected all reviewer comments. Below, you will find our responses to the comments (in italics and blue). As suggested by Reviewer #1, we extended the sensitivity analysis regarding the fixed exchange ratios of gross assimilation, stem and soil respiration. Furthermore, we discussed the influence of dilution and displacement effects (non-diffusive transport) as suggested by the community comment and Reviewer #2.

We uploaded a version of the manuscript where all changes with respect to the previous version have been marked (track-changes). The line numbers in the following reply refer to the revised manuscript version including the track-changes.

We hope that you will find the result satisfying.

## Sincerely,

Yuan Yan, Anne Klosterhalfen, Fernando Moyano, Matthias Cuntz, Andrew C. Manning, Alexander Knohl

## **Reviewer #1**

The reviewed manuscript presents an interesting study that models the  $O_2$  and  $CO_2$  fluxes in and above a forest canopy, and aims to determine if the actual measurement of such fluxes will enable the partitioning of the  $CO_2$  fluxes into its components. This is a new and interesting modeling exercise, and the manuscript is generally well-written and clear. *Thank you for the positive feedback.* 

Major comments:

I find the way the manuscript is structured somewhat confusing. In the method section, the effect of nitrate assimilation on the ER is ignored, and a fixed value for stem and soil ER is assumed, although the introduction mentioned a range found in field studies. That leaves the reader to wonder why these important variations are ignored. Then the results are detailed, based on the simplified assumption of a fixed ER, and only in the discussion, the variability in the sources ER is discussed in detail and a sensitivity test is performed. If the authors want to keep this structure, they should state clearly in the methods and the results sections, that the effect of variability in ER will be discussed and tested later. For me, it seems it will be even better if some of this discussion will be moved to the introduction and the sensitivity analysis will be included in the methods and results.

This issue has also important implications for the conclusions. If chamber studies at a given site show a constant and large difference between the respiration components, there is a much better chance to use the  $O_2$  approach for  $CO_2$  fluxes partitioning. Maybe this could be also demonstrated by a test run of the model.

We revised the structure as suggested to show more clearly why and how we used, for the most part, fixed exchange ratios (ER) as model parameters and their spatial and temporal variability as model output on ecosystem scale. We are aware of the role of N assimilation on ER but decided deliberately to leave this out of the current manuscript to keep a clear focus. We are currently working on a study investigating the N assimilation effect on ER variability. As the reviewer suggested, we extended the sensitivity analysis and restructured the manuscript accordingly by adding information in the Methods, Results and Discussions sections.

#### Methods:

Lines 205-209: "To quantify the dependency of the CANVEG model regarding these fixed ER parameters, we also conducted a sensitivity analysis, where we changed each of ER<sub>A</sub>, ER<sub>stem</sub> and ER<sub>soil</sub> by  $\pm 10\%$  and estimated the resulting relative changes in simulated O<sub>2</sub> fluxes. Furthermore, the impact of changed ER parameters was also investigated in the following parts of this study (see sections 2.3 and 2.5 below)."

Lines 260-261: "Moreover, we assessed the impact of the model parameters  $ER_A$ ,  $ER_{stem}$  and  $ER_{soil}$  by changing each by  $\pm 10\%$  on estimates for  $ER_{eco}$  and  $ER_{An}$  within the sensitivity analysis."

Lines 357-358: "Moreover, we assessed the impact of the model parameters  $ER_A$ ,  $ER_{stem}$  and  $ER_{soil}$  by changing each by  $\pm 10\%$  on the source partitioning results by estimating the absolute change in the a posteriori  $\sigma_{F_A}$ ."

Results:

Lines 372-377: "Due to potential variations in the ER model parameters (which were here taken from literature), we conducted a sensitivity analysis to show how these parameters affected the modeled  $F_{O_2}$ . If ER<sub>A</sub> was increased or decreased by 10%, the modeled  $F_{O_2}$  sum of the entire study period increased or decreased on average by 20.3% correspondingly. Similarly, a change by plus or minus 10% increments on ER<sub>soil</sub> and ER<sub>stem</sub> caused the  $F_{O_2}$  sum to decrease or increase by 8.6% and 1.7%, respectively. These results directly followed Eq. (1) where the derivative with respect to a specific ER gives the corresponding flux in percent. Oxygen fluxes were hence most sensitive to the ER of the largest carbon fluxes."

Lines 400-407: "Within the sensitivity analysis, the initial annual median  $ER_{eco}$  of 1.08 mol mol<sup>-1</sup> changed only by up to 0.02 mol mol<sup>-1</sup> due to the change in  $ER_A$  or  $ER_{stem}$  by ±10%. Increasing or decreasing  $ER_{soil}$  had the largest impact, where median  $ER_{eco}$  increased or decreased to 1.00 or 1.17 mol mol<sup>-1</sup>, respectively. Also here, the interannual difference between years was very small. A similar pattern could be found for the annual mean  $ER_{eco}$ , which varied between 1.04 and 1.15 mol mol<sup>-1</sup> depending on  $ER_A$  and  $ER_{stem}$ , and varied even between 1.00 and 1.24 mol mol<sup>-1</sup> due to  $ER_{soil}$ .

The median and mean of hourly  $O_2$ :  $CO_2$  net assimilation ratio ( $ER_{An}$ ) were 0.99 mol mol<sup>-1</sup> and 0.97 mol mol<sup>-1</sup>, respectively, for all growing seasons during the simulation period, and did not vary between years. In the sensitivity analysis,  $ER_{An}$  was only slightly impacted by changes in the model parameter of  $ER_A$  ( $ER_{stem}$  and  $ER_{soil}$  had no impact)."

Lines 556-557: "In regard to the sensitivity analysis,  $\sigma_{F_A}$  was only slightly impacted by ER<sub>A</sub>.  $\sigma_{F_A}$  ranged from 1.42 to 4.83 µmol m<sup>-2</sup> s<sup>-1</sup> for the case of the lower a priori uncertainty (with  $\sigma_{F_{CO_2}} = 0.5 \mu mol m^{-2} s^{-1}$  and  $\sigma_{ER_B} = 0.001 mol mol^{-1}$ )."

Discussions:

Lines 630-636: "Due to this high variance between derived ER of these different studies, we conducted a sensitivity analysis by changing  $ER_A$ ,  $ER_{stem}$  or  $ER_{soil}$  by  $\pm 10\%$  to show how these

parameters affected the modeled  $F_{O_2}$ ,  $ER_{eco}$  and  $ER_{An}$ . Furthermore, we assessed the impact of these model parameters on the source partitioning results. In summary, the model simulations showed a small sensitivity towards the model parameter settings. The modeled  $F_{O_2}$  sum was mostly sensitive to  $ER_A$ , which corresponded to the largest flux component.  $ER_{eco}$  and  $ER_{An}$ changed by less than 10% in each case. The uncertainty in the source partitioning results were mostly driven by the uncertainty of  $O_2$  flux estimates ( $\sigma_{FO_2}$ ) and much less by the ER parameters. Generally, all model simulations yielded the same tendency and pattern of exchange ratios."

In the following tables, we listed the results of the sensitivity analysis in greater detail. However, we have not added them to the manuscript.

⊿parameter	$\Delta F_{02}$ (%)
<b>ER</b> <sub>A</sub> -10%	-20.30
<b>ER</b> <sub>A</sub> +10%	20.30
<b>ER</b> soil -10%	8.60
<b>ER</b> soil +10%	-8.60
<b>ER</b> stem -10%	1.70
<b>ER</b> <sub>stem</sub> +10%	-1.70

Tab.: Changes in the sum of F<sub>02</sub> due to 10% variation of ER parameters

Tab.: Changes in mean or median annual  $ER_{eco}$  and  $ER_{An}$  due to 10% variation of ER parameters. The range of the five years of the study period are given.

Anavamatan	mean annual	median annual	mean annual	median annual
⊿purameter	<b>ER</b> <sub>eco</sub>	<b>ER</b> <sub>eco</sub>	<b>ER</b> <sub>An</sub>	<b>ER</b> <sub>An</sub>
original	1.06-1.12	1.082-1.084	0.528-1.097	0.996-0.997
ER <sub>A</sub> -10%	1.04-1.15	1.076-1.079	0.591-1.081	0.996-0.997
<b>ER</b> <sub>A</sub> +10%	1.09-1.1	1.092-1.093	0.464-1.110	0.996-0.997
ERsoil -10%	0.998-0.999	0.9986-0.9989	-	-
<b>ER</b> soil +10%	1.13-1.24	1.16-1.17	-	-
<b>ER</b> stem -10%	1.05-1.09	1.062-1.066	-	-
<b>ER</b> <sub>stem</sub> +10%	1.08-1.14	1.101-1.102	-	-

Tab.: Variations of  $\sigma_{F_A}$  (µmol m<sup>-2</sup> s<sup>-1</sup>) due to 10% variation of ER parameters. Panel (a), (b), and (c) refer to Figure 7 in the manuscript representing the various settings of a priori uncertainties.

⊿parameter	panel (a)	panel (b)	panel (c)
original	27-193	4.74-4.87	1.43-4.47
<b>ER</b> <sub>A</sub> -10%	30-194	4.74-4.87	1.47-4.47
<b>ER</b> <sub>A</sub> +10%	29-212	4.74-4.87	1.42-4.83
<b>ER</b> soil -10%	28-195	4.74-4.87	1.43-4.48
<b>ER</b> soil +10%	28-193	4.74-4.87	1.44-4.47
<b>ER</b> stem -10%	27-193	4.74-4.87	1.43-4.47
<b>ER</b> <sub>stem</sub> +10%	27-193	4.74-4.87	1.43-4.47

#### Minor comment 1:

Line 35: I guess there are much older references for this, or this can be just assumed as common knowledge.

Yes, we agree that there are older references. Nevertheless, we prefer these two references cited as they nicely summarize the exchange processes of  $O_2$  and  $CO_2$ , both at the land and the ocean interface. Some older references were also added (lines 36-37):

- *Krogh A (1919): The composition of the atmosphere. Det Kongelige Danske Videnskabernes Selskab 1, 1-19.*
- *Keeling RF and Shertz SR (1992): Seasonal and interannual variations in atmospheric oxygen and implications for the global carbon-cycle. Nature 358, 723-727.*

#### Minor comment 2:

# Line 49: How important is this 0.05 Pg uncertainty compared to other uncertainties, like the effect of ocean warming on $O_2$ solubility?

Following the reference (Keeling and Manning, 2014), ocean warming of 1 Watt per square meter of ocean area would lead to a correction of the global and ocean sinks by about 0.1 Pg C per year due to the combined  $N_2$  and  $O_2$  solubility effect (section 5.15.4.6 in Keeling and Manning (2014), citing Manning, 2001). So, the 0.05 Pg C per year uncertainty due to the uncertainty in ER is smaller than the effect of  $O_2$  solubility under 1 Watt per square meter warming, nevertheless still relevant. A better understanding of the ER of land-atmosphere exchange could help to reduce this uncertainty.

## Minor comment 3:

Line 707: As in the major comments above – is it worth showing some sensitivity test for this? The application and results of the sensitivity analysis by testing a change of  $\pm 10\%$  in ER<sub>A</sub>, ER<sub>stem</sub>, and ER<sub>soil</sub> (model parameters) were described in the Methods, Results and Discussion sections. Please refer to the major comment above.

We further added the following to the Conclusions (lines 810-813): "The annual mean  $ER_{eco}$  ranged from 1.06 to 1.12 mol mol<sup>-1</sup> during the five years' study period and depended significantly on our assumptions about the fixed model parameters describing the exchange ratios of the ecosystem components: leaves, stem and soil ( $ER_A$ ,  $ER_{stem}$ ,  $ER_{soil}$ ). Especially, changes in  $ER_{soil}$  by ±10% yielded annual mean  $ER_{eco}$  from 1.00 up to 1.24 mol mol<sup>-1</sup>."

#### **Reviewer #2**

Major comments:

This work by Yan et al. is a solid, model-based examination of the ways in which real measurements of atmospheric oxygen (with their limited speed and precision) can be used to assess the exchange ratio of forested ecosystems. The authors also explore the potential for these measurements to separate net fluxes into the gross fluxes that occur simultaneously.

Overall, I find the reasoning sound, the organization appropriate and the writing generally quite good.

Thank you for the positive feedback.

I have two scientific questions I would like to see addressed before publication:

First, the prose in line 194 led me to wonder if you really can claim that you're truly predicting the full measure of interannual variability if you're using static values for leaf phenology and LAI and WAI profiles. Please clarify this.

Unfortunately, direct measurements of LAI and WAI were only conducted in 2015, and thus used for all simulation years. The effective LAI was at maximum 4.8 m<sup>2</sup> m<sup>-2</sup> in the growing season in 2015 (Braden-Behrens et al., 2017). Thus, the interannual variability in our simulations is mainly driven by the meteorological conditions.

However, considering estimates by MODIS (Myneni, R., Knyazikhin, Y., Park, T. (2021). MODIS/Terra+Aqua Leaf Area Index/FPAR 4-Day L4 Global 500m SIN Grid V061. NASA EOSDIS Land Processes DAAC. Accessed 2023-05-04 from

https://doi.org/10.5067/MODIS/MCD15A3H.061), the magnitude of LAI did not vary significantly between years from 2012-2016 (see Figure below). The variability of the LAI estimate within one year was larger and the standard deviation is quite large in this data set. Furthermore, the fraction of absorbed photosynthetic active radiation (FPAR) did not differ significantly during growing seasons between years.

In general, the start and end of the season (phenology) can differ between years. Based on the net ecosystem  $CO_2$  flux measurements obtained with the eddy covariance technique, the start of the season varied by up to 18 days within May and the end of the season by only 5 days within November during our study period. Deriving the start and end of season based on canopy photos or satellite data would yield different days.

Implementation of interannual variable leaf phenology in our model simulations would improve the comparison between observations and simulations during the few days of leaf out and leaf fall, but not during the main part of growing seasons. This would mainly decrease the scatter in Figure 2 in the manuscript, but will not have a large impact on the other results, in our opinion. Thus, we like to refrain from changing our model set-up.



*Fig.: Leaf area index (LAI) and fraction of absorbed photosynthetically active radiation (FPAR) derived from remote sensing MODIS data (Myneni et al., 2021). All data was included and quality flags were not considered.* 

Second, I am a little uncomfortable with your choice of "ppm" (i.e. mole fraction) for oxygen values. Because oxygen is not a trace gas, dilution effects can be significant. For this reason, the measurement community uses per-meg units when comparing ambient oxygen to reference gases (e.g. Keeling et al, JGR 103, D3, 3381-3397, 1998). I encourage the authors to switch to per-meg throughout this paper for oxygen.

Throughout the entire manuscript, we report  $O_2$  and  $CO_2$  concentrations as mole fractions regarding dry air (mixing ratios) in ppm. Thus, diluting effects should be excluded. We prefer to keep it this way, because we applied micrometeorological methods, such as the flux-gradient method and the source partitioning approach, and also like to address the eddy covariance community with our study. Within this community, mole fractions are usually reported in ppm and fluxes correspondingly in µmol m<sup>-2</sup> s<sup>-1</sup>. Further, we like to be consistent in regard to the calculation of  $O_2$ : $CO_2$  exchange ratios, which are usually presented in mol mol<sup>-1</sup>. We have added the following sentence to the Methods section in lines 239-244: "In general, the CANVEG model only considered dry mole fractions of  $O_2$  and  $CO_2$ . Usually,  $O_2$  measurements are reported in per meg, which describes the change in the  $O_2$  to  $N_2$  ratio relative to a reference. To convert from ppm to per meg, the factor 1/0.2095 = 4.8 per meg ppm<sup>-1</sup> can be used, where 0.2095 represents the  $O_2$  mole fraction of air in mol mol<sup>-1</sup>. In this study, we chose mole fraction as unit for  $O_2$  to be consistent in regard to the calculation of  $O_2$ : $CO_2$  exchange ratios, which are usually presented in mol mol<sup>-1</sup>.

This question of dilution and units ties in with the thoughtful comments left by Andrew Kowalski. I am glad to see the authors' recent reply. I am far from expert in this area and can't assess the relative merits of the comments or the reply, but two things come to mind: First, it is worth emphasizing that that air samples are cryogenically dried before they are analyzed, so water vapor *should* be disregarded in the model output when characterizing mixing ratios for

comparison with observations. This is unrelated to Stefan flow, but connects to my next point. Second, as I understand it, Kowalski is essentially comparing the rates of Stefan flow and *molecular* diffusion. This might be appropriate when considering the stagnant boundary layer at a leaf's surface, but I believe it is irrelevant at the branch/canopy/tree scale where air parcels (and their properties) are being rearranged by turbulent eddies. My instinct (and it's nothing more than that) is that Stefan flow is much less significant than eddy diffusion. If a moist, O<sub>2</sub>-rich parcel of air in the canopy is ascending through bulk (eddy) transport, while a dry, O<sub>2</sub>-poor parcel is descending, there will be a net transport of O<sub>2</sub> upward if molar mixing ratios are calculated for the samples *after water is removed*. I recognize that I may be wrong about the relative significance of Stefan flow and turbulent transport, or I may have misunderstood some other aspect of Kowalski's argument. Nonetheless, I would like to see my thoughts addressed by the authors.

We added the information that CANVEG only considers mole fractions regarding dry air in the model simulations to the Methods section. Further, we added the following paragraph in the Discussions section, addressing the diffusive and non-diffusive transports and their meaning for our study (lines 742-785):

"In general, mass is transported in air due to diffusive and non-diffusive processes. Diffusive transport can be induced due to random turbulent or molecular motions acting against a gradient. As shown in Figure 5, an exemplary vertical profile or gradient of CO<sub>2</sub> mole fraction regarding dry air shows a higher mole fraction close to the soil surface due to respiratory processes and a lower mole fraction within the forest canopy due to net assimilation during daytime. Above the canopy the  $CO_2$  dry air mole fraction increases slightly again within the boundary layer. The vertical  $O_2$  profile is mirrored to this  $CO_2$  profile (when dry air mole fractions are considered). Because of the processes of evaporation and transpiration from the soil surface and canopy, water vapor is also added to the air column, where the vertical water vapor profile usually shows a decreasing water vapor mole fraction with increasing height. The addition of water vapor molecules to an air package dilutes the other molecules in that air package such as N<sub>2</sub>, O<sub>2</sub>, and CO<sub>2</sub> by replacing some of them. Thus, the ratio between number of  $O_2$  or  $CO_2$  molecules and total number of air molecules (= mole fraction regarding moist air) decreases and therefore the vertical  $O_2$  and  $CO_2$  gradients change. Furthermore, due to the addition of water vapor molecules, other air molecules are being displaced and moved away from the evaporating surface. This displacement effect yields in a non-diffusive transport (also known as Stefan flow) that does not necessarily follow a gradient (Kowalski, 2017; Kowalski et al., 2021). The magnitudes of the dilution and displacement effects depend on the mass fraction of each gas (number and weight of molecules per mass of air), where  $O_2$  is more affected than *CO*<sup>2</sup> due to its high abundance (Kowalski et al., 2021). Considering the above described vertical profile,  $O_2$  diffuses downwards towards the evaporating surface following the increased gradient due to the dilution effect. However, this downward motion can be offset by the displacement effect.

To analyze the transport of and the relationship between  $O_2$  and  $CO_2$  molecules, the dilution and displacement effects have to be considered - also in relation to the turbulent transport. The magnitudes and directions of diffusive (turbulent and molecular diffusion) and non-diffusive transport are variable and need to be quantified experimentally for various atmospheric conditions, various ecosystems and heights above the ecosystems. Thus, the significance and impacts of the various transport types are unknown and currently under discussion. In regard to the many open questions towards non-diffusive transport, we have not implemented the Stefan flow within CANVEG until now.

*The CANVEG model considers mole fractions regarding dry air (removing all the water vapor)* for  $O_2$  and  $CO_2$ , and therefore the dilution effect is excluded from the model simulations and vertical gradients do not change due to the process of evapotranspiration. This allows comparison to O<sub>2</sub> measurements where it is common practice to cryogenically dry the air before analysis for O<sub>2</sub> (Pickers et al., 2017). The non-diffusive transport (Stefan flow) would play a role in our study within the application of the flux-gradient method and the estimation of  $ER_{conc}$ . By the modification of the vertical gradients due to the non-diffusive transport, flux estimates based on the flux-gradient method would differ (personal communication with Andrew S. Kowalski). However, our study considered mostly net ecosystem fluxes in this application. Further, Kowalski et al. (2021) determined that the Webb, Pearman and Leuning (WPL) methodology, based on perturbations in the dry air mass fraction, correctly estimated biogeochemical fluxes (for both water vapor and CO<sub>2</sub>) despite incorrectly describing transport mechanisms. Therefore, the WPL methodology predicts that artificially eliminating the effects of water vapor (dilution and displacement) and expressing each gas with reference to dry air will yield the equivalent flux-gradient relationships. Furthermore, by assuming all scalars (temperature, water vapor,  $CO_2$  and  $O_2$ ) are transported similarly (and thus assuming the eddy diffusivities  $K_o$ ,  $K_c$ ,  $K_T$  and  $K_v$ are the same), we have added an additional uncertainty. Also due to the change in the vertical gradients, the estimation of  $ER_{conc}$  will be affected, because the displacement by evapotranspiration has a different impact on  $CO_2$  and  $O_2$ . However, again for the mole fractions regarding dry air, the effect should be small. Also, the estimated  $ER_{conc}$  (and also  $ER_{eco}$ ) were reasonable and in line with current process understanding."

#### Minor comment 1:

Throughout the paper: I believe all instances of "a posteriori" and "a priori" should be italicized. Also, throughout, I am pretty sure that "et al." should also be italicized. *Yes, done a suggested. All the* "a posteriori" *and* "a priori" *are in italic now. Following the author's guide of Biogeosciences, "et al." does not need to be italicized.* 

#### Line 13: Please provide a citation for the 1.10 value of ER

The corresponding citation for the ER value 1.10 is Severinghaus (1995), doi:10.2172/477735. However, we would prefer not have a reference in the abstract, but leave it to the editor and reviewer to decide if we should include it or not. The reference is given later in the introduction.

Line 16 and elsewhere: Please choose a tense for the manuscript and make it consistent throughout. I suggest the past tense, so in line 16, change "explore" to "explored". *Done as suggested. We checked the entire manuscript.* 

Line 20: Please change to "that the modeled annual mean..." to make it very clear that this is *not* an observational result. *Done as suggested (line 20).*  Line 24: This wording here is confusing. I think you mean "...could be derived with the fluxgradient method using measured vertical gradients in scalar properties, as well as fluxes of CO<sub>2</sub>, sensible heat, and latent energy, all derived from eddy-covariance measurements." Please use this, or some other clarifying wording.

Done as suggested (lines 23-25).

Lines 38-39: This should read " – ranging from hourly to decadal, and from leaf to global, respectively. Since the relationship of  $O_2$  and  $CO_2$  fluxes…" We rephrased it as follows (lines 39-40): "– ranging from hourly to decadal scales temporally and from leaf to global scales spatially, respectively."

Line 50: This should read "...indicating that the ER needs to be..." *Done as suggested (line 52).* 

Line 56: This should read "over a six-year period with" *Done as suggested (line 58).* 

Line 67: This should read "...in this study. Very few studies..." *Done as suggested (line 69).* 

Line 76: This should read "(Seibt et al., 2004). As described by Battle et al. (2019)" *Done as suggested (line 79).* 

Line 119: This should read "...of ER variations at the ecosystem scale" *Done as suggested (line 123).* 

Line 129: This should read "...and ER can be plausibly simulated for" *Done as suggested (line 132).* 

## Line 152: Are these properties measured at 44m above the forest canopy (as stated) or 44m above the forest floor?

Thank you for catching this error. The eddy covariance measurements are conducted at 44m above the ground level (line 156).

#### Line 171: I'm not sure to what fit this R<sup>2</sup> value refers.

For clarification we rephrased the paragraph as follows (lines 174-179): "Atmospheric  $O_2$  mole fraction ( $O_2$  atm) as input for the model was deduced from a fixed  $O_2$ :  $CO_2$  mole ratio of -1.15 mol mol<sup>-1</sup> and continuous  $CO_2$  mole fraction measurements at the site (Table 1). The fixed  $O_2$ :  $CO_2$ 

mole ratio was derived from measurements at the University of Göttingen from November 2017 to January 2018 using a high-precision  $O_2$  measurement system developed by Dr. Penelope Pickers (University of East Anglia, UK) and very similar to the system described in Pickers et al. (2017). For these measurements, the correlation between  $O_2$  and  $CO_2$  mole fractions had an  $R^2$ = 0.99."

Line 178/179: No line break *Done as suggested (line 183).* 

Line 184: This should read "LAI increased and decreased linearly, respectively." *Done as suggested (line 190).* 

Line 184-186: The sentence beginning "The maximum LAI..." seems to me like it really belongs in the site description.

*Yes, please see lines 150-151: "The canopy height (ht) was 37.5 m and the effective leaf area index (LAI) was at maximum 4.8 m<sup>2</sup> m<sup>-2</sup> in the growing season in 2015 (Braden-Behrens et al., 2017)."* 

Line 200: This should read "...2014 to 2016. To quantify the model..." *Done as suggested (line 210).* 

Line 230: This should read "For the model simulations, ER can be obtained for the entire ecosystem, the net assimilation at the leaf level, or for only respiratory processes by considering..."

Done as suggested (lines 245-246).

## Line 275: Is the gradient of O2 best represented by " $\Delta$ o" or " $\Delta$ o/ $\Delta$ z"?

In the entire manuscript, we now use ' $\Delta$ variable' for differences of a variable (CO<sub>2</sub>, O<sub>2</sub>, temperature, etc.) between two heights, between measurements and simulation, or between fluxes derived by simulations or based on flux-gradient method (see comment below). ' $\Delta$ variable/ $\Delta z$ ' always refers to a vertical gradient.

Line 315: I don't understand the use of the word "even" here. *We deleted now the word 'even' (line 336).* 

Line 436: Here and afterward, I suggest you use " $\Delta$ " instead of "diff". I find "diff<sub>xxx</sub>" very visually distracting. With "Fxxx" all as a subscript, there won't be any confusion with other  $\Delta$  terms. *Done as suggested throughout the entire manuscript*.

Lines 439-445: This information all really belongs in a table. Having one to which we can easily refer (and changing "diff" to " $\Delta$ ") will make this section much, much easier to read. *Done as suggested. We have added the following table to the manuscript (lines 486-492):* 

Table 3. Difference between the  $F_{0_2}$  estimations derived by the flux-gradient method ( $F_{0_2,(c,T,v)}$ , based on  $F_{C0_2}$ ,  $H^{\sim}$  or  $LE^{\sim}$  and their respective vertical scalar profile) and by model simulations ( $F_{0_2,CANVEG}$ ) for above canopy fluxes and for day- and nighttime individually. Results of the two-height approach are shown as the mean and standard deviation of flux-gradients derived between z/ht = 2 and each layer below above the canopy. Also results of the three-height approach are shown, where the flux-gradient was derived between three fixed heights (z/ht = 1.05, 1.45 and 2 with ht = 37.5 m).

variables	two heights		three heights	
$(\mu mol \ m^{-2} \ s^{-1})$	daytime	nighttime	daytime	nighttime
$\Delta F_{O_2,c}$	$0.030 \pm 0.09$	$-0.53 \pm 0.04$	-0.13	-0.50
$\Delta F_{O_2,T}$	$1.55 \pm 0.54$	$-1.98 \pm 0.20$	-4.31	-2.41
$\Delta F_{O_2,v}$	$-4.26 \pm 0.63$	$-0.47 \pm 0.24$	4.72	-0.66

Line 453: This should read "...the heights with" and "...1.05 were used in" ("finally" is confusing to me)

We rephrased the sentence as follows (lines 499-500): "To guarantee a large gradient, the heights with z/ht = 2 and z/ht = 1.05 were used in inferring  $F_{O_2}$  from vertical CO<sub>2</sub>, temperature and water vapor gradients for the following analysis."

## Line 469: Shouldn't this be "net assimilation" (rather than gross)?

For clarification, we rephrased the sentence as follows (lines 515-517): "..., when  $O_2$  mole fractions increased with decreasing height above the canopy due to prevailing gross assimilation over respirations during daytime."

Figure 5 caption: The organization of the plots by column (day and night) is good, but please put labels ("day" and "night") in the individual plots themselves so we can immediately interpret them. Also, in the legend of panel c, you use  $\Delta C$  for CO2, when in fact it's not a difference or anomaly (unlike the O2). Better to just use "CO2". Also, for oxygen, I'd prefer the legend read "O2" or "O2 anomaly", or at the very least " $\Delta O2$ "

We have applied the suggested improvements of the figure and legends (lines 521-529).

Figure 6 caption: The last sentence is ambiguous. It's not clear whether it applies to only Plot D, or to all of them. Again, I would prefer something other than " $\Delta o$ " for the oxygen anomaly. *The last sentence refers only to panel (d). To clarify, we rephrased the sentence as follows (lines 539-540): "In order to include daytime hours with an active canopy for the estimation of*  $\sigma_{F_{O_2}}$ ,  $\Delta o \ge 1$  ppm was used as a filter, assuming higher oxygen dry air mole fractions close to the canopy than in the top domain layers."

## Line 532: What is meant by "lower performance"? Are the predicted energies lower, or is there some metric of agreement to which you're referring? Please clarify.

Yes, we meant the model performance in regard to some metrics. We added this information as follows (line 584): "The model performance (in regard to the slope,  $R^2$  and RMSE) in the energy fluxes was generally lower than for  $CO_2$  flux simulations."

Line 565: This should read "...2019). In addition, dry or wet" *Done as suggested (lines 617-618).* 

Line 568: This should read "...level. Worrall et al. (2013) also derived" *Done as suggested (line 620).* 

Line 573: This should read "bulk soil, measured ERsoil varied" *Done as suggested (line 625).* 

Line 575: This should read "processes strongly suggest that" *Done as suggested (line 627).* 

Line 581: This should read "change by 10% increments" *Done as suggested. We have moved the paragraph to the Results section (line 375).* 

Lines 587-588: This should read "...(ERzeco). The temporal variations in EReco arose from diel and..." *Done as suggested (line 646).* 

Lines 589-590: As it stands, this is not a sentence (and it's confusing). Please correct/clarify. *To clarify, we rephrased the sentence as follows (lines 647-649): "Since assimilation and respiration are two individual processes, which are influenced by two differing main drivers - photosynthetic photon flux density and temperature - they usually show shifted diel cycles."* 

Line 591: This should read "fluxes from respiration" *Done as suggested (line 650).* 

Line 595: This should read "information about the turbulent flux exchange, as well as the" *Done as suggested (line 654)*.

Line 600: I am puzzled by "between our studies". I think you mean "between Seibt et al's

work and ours" *Done as suggested (lines 659-660).* 

Line 610: This should read "by the utilization of varying nitrogen sources". Also – haven't you made an effort to include some of these diverse sources of nitrogen in your model? Perhaps you're saying that the balance of nitrogen sources in the model might be wrong, but as written, it reads as if your model has no nitrogen sources at all.

Done as suggested (line 669). In the here used model version, we do not consider nitrogen. Another model study about the effects of nitrogen sources on  $O_2$ :  $CO_2$  exchange ratio of gross assimilation is under preparation.

Line 613: This should read "and sinks, and the turbulence" *Done as suggested (line 672).* 

Line 616: This should read "recently found by Fassen et al. (2022). We also" *Done as suggested (line 675)*.

Line 619: This should read "forest over a six-year period" *Done as suggested (line 678).* 

Line 630: This should read "modeled ERzconc was excessively influenced" *Done as suggested (line 689).* 

Line 632: This should read "which have become" and "at eddy covariance sites in forests." *Done as suggested (lines 691-692).* 

Line 641: This should read "mole fraction gradients, we confirmed that the selected heights should both be above the canopy." *Done as suggested (lines 701-702).* 

Line 670: This should read "We also test this three-heights" *Done as suggested (line 730).* 

Line 694: This should read "due to leaf temperature. Implementing variable" *Done as suggested (line 798).* 

Line 698: This should read "derived using the eddy" *Done as suggested (line 802).* 

Line 725: This should read "based on, for example, long term chamber measurements, will greatly help"

Done as suggested (line 830).

## **References**

Braden-Behrens, J., Yan, Y., and Knohl, A.: A new instrument for stable isotope measurements of 13C and 18O in CO2 – instrument performance and ecological application of the Delta Ray IRIS analyzer, Atmos. Meas. Tech., 10, 4537-4560, 10.5194/amt-10-4537-2017, 2017. Keeling, R. F. and Manning, A. C.: 5.15 - Studies of Recent Changes in Atmospheric O2 Content, in: Treatise on Geochemistry (Second Edition), edited by: Holland, H. D., and Turekian, K. K., Elsevier, Oxford, 385-404, doi:10.1016/B978-0-08-095975-7.00420-4, 2014. Kowalski, A. S.: The boundary condition for vertical velocity and its interdependence with surface gas exchange, Atmos. Chem. Phys., 17, 8177-8187, 10.5194/acp-17-8177-2017, 2017. Kowalski, A. S., Serrano-Ortiz, P., Miranda-García, G., and Fratini, G.: Disentangling Turbulent Gas Diffusion from Non-diffusive Transport in the Boundary Layer, Bound-Lay Meteorol, 179, 347-367, 10.1007/s10546-021-00605-5, 2021. Pickers, P. A., Manning, A. C., Sturges, W. T., Le Quéré, C., Mikaloff Fletcher, S. E., Wilson, P. A., and Etchells, A. J.: In situ measurements of atmospheric O2 and CO2 reveal an unexpected O2 signal over the tropical Atlantic Ocean, Global Biogeochem Cy, 31, 1289-1305, doi:10.1002/2017GB005631, 2017. Severinghaus, J.: Studies of the Terrestrial O2 and Carbon Cycles in Sand Dune Gases and in Biosphere 2, doi:10.2172/477735, 1995.