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Interactive comment on "Estimating global gross primary productivity using chlorophyll fluorescence and a data assimilation system with the BETHY-SCOPE model" *by* Alexander J. Norton et al.

Alexander J. Norton et al.

nortona@student.unimelb.edu.au

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We thank the referee for their comments. Here we provided a response to each comment. We hope that this new version is much improved. Note that original referee comments are enclosed in < > symbols.

While we have made the necessary changes following the referee comments, we have also rearranged and clarified parts of the discussion. We also noticed that we include one figure both in the manuscript and in the supplementary material. This has been

removed from the supplementary material

<GPP is the largest carbon flux and constraining it is very important for understanding the terrestrial carbon sources and sinks. This paper presents a method to estimate the GPP in a data assimilation system based on the OCO2 SIF products. Compared to previous studies mainly based on the linear relationship between SIF and GPP, this paper adopts the process-based manner in which terrestrial biosphere model explicitly simulates the GPP and SIF. It is a new pathway to constrain GPP using the satellite SIF products.

Also, there are some concerns about the results. I list them as follows: Several major concerns:

(1) Actually I also noticed your previous online version about this paper (Norton et al., 2018, Biogeosciences Discuss). I find that GPP can be largely increased by 31% in this new manuscript, while it was only increased by 7% in the previous one. So what's the difference in the background assimilation process? I carefully compare the prior parameter values in the Table A1, and find the only differences in the chlorophyll ab content (Cab). Is this the only difference? >

Given that RC1 made a similar comment made, we provide the same response that we gave to RC1: Given the questions from both referees, it is perhaps helpful to point out the specific differences between our last assimilation setup and the present one. While it is not a focus of the paper to distinguish between these two, it is useful to present this in more detail here than is feasible in the manuscript. Here are the major differences in the assimilation setup between our current manuscript and the previous version to which the referee refers to: (i) The prior chlorophyll (Cab) parameters are set to be higher. The prior Cab parameters presented in the earlier version were too low (with a PFT average of 13 μg cm-2). This is not considered realistic as anything below ~20 μg cm-2 suggests light interception is very low and will strongly limit photosynthesis (see Fig. 3.4 in Bjorkman, 1988); this is not expected under most natural conditions.

This change in prior Cab values means our sensitivities (the slope of SIF with respect to Cab) were too large, as the expected change in SIF from Cab would be very large given it is strongly light-limited. The effect of more realistic Cab values would be an increase in APAR and increase in GPP. We also set the 1-sigma prior uncertainty of all Cab parameters to be a consistent 10% of the mean value. (ii) The APAR provided to the photosynthesis module was total APAR in the previous version. In the SCOPE model, the total APAR represents the absorbed radiation by all canopy leaf elements. However, only green chlorophyll directs absorbed radiation to photochemistry. The model was therefore altered so that the green APAR was provided to the photosynthesis module, a change that has also been made to a more recent version of the SCOPE model. The effect of this more realistic model setup would be a decrease in APAR provided to GPP, hence a decrease in GPP. (iii) The version of Fluspect used in our last submission was not actually that of SCOPE v1.53. Therefore, we had to update the version of Fluspect in our model. Fluspect simulates the leaf level fluorescence and calculates the leaf level reflectance, transmittance and absorbances. The main issue was that the fluorescence quantum efficiency used in Fluspect (termed "fqe") was the same for photosystem I and II, but actually the values should be such that photosystem I is one fifth the value of of photosystem II. Therefore, the simulated SIF would have too high a contribution from PSI, which is not affected by physiological changes e.g. Vcmax.

These changes therefore include a change in model formulation and the prior parameters. We are confident that these changes make the model more realistic. The first two changes, i and ii, also have opposing effects on GPP, hence the prior GPP is similar between the current manuscript and previous version. The major difference is therefore in the sensitivities between SIF and the parameters, particularly Cab. This means our Jacobian matrix (H) is also different. The third change, iii, changes SIF but not GPP, but it will change the Jacobian matrix (H) as the contribution photosystem II to canopy SIF is larger and it is this photosystem that is regulated by physiological feedbacks. In layman's terms, the assimilation has different knobs and dials that it can use to minimise the cost function. If the model formulation or the Jacobian changes, these knobs

and dials will change in size and strength, thus the posterior will also change.

There are a couple of notable differences in the posterior parameter set that probably cause the higher global GPP is in this version: (i) posterior Cab and leaf angle distribution (LIDF) parameters are different, with Cab being higher on average than our previous version (average of 13 PFTs is 22 μg cm-2 compared to 5 μg cm-2 in the last version), hence the new parameter set has higher APAR; (ii) the posterior Vcmax is slightly higher than the last version, with a PFT average of 61 μmol m-2 s-1 in the current version and 57 μmol m-2 s-1 in the previous version. This results in a higher APAR and higher LUE, hence higher GPP.

To address this, we have added a model version (now BETHY-SCOPE v1.1) to the methods to distinguish this version of BETHY-SCOPE from the previously submitted manuscript as well as the one used Norton et al. (2018) GMD paper (BETHY-SCOPE v1.0). We have also added a comment in the model description section of the Methods to highlight the changes: "In BETHY-SCOPE v1.1, the key changes are (i) the correction of an error in the Fluspect module where the fluorescence quantum efficiency (fqe) for PSI and PSII were set to be equal, while SCOPE v1.53 sets fqe for PSI to be one fifth that of PSII, and (ii) the leaf biochemistry module is now driven by green APAR (as mentioned above), rather than total APAR that is used in SCOPE v.153."

<You mentioned that the Cab is set more in line with physiological understanding here (P6 Line 33-34). So what's the reference? > The reference is Bjorkman (1981). This study showed how chlorophyll concentrations below about 15-20 ug cm-2 cause steep declines in photosynthetic efficiency as only a very small fraction of light is intercepted at these concentrations. Optimal plant behaviour will act to prevent this.

<If only tuning the prior Cab values makes the large difference, how to explain? The Cab value is only related to SIF not to GPP.> Firstly, please refer to our extended response to your concern (1) above, as this addresses this comment as well. Briefly, we note that changing the prior Cab values causes a change in the Jacobian matrix

and will subsequently change how the assimilation minimises the cost function. We also note that Cab is actually strongly related to both SIF and GPP via APAR.

<(2) As you mentioned that the calculation of observation uncertainties is an important aspect of the data assimilation study. You calculate the observation uncertainty with a scale of 1/2 (Equation 4, P8 Line 11-20). How do you determine this scale? Sensitivity experiments? >

This scale, as we point out in the methods section 2.3.1, places our uncertainties roughly in the middle of the two extreme (and incorrect) ways of determining uncertainties. While rather arbitrary, in the end it's the reduced chi-squared statistic that determines whether we have selected appropriate uncertainties, including our choice of a $\frac{1}{2}$ scaling. We perhaps did not make this clear enough in section 2.3.1. So, we have added a specification in section 2.3.1 that the statistical tests used to test whether this is appropriate is the chi-squared test. This sentence now reads: "Statistical tests on the results, using the so-called reduced chi-squared statistic, allow us to test whether these observational uncertainties are consistent with other aspects of this data assimilation process, as outlined further below."

We also make a change in the results section where we report the posterior reduced chi-squared test. We make sure to refer back to the uncertainty calculation and the use of the $\frac{1}{2}$ scaling. This now reads: "The global χ_r^2 fit is strongly reduced from 2.45 to 1.01. This is close to the optimal value of one, demonstrating the ability of the optimized model to fit the observed patterns of SIF and validating our chosen uncertainties as far as is practicable, including the choice of the scaling used to calculate observational uncertainties in Eq. \ref{eq:1}."

<(3) P19 Line 9-10. You say that the changes in the posterior GPP can differ in sign and magnitude from the changes in posterior SIF. You explain it as a result of the non-linear effect in the process-based approach. First, you use the same SIF module as your previous manuscript (Norton et al., 2018, Biogeosciences Discuss)? It seems that

the non-linear effect is not obvious in the previous one, but significant in this one, why? >

In fact the same effect could occur in the previous manuscript and it did in some areas. We just hadn't highlighted it as a result. We believe it is an important result and a distinction of this process-based method that separates this study from those using empirical, linear relationships between SIF and GPP. We discuss this in detail in the Discussion section (P25, L26-35).

To clarify this, we have changed this line to: "We note that these changes in model GPP can differ in sign and magnitude from the changes in model SIF (see supplementary material Fig. S18 and S19). This can occur as SIF and GPP have differing sensitivities to the underlying parameters, a result of the process-based approach."

<Second, If the nonlinear effect is obvious, how can we determine the GPP can be truly optimized? > Just because the relationship is non-linear, this doesn't mean it is non-unique. Weather forecasting uses non-linear models for example. Many other inverse problems handle this. The problems arise if solutions are not unique. We do not see any suggestion that this is an issue. The posterior parameter values would likely reach into unphysical values if this was the case.

<(4) P15 Line 1-3. You say that the SIFprior does not show this systematic underestimation, but has a poorer global fit (Fig. S3). If we look at the Figure S3, we can find that modeled SIF in lots of grids keep near constant (below 0.5). Or actually the scattering turns out the linear relationship is not statistical significant. But you show the $p < 0.001$, I think it is because you do not calculate the effective degrees of freedom, instead that you use the number of the points to calculate the p values. So the SIF module itself has large model errors. > We calculate the reduced chi-squared statistic to evaluate the prior and posterior fit to the observations (Figs. S3 and S4), not the linear regression line or p-value. The reduced chi-squared statistic takes into account the number of degrees of freedom. The p-value you refer to is a simple p-value from

the linear regression. We used the linear regression simply to show what a linear regression fit looks like when fitted to the model vs observed data (i.e. is the slope near to one?), not as an actual test of the fit. We only report the reduced chi-squared statistic in the manuscript text. To ensure the p-value is not misleading other readers, we have removed it from the figure altogether.

<(5) In Section 3.2, you show the results about the posterior parameters. You say "we can be more confident in parameters that see large reductions in uncertainty. Conversely, parameters with little reduction in uncertainty following optimization should be accepted cautiously." Actually, in the data assimilation, the uncertainty should be more or less reduced owing to the mathematics. But the reduction of the uncertainty does not mean the optimized parameters are more accurate, because parameter optimization accounts for the LAI uncertainty, model structural uncertainty etc. In fact, posterior parameters can only partially improve the SIF simulation. In Figure 4, we can see the posterior SIF is more in line with the observed SIF. Therefore, the posterior parameters may be over-tuned. So is it possible to validate the posterior parameters based on the other datasets. > Yes, the referee is, in principle, correct. The uncertainty reductions are somewhat a measure of how exposed the parameters are to the observations (accounting for uncertainties of course). We cannot be sure that the parameters are accurate. This is relative though. Ultimately, a parameter that has no uncertainty reduction should not be accepted as being "constrained" by the data. A parameter that has a large uncertainty reduction should not be accepted as being accurate but can be relatively more accepted than one with no uncertainty reduction. As this statement is just relative, we have added "more" before cautiously.

Specifics:

<(1) P1 Line 19. "(see Anav et al., 2015)/P2 Line 7 (see Baccour et al., 2015; . . .)" ->remove the 'see". > Done, thank you.

<(2) P 6 Line 11 "Overall, the modelled link between SIF and GPP occurs via the

above equations" ->actually it is not clear according to the above three equations. > If you consider that Ag is gross photosynthetic rate and ÐďF is the fluorescence yield, then these equations outline how the model links the two. However, if the referee can indicate what is not clear about these equations, or how to make it better, we're open to making changes.

<(3) P9 Line 11. Miss an "and". Should be "by the uncertainties in the observations Cd and model parameters Cx, respectively". > Good catch thank you. Amended.

<(4) P11 Line 7-8. I cannot clearly understand the sentence "... but forced by the respective monthly mean diurnal cycle such that a single diurnal cycle is simulated for each month". > Yes, I can see how this might be confusing. This has been changed to ". . .a single, average diurnal cycle of meteorological forcing for each month is used to simulate photosynthesis and fluorescence. This allows the computation of SIF at the equivalent overpass time as the satellite data (1:00 - 2:00 p.m. local time)."

<(5) Figure2 and Figure 3 can be presented in the same color bar. > Does the referee suggest combining these two Figures into one and just using a single color bar? This can probably be done during the typesetting phase.

<(6) P13 Line 14 "underestimate large observed SIF values > 0.5 W/m2/sr/um". > The systematic underestimation of SIF only occurs beyond about 1.0 W m-2 sr-1 um-1. We can see from Fig. S4 that there a numerous spatiotemporal grid cells where model SIF is > 0.5 W m-2 sr-1 um-1. Hence, we have kept this as 1.0 W m-2 sr-1 um-1.

<(7) P15 Line 5 "This is largely because of observed SIF values that are slightly negative". Can it be shown in Figure 1 with the negative color bar. > Okay, we have changed Fig. 1 so that grid cells with negative values show up as white, and a new color bar that reflects this. Thank you for the suggestion.

<(8) Section 3.1.3 "A case with seasonally Varying Parameters" can be regarded as a discussion in the Section discussion. > Okay. We discussed this ourselves about

where best to place this. Note what comes next. There are new results presented based on this seasonally varying case in section 3.1.4 “Fit to the Seasonal Cycle”, which would not make sense if the “case with seasonally Varying Parameters” was in the discussion. Therefore, we have kept these results where they are.

<(9) P16 Line8-12 Is it possible add an equation here. > Okay, we’re happy to add the equation into the supplementary material, perhaps a better place as readers can find it if they’re interested. We don’t think it’s pertinent to understanding our sensitivity test.

<(10) P 16 Line 17-18 “..with R2 increasing from 0.74 to 0.77 and the slope increasing from 0.67 to 0.71. This indicates that the systematic under- estimation of large observed SIF values may be improved.” This conclusion is vague without the figures. > Ah yes, good point. We should have included them. We have added in the required figures to the supplementary material.

<(11) P20 the comparison between FLUXCOM and posterior GPP over the North America. The spatial correlation has an improvement with increasing correlation coefficient from 0.89 to 0.95. However, the amplitude is much larger than the FLUXCOM GPP. So it is improved or turns out poorer because you also mentioned the FLUXCOM GPP over north American and Europe may represent the actual GPP? > The simplest answer is that the spatiotemporal patterns are ‘improved’ but the magnitude gets ‘worse’ with respect to the FLUXCOM product. As discussed to the first referee, the true GPP is not known so we cannot be sure which estimate is correct. They’re probably both wrong. So, we have removed the comment on “and thus where we expect it to better represent actual GPP”. Nevertheless, we think this is the best comparison we can do between FLUXCOM and our SIF-based GPP considering the spatial scale. If the referee has a better idea of how to validate GPP we’re open to suggestions.

<(12) Maybe can adjust the orders of the Appendix figures. You first describe the Figs. B5 B6, then describe the Figs. B2 B3. > Amended.

<(13) P22 Line6. You say “In both of these studies an increase in tropical GPP was

found”, In Macbean et al., 2018, the posterior GPP seems a reduction? > Thanks for catching this. We are actually referring to the relative contribution to global GPP, in which their study sees the tropics increase relative to extratropics. Even so, in this paragraph our comment on our own results was not quite correct. We have actually changed this paragraph altogether, so this issue is no longer present.

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