

Zhu et al. present a new assimilation model NUCAS v1.0 for simulating carbonyl sulfide (COS) fluxes at ecosystem scale. The model is a good addition to the COS modeling pool, but the study requires some modifications and the paper lacks important information and is in many places too ambiguous and inconsistent.

General comments:

The paper lacks consistency on terminology used throughout the paper. Examples: in Eq. 1 observation is marked with O and model with M while in Eq. 12 they are marked with c and s and in Eqs. 14-16 they are marked obs and sim, respectively. Soil moisture is sometimes marked with SWC and sometimes as  $\Theta$ . Section 2.1.3 is full of examples (listed below in more detail). This makes the paper very difficult to follow for the reader.

The authors model soil and plant COS fluxes separately but only report the total ecosystem flux. However, it would be interesting to see the simulated soil and plant fluxes separately and see how they compare with measured chamber COS fluxes from the different sites and also with e.g. other soil models.

Some coefficients and uncertainty estimates used in the paper are very poorly explained. Where does a perturbation rate of 0.4 come for some sites while for others it is 0.2? How do the authors come up with an uncertainty of  $1 \text{ pmol m}^{-2} \text{ s}^{-1}$  for the prior simulated COS flux (L275)? Section 2.1.3 is also filled with these coefficients, listed in more detail below.

The benefit of the “multi-site” assimilation is unclear since it produces more or less similar results as the single-site assimilation. This is primarily due to using only two sites in this assimilation. The use of the word “multi” is thus exaggerated and I suggest leaving this part totally out of the paper, since it does not bring any notable improvement to the model. I understand that using only two sites is due to lack of in-situ COS flux measurements in similar ecosystems, but I don’t really see a point doing a two-site assimilation since the results will be very similar to single-site assimilation.

I have several comments regarding the use of measured COS flux data:

- all sites: The authors do not specify any quality criteria used to filter the measured fluxes. Usually eddy covariance flux data are given a quality flag from 0 to 2; 2 indicating poor quality fluxes that should not be used, 1 indicating medium quality fluxes that are fine for budget calculations and 0 indicating the best quality that should be used for functional relationships and modelling. Please specify if you have used quality filtering in the data and if not, please give reasons why.
- US-Wrc: The dataset provided by Rastogi et al. 2018 does include the ready calculated gradient fluxes, and it is unclear why the authors are not using those fluxes but give a very ambiguous explanation of their own gradient flux parameter calculations. Moreover, since US-Wrc fluxes were calculated partly from the simulated COS fluxes in this study, this introduces a huge bias to these fluxes which gives even more reason not use this site in the “multi”-site assimilation.
- FI-Hyy: The dataset provided in Vesala et al. 2022 and Kohonen et al. 2022 already include storage corrected COS fluxes and it is not clear why the author have decided to do another storage correction for this site but not to other sites. In addition, this dataset includes gap-filled COS fluxes and it is not clear if the authors have used the gap-filled fluxes or the direct measured fluxes since the authors have not given any information on quality filtering.

Simulation of sensible and latent heat fluxes as well as SWC seems quite out of place. Can you explain how COS fluxes should be related to sensible heat flux, and why assimilating COS fluxes should

improve simulated sensible heat flux and soil moisture? Simulated sensible heat flux has even a different direction than the measured one. I suggest to leave this part out of the paper.

The abstract is too ambiguous and no concrete results are given. The authors use expressions “various processes” and “various ecosystems” without providing any details that would be useful for the reader.

The authors need to mention in the method section if they use one-sided or all-sided LAI data, and if that applies everywhere in the paper or not. Also specify if negative fluxes mean uptake or emission. The word “significantly” is thrown around a lot, without any relation to statistical significance, it seems.

Section 2.1.3 needs to be rewritten, especially regarding the equations that are inconsistent and lacking information. Specifically:

- Where is  $F_{cos,leaf}$  used in the model? It is not present in any other equations after Eq. 3
- The authors need to explain where the different coefficients (e.g., 1.94 and 1.56 in Eq. 3; 1.4, 1.0, 5.33, -0.45 in Eq. 4; 0.437 and 0.0984 in Eq. 6; -0.00986, 0.197, -9.31 in Eq. 9; -0.119, 0.110, -1.18 in Eq. 10, and 0.28 and 14.5 in Eq. 11) come from; what they represent and what is the reference.
- What is  $f_{sw}$  (how it is defined, is there an equation, what unit does it have and what kind of variation does it have) exactly.
- $V_{cmax}$ ; what is the unit and how do you get values (and which values) for it?
- $F_{cos,biotic}$  suddenly changes to  $F_{\theta g}$  in the switch from Eq. 7 to Eq. 8, if I got it right. Be consistent with the terms, as this is impossible to follow as a reader!! Also, where does  $\Theta_i$  go in between these equations?? Is it switched to  $\Theta_g$ ?
- How is “optimum soil moisture” defined? Optimum in terms of what?

In general, there is lot of repetition throughout the paper and the text could certainly be condensed.

Finally, I would like to see scatter plots in addition to the diurnal variation comparison, to better see how the model is able to simulate the COS fluxes and GPP.

Specific comments:

L19: “various processes” is too ambiguous

L25: “various ecosystems”; please specify which ecosystems

L26: “can significantly improve”; how much did it improve, which timescale, which ecosystem(s) etc?

L34: “carbon dioxide (CO<sub>2</sub>)” since this is the first time

L 47-49: I don’t really see a point in repeating the same references twice in the same sentence

L55: Wohlfahrt et al 2012 and Kooijmans et al 2019 present an empirical model for leaf relative uptake (the uptake ratio of COS and CO<sub>2</sub> at the leaf scale) but do not model COS flux itself

L58-60: This sentence is very unclear and I am not sure what the authors want to emphasize here. Please rephrase

L71-75: Please rephrase this sentence and preferably split it in two. At the moment it reads like Liu et al 1997 developed a model for simulating COS fluxes (which is not the case).

L78: Since you do not assimilate COS fluxes in all ecosystems existing, please specify which ecosystems you are talking about here

L79: Controlling factors in which time scale of variability? E.g., in yearly scale temperature and radiation are for sure the most important drivers for carbon fluxes since they drive the seasonality, but this might not be the case in sub-daily time scales.

L81: List the ecosystems

L96: all-sided or one-sided LAI?

L98: "phenology is driven by LAI" but isn't it the other way around?

L103: remove one "of the"

L148: "pmol/m<sup>2</sup>/s" -> should be pmol m<sup>-2</sup> s<sup>-1</sup> and units are not supposed to be written in italic. Check this everywhere in the paper, also with other units like m<sup>2</sup> m<sup>-2</sup>

L153: "And the leaf-level" -> "The leaf-level"

L156: Are the conductances different for shaded and sunlit leaves?

L179: Do you perhaps mean Table S2?

L187-195: It is quite strange to cite here not the papers whose data you use but other papers from those same sites. Please cite the papers whose data you are using.

L189: ICOS is not defined (Integrated Carbon Observation System)

L199-201: Specify that you use ecosystem scale eddy covariance (or gradient) flux measurements.

Sect. 2.4.1: I don't understand how the authors decided that the GLOBMAP LAI product was too low for the DK-Sor site but not for other sites. I did not find this information from Spielmann et al. 2019, as the authors claim. Please elaborate.

L224-226: I am sure US-Ha1 site has some radiation data, at least PPF data if not shortwave radiation, as well as air temperature and relative humidity. In-situ data is for sure better than the ERA5 data.

L235: Table 1 does not list soil measurement information (and not the references either)

L248-250: Now this is very confusing. In Kohonen et al 2020 the uncertainty is high **with low absolute fluxes**, the fact there is a stronger peak in negative fluxes is simply due to lack of observations of positive fluxes. In Kohonen et al. 2020 the negative fluxes are defined as uptake by the biosphere. In any case there should be no reason to remove either positive or negative fluxes, unless the quality criteria are not filled!

L254: "gross primary productivity" -> "GPP"; "sensible heat" -> "H"; "latent heat" -> "LE"

L257: Cite Reichstein 2005 for the nighttime partitioning method

L260: How is nighttime defined?

L280: "And as a..." -> "As a.."

L296: Do you really mean that only one set of model parameters is required, independent of the ecosystem type? I would assume e.g. Vcmax to be quite different for different ecosystems and PFTs.

L307: I don't understand where the number 76 comes from. In table S2 there are 11 different parameters and their values are repeated as a constant value to get to 76, but there are certainly not 76 different parameters?

L310: "correlation" -> "coefficient"

L330: "dozens" -> please give an exact number

L335-337: This sentence is too vague. Please be more specific.

L337-339: Where are these parameters used? Not in the COS model presented earlier

L353: 1.64% is very low, how do you explain that?

L357: Figure 3 comes in the text before Figure 2 is presented

L360: Could this have something to do with the dry conditions and stomatal limitations, discussed in Vesala et al. 2022 regarding the low COS fluxes at FI-Hyy in July and August 2014?

L378: "for all experiments" -> not true for IT-Soy and US-Ha1!

L385: Can this even be called an increase? In any case very low correlation coefficient.

L387: Why are the simulated nighttime fluxes unchanged?

L400: "due to high value of observation" or rather underestimation by simulation?

L412: I would not call two sites multiple sites....

L422: Can the ratio between PAR and SW really change that much? Why is it allowed to change so much?

L429: Either "In particular," or "Particularly"

L444: "underestimated (by 55.72%), ..."

L444: "greatly increased"; how much?

L445: "...simulations of COS **flux** at FI-Hyy.."

L468: "forest sites (DK-Sor, FI-Hyy, US-Ha1, US-Wrc) compared to grassland and savanna (AT-Neu and ES-Lma)"

L489-491: GPP cannot be observed directly, it is always a model!!

L502: "excellent match" needs quantification

L513-515: Not a very convincing result with the multi-site assimilation though

L515-520: How would the results be without COS assimilation?

L523: It is not possible that there would not be sensible heat flux measured at a site where other eddy fluxes are measured, since it comes directly from the sonic anemometer used for wind measurements. If the authors have not published their sensible heat flux data, you can ask for it from the authors.

L525: "And the assimilation.." -> "The assimilation.."

L536 & L554-556: Refer to the supplement figs

L571: "not significant" by what metric? What is a "short period of time"?

L573: “almost no diurnal...” very vague, be more specific

L578-580: This is not really true, especially in the end of August (but other months are also underestimated)

L583-585: Refer to the supplement figs

L592: “COS fluxes of soil” -> “soil COS fluxes” or “COS fluxes from soil”

Sect 4.1: Would it make sense to limit  $f_{\text{leaf}}$  and  $V_{\text{cmax25}}$  variability to reasonable scales?

L635: But since soil COS fluxes are low, wouldn't that lead to higher change in the parameters, to compensate for low fluxes..?

L652-655: Already mentioned in the previous section”

L662: Could this be due to drought/ drier than normal conditions at FI-Hyy reported in Vesala et al. 2022?

L691: Table 1 perhaps?

L706: Which in-situ LAI data was used for FI-Hyy? Maybe the other one is all-sided and the other one-sided LAI?

L720: Start a new sentence “More laboratory...”

L728: Why are the authors not already refining the uncertainty of prior values in this study?

L735-738: Given that this is already known, why is the COS concentration variation not already taken into account in this model?

L749: Plants in lower rainfall conditions could also be e.g. CAM plants?

Data availability section: Please include also citations to all datasets used

Figure 1: How about mesophyll conductance? What does the dashed box represent?

Figure 2: Are there any boundary values given to the parameters? How are these normalized? Add a similar plot from each site to same figure (as subplots) and put the figure to the supplementary material.

Figure 3: I don't think these colors are color-blind friendly. Fig. 3 m: How is the RMSE in posterior lower, even though it looks worse than prior? Are the times presented here local time? For FI-Hyy the dataset is in local winter time (UTC +2). Please include the variability of the circle size (and what it means) to the figure legend. Why are you using mean instead of median diurnal variability?

Figure 4: I suggest to remove this fig with the whole “multi-site” analysis

Figure 5: Add in legend what the different colors mean. It is not clear from the caption what do the thick bars and the errorbars represent.

Figure 6: Same comments as for Fig. 5; you could combine these two figs in one as two different rows

Figure 7: same comments as for Figure 3.

Figure 8: Very weird pattern in simulated H. Solid and hollow circles are not distinguishable. I suggest to remove this fig with the analysis of H and LE.

Figure 9: Suggest to remove or move to supplement.

Figure 10: Not cited in the results section. What are “four LAI data”?

Table 1: Better reference to FI-Hyy would in this case be Vesala et al. 2022, since that paper presents the COS fluxes while Kohonen et al 2022 is about GPP.

Table 4: Suggest to remove.

Table S2: Not clear why the constant parameter values are repeated so many times