

We would like to thank both reviewers for their detailed and insightful comments. These comments have helped improve and clarify the submitted manuscript. Below we reply to each comment point by point, showing the reviewers' comments in black and our responses in blue. Changes to the original manuscript are highlighted in **bold blue**. Note that the line numbers in the response are updated based on the revised manuscript, which we provide with our response..

We note already here that we reran all our numerical experiments, in response to two comments of Reviewer #2, one on the processing of COS flux observations and one on the prior uncertainty specified for the parameter  $f_{leaf}$  and to one comment by reviewer # 1 on the size of the perturbation for the starting point of the twin experiments.

Reviewer #1

The paper by Zhu et al. presents an interesting study of data assimilation of carbonyl sulfide (COS) using the BEPS model. They used adjoint method to assimilate the COS fluxes as NUCAS v1.0. This is a new model tool to the modelling science and is useful for study of carbon cycle. The novelty of the model is that it assimilates COS flux to improve the model performance of GPP and other model parameters. Therefore, the research is within the scope of GMD and could be considered as publishable. However, there are some issues the authors should address before publication.

Response: We thank the reviewer for this comment. We will address these issues in order to make this paper publishable in GMD.

First of all, the adjoint code used in this paper is based on the automatic differentiation tool TAPENADE (Hascoët and Pascual, 2013). Yet, the authors did not validate the adjoint method or did not write it clearly. The question is: how do you justify that the adjoint codes will produce correct optimization?

Response: We extended the text as follows "In this study, all derivative code is generated from the model code by the automatic differentiation tool TAPENADE (Hascoët and Pascual, 2013). **The derivative with respect to each parameter was validated against finite differences of model simulations, which showed agreement within the accuracy of the finite difference approximation.**" (Line 125-127)

Secondly, the logic of the paper is lost in some places. Section 3.7 and 3.8 showed results of comparison and evaluation of simulated H and LE, and SWC. But it is unclear how data assimilation of COS flux can impact those parameters, and the performance is less satisfactory than evaluations of COS fluxes and GPP. The question: is there causality between assimilation of COS fluxes and H, LE, and SWC? What is your hypothesis that COS fluxes are linked to H, LE and SWC? Consider adding details in Section 2.

Response: Since the leaf exchange of COS, carbon dioxide (CO<sub>2</sub>) and water vapor are tightly coupled through stomata, COS has been proved as a useful tracer of photosynthesis, stomatal conductance and transpiration (Sandoval-Soto et al., 2005; Wohlfahrt et al., 2012). Transpiration is closely linked to soil moisture because the water it dissipates originates from the soil (Berry et al., 2006). This process of water turning from liquid to vapor requires energy,

and that energy is a crucial part of the ecosystem latent heat (LE) (Gupta et al., 2018). The energy is obtained from the surrounding leaf cells, leading to a decrease in temperature within the leaf (so called “cooling effect”) (Gates, 1968; Gupta et al., 2018). Thus, the sensible heat (H) can be linked to transpiration since the leaf-to-air temperature gradient is a key control factor of it (Monteith and Unsworth, 2013; Dong et al., 2017). Therefore, our hypothesis is that the assimilation of COS is expected to improve the modelling of LE, H and SWC due to the ability of COS to indicate transpiration and the mechanism of transpiration (i.e. the corresponding energy transfer, cooling effect and water source).

We have added detailed in Section 2.4.3: **“Due to the coupling between leaf exchange of COS, CO<sub>2</sub> and H<sub>2</sub>O, GPP and LE data are selected to evaluate the model performance of COS assimilation in this study. In addition, we further explored the ability of COS to constrain SWC as well as H simulations since the water dissipated in transpiration originates from the soil (Berry et al., 2006) and the transpiration contribute to a decrease in temperature within the leaf (so called “cooling effect”) (Gates, 1968; Konarska et al., 2016).”** (Line 276-279)

Another recent paper By Cho et al. is worthy of a comparison and discussion: Cho, A., Kooijmans, L. M. J., Kohonen, K.-M., Wehr, R., and Krol, M. C.: Optimizing the carbonic anhydrase temperature response and stomatal conductance of carbonyl sulfide leaf uptake in the Simple Biosphere model (SiB4), *Biogeosciences*, 20, 2573–2594, <https://doi.org/10.5194/bg-20-2573-2023>, 2023

Response: Based on previous studies on the temperature response of carbonic anhydrase (CA), Rubisco enzyme and LRU, Cho et al. (2023) proposed a new COS plant uptake scheme for CA with the argument that different enzymes have different physiological characteristics. Through data assimilation, they combined COS and GPP observations with the Simple Biosphere model (SiB4) simulations to optimize stomatal conductance parameters  $b_0$  and  $b_1$ , empirical parameter  $a$ , and CA enzyme optimum temperature, and thus improved the model performance of stomatal conductance, ‘interior’ conductance, and COS leaf uptake. This study provides new insights into achieving accurate modeling of COS plant uptake, which is worthy of comparison and discussion.

Firstly, precise modeling of carbonyl sulfide (COS) is fundamental for the utility of COS observations in optimizing model parameters associated with COS. The remarkable contribution of Cho et al. (2023) to COS modeling would undoubtedly benefit the work in utilizing COS as a probe to explore the ecological processes such as water-carbon exchange and energy flow within ecosystems.

Secondly, while the study by Cho et al. (2023) focused on optimizing COS-related and stomatal-related parameters, our investigation concentrates on refining parameters associated with photosynthesis and soil hydrology. Although the parameters optimized in our study influence stomatal modeling, our results reveal that the optimization of transpiration-related variables (LE, H, SWC) is comparatively less successful than that of COS and GPP. The insights gained from Cho et al. (2023)'s work underscore the potential for achieving improved optimization of transpiration-related variables by utilizing COS to directly constrain parameters associated with stomatal conductance.

Thus, we extended the text as follows: “This result is also proved by Resco De Dios et al. (2019), which found that the median  $g_n$  in the global dataset was  $40 \text{ mmol m}^{-2} \text{ s}^{-1}$ . **Therefore, utilizing COS to directly optimize stomatal related parameters should be perused. Cho et al. (2023) has proven the effectiveness of optimizing the minimum stomatal conductance as well as other parameters by the assimilation of COS. Besides, with the argument that different enzymes have different physiological characteristics, Cho et al. (2023) proposed a new temperature function for the CA enzyme and showcase the considerate difference in temperature response of enzymatic activities of CA and RuBisCo enzyme, which also provided valuable insights into the modelling and assimilation of COS.**” (Line 701-706)

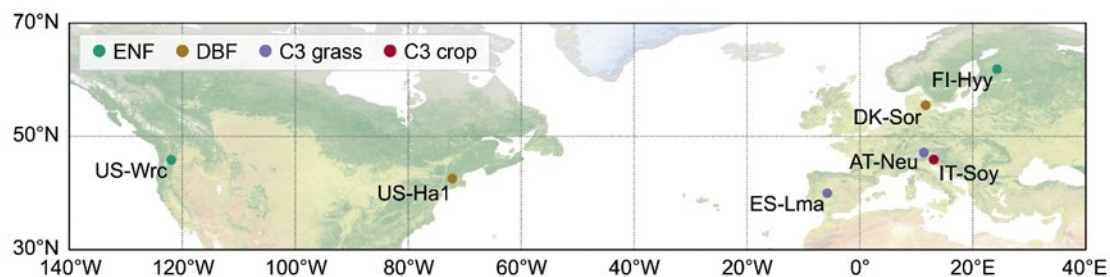
Other minor comments:

Line 142: “For NUCAS, we use the same soil texture” to “we used the same soil texture.”

Response: Corrected.

Line 185: the sites used in the study is better to be shown in a Figure to give a general idea of the locations of those sites.

Response: Thanks for your suggestion, we have added such a figure to our manuscript, as shown below.



**Figure 2.** Locations of the 7 studied sites. Sites sharing the same plant function type are represented with consistent colors. The background map corresponds to the “Nature color I” map (<https://www.natureearthdata.com>). ENF and DBF denote evergreen needleleaf forest and deciduous broadleaf forest, respectively.

Line 197: “the  $\text{CO}_2$  and COS mole fractions in the bulk air were assumed to be spatially invariant.” What is the value of  $\text{CO}_2$  and COS mole fractions in your case?

Response: Thanks for your comment. we extended the text as follows: “The  $\text{CO}_2$  and COS mole fractions in the bulk air were assumed to be spatially invariant over the globe and to vary annually. **The  $\text{CO}_2$  mole fraction data utilized in this study are taken from the Global Monitoring Laboratory (<https://gml.noaa.gov/ccgg/trends/global.html>). For the COS mole fraction, the average of the COS mole fraction observations from sites SPO (South Pole) and MLO (Mauna Loa, United States) was utilized to drive the model, the data are publicly available on line at: <https://gml.noaa.gov/hats/gases/OCS.html>.**” (Line 219-223)Line 227: “in situ” to “*in situ*”, and all elsewhere.

Response: Thanks for your reminder, we have changed to “*in situ*” throughout the manuscript.

Line 284: “For all cases where the PFT is evergreen needleleaf forest, a perturbation ratio of 0.2 was used. And for the remaining six single-site twin experiments, a perturbation rate of 0.4 was used.” Please specify the reasons to those perturbation rate as 0.2 or 0.4.

Response: Thanks for your comment. The settings of the prior parameter uncertainties in this study refer to previous studies, e.g., Chen et al. (2022), Ryu et al. (2018). Now, the prior uncertainty of most model parameters was set to 25% of the prior value, while the prior uncertainty of  $f_{leaf}$  was estimated using the datasets provided by Ryu et al. (2018) and was about 7 % of the prior value. These studies also provide us with reference for understanding the degree of parameter variability and choosing the perturbation rate. Now, we chose a perturbation ratio (0.2) that falls between these two values (7 % and 25 %), but is closer to the prior uncertainty with most of the parameters, and reran all the twin experiments.

Line 440: “very reasonable”. Is there another way to say “very”?

Response: Thank you for the suggestion. The relevant parts have been re-written in the revised manuscript.

Line 450: “very similar”. The same as Line 440. And check all elsewhere.

Response: Thanks for your comment. The relevant parts have been re-written in the revised manuscript and we have checked all elsewhere.

Line 513: “assimilation using COS observations from multiple sites can also improve GPP simulations, and the assimilation is sometimes”, it is vague to use sometimes to describe results.

Response: Thanks for your comment. We have reorganized the sentences to avoid vagueness.

Line 1165: Figure 4, it is not easy to see clearly the green and gray shading. Please consider better visualization.

Response: Thanks for your comment. We have remade our figures so that the results can be easily distinguished.

Line 1170 and 1175: Figure 5 and 6, why there are error bars for some sites but no error bars for other sites?

Response: Thanks for your comment. In this study, FI-Hyy and US-Ha1 are the only two sites with multi-year COS observations, which provides an opportunity to investigate the optimization results of COS-related parameters and the effectiveness of COS assimilation in different years. For these two sites, error bars were plotted to represent the maximum and minimum of the posterior parameter values. In contrast, no error bars were plotted for the other sites due to the lack of multi-year COS observations. We have described in the manuscript that we plotted error bars for sites with multiple years of COS observations. In response to your question, we have added a note to the figure legend of the revised manuscript: “**For those sites lacking multi-year COS observations, no error bars were plotted.**” (Line 1177-1178)

Line 1185: Figure 8. It is hard to see difference between green and gray. The dots in c and f are maybe too big.

Response: Thanks for your comment. We have reorganized the figure using smaller dots and

changed the colours for better visualization.

## Review #2

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.

Response: We thank the reviewer for this comment. In response to this comment, we have refined the manuscript to enhance clarity and ensure consistency. The necessary information has been incorporated, rendering the manuscript comprehensive and informative.

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.

Response: We thank the reviewer for this comment. To enhance readability, we have revised the manuscript to ensure consistency in terminology. In the revised manuscript, we have designated observations as 'O' and the model as 'M.' Soil moisture is identified by 'SWC.' Furthermore, to mitigate ambiguity with 'C' in Eq.1, we now use 'F' to represent the corrected COS fluxes. Additional details regarding the rationale for utilizing corrected COS data from the US-Wrc site have been elaborated below.

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.

Response: Thanks for this valuable comment. Actually, there are many difficulties in evaluating COS soil and plant fluxes separately for the sites used in this study. The five-year COS ecosystem flux data at FI-Hyy provided us an opportunity to investigate the difference of assimilation performance of COS. However, the soil COS flux data at FI-Hyy are only available in 2015, which makes it impossible for us to separately evaluate COS plant flux and soil flux for the vast majority of experiments conducted at FI-Hyy. In addition, Whelan et al. (2022) have evaluated the model performance at FI-Hyy in 2015 and US-Ha1 using a similar soil model. At US-Wrc, only the raw COS concentration data at different altitudes are provided in Rastogi et al. (2018), while the values of the parameters needed to calculate the COS fluxes by the aerodynamic gradient method are not provided. Thus, there may be significant biases in our estimates of both plant and soil fluxes at US-Wrc. As for DK-Sor, ES-Lma and IT-Soy, a random forest regression model was trained for each site in order to simulate the soil COS exchange, and only the modelled COS soil fluxes are provided in Spielmann et al. (2019) while the observational data for COS soil flux is lacking. Overall, given the insufficient and inconsistent availability of separate COS soil and plant data, we face considerable obstacles in separately

assessing simulated COS soil and plant fluxes.

Additionally, in NUCAS, the resistance analog model of COS plant uptake and the empirical model of soil COS flux were embedded in the BEPS model, and the model performance of these COS models have been evaluated in numerous previous studies (Berry et al., 2013; Whelan et al., 2016; Kooijmans et al., 2021; Maignan et al., 2021; Whelan et al., 2022; Chen et al., 2023; Cho et al., 2023). These studies have demonstrated the usefulness and robustness of these models to simulate COS plant and soil fluxes, thus founded the basis for us to assimilate COS ecosystem flux in this study.

Last but not least, we do agree with your opinion and we also believe that assimilating the component fluxes of COS individually should be pursued in the future as this assimilation approach would provide separate constraints on different parts of the model. We expect the observational information on the partitioning between the two flux component to provide a stronger constraint than using just their sum.

Therefore, we extended the text in the conclusion: **“Specifically, with the lack of separate COS plant and soil flux data, the ecosystem-scale COS flux observations were utilized in this study. However, we believe that assimilating the component fluxes of COS individually should be pursued in the future as this assimilation approach would provide separate constraints on different parts of the model. We expect the observational information on the partitioning between the two flux components to provide a stronger constraint than using just their sum.”** (Line 739-743)

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.

Response: Thanks for your comment. Reviewer #1 asked a similar question about the choice of the perturbation size, please refer to our previous answer. Besides, we have changed the uncertainty of the prior simulated COS flux in twin experiments, and reperformed the experiments. Now, the uncertainty of the prior simulated COS flux was estimated as the standard deviation of the prior simulated COS fluxes within 24 hours around each simulation.

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.

Response: We appreciate the reviewer’s understanding of the lack of *in situ* COS flux measurements in similar ecosystems. Therefore, we only performed a “multi-site” or “two-site” assimilation experiment at evergreen forest sites FI-Hyy and US-Wrc. Our two-site setup constitutes a challenge for the assimilation system, the model and the observations. In this setup the assimilation system has to determine a parameter set that achieves a fit to the observations

at both sites, and NUCAS passes this important test. NUCAS was designed as a platform that integrates multiple data streams to provide a consistent map of the terrestrial carbon cycle, although only ecosystem COS flux data were used to evaluate the performance of NUCAS in this study. The “two-site” assimilation experiment conducted in this study gives us more confidence that the calibrated model will provide a reasonable parameter set and posterior simulation throughout the plant functional type. In other words, what we present here is a pre-requisite for applying the model and assimilation system at regional to global scales. We did, however, replace the formulation "multi-site" by "two-site".

Also, we have extended the text in the conclusion: **“Our two-site setup constitutes a challenge for the assimilation system, the model and the observations. In this setup, the assimilation system has to determine a parameter set that achieves a fit to the observations at both sites, and NUCAS passes this important test.** It should be noted that the NUCAS was designed as a platform that integrates multiple data streams to provide a consistent map of the terrestrial carbon cycle although only ecosystem COS flux data were used to evaluate the performance of NUCAS in this study. **The “two-site” assimilation experiment conducted in this study gives us more confidence that the calibrated model will provide a reasonable parameter set and posterior simulation throughout the plant functional type. In other words, what we present here is a pre-requisite for applying the model and assimilation system at regional to global scales.”** (Line 744-751)

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.

Response: Thanks for this comment. In the dataset for FI-Hyy (Vesala et al., 2022), No quality flags are provided, but measured COS fluxes as well as gap-filled COS fluxes are provided. In this study, only the measured COS fluxes are utilized and we have provided additional clarification on this (Line 260-261). For US-Ha1 and US-Wrc, no quality flag or gap-filled data is provided. At the remaining four sites, “COS filter” flag was provided to mark whether the COS observations are without flux detection limits. In this study, we do not use the detection limits to filter the COS flux data because such filtering would cause us to lose all values close to zero.

- 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.

Response: Thanks for this comment. The dataset (<https://zenodo.org/records/1422820>)

provided by Rastogi et al. (2018) **does lack** readily available gradient fluxes. Consequently, we implemented a bias correction to align the simulated and estimated COS fluxes for the US-Wrc site, drawing upon methodologies outlined in previous studies (Leung et al., 1999; Scholze et al., 2016). In addition, we have reached out to the corresponding authors via email to kindly request assistance in obtaining their readily-calculated flux data. Unfortunately, as of now, we have not received a response.

We acknowledge that the absence of precise COS flux data at US-Wrc poses challenges to our two-site assimilation experiments. Nevertheless, we maintain the importance of conducting two-site experiment, as detailed before.

- 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.

Response: Thank you for pointing this out. We deleted the sentence: “We then corrected the COS fluxes from FI-Hyy using the storage-correction method (Kooijmans et al., 2017).” At FI-Hyy, only the direct measured COS flux data were utilized in the assimilation experiments, and we have clarified this (Line 260-261).

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.

Response: Thanks for this comment. Reviewer #1 asked a similar question, please refer to our previous answer.

In this study, the diurnal variability of the simulated sensible heat fluxes using the BEPS model exhibited misalignment with observations, mainly at FI-Hyy. However, the simulated sensible heat showed good agreement with observations at the remaining sites. Moreover, the optimization of H was demonstrated successfully at FI-Hyy, despite the different direction of the simulated sensible heat and the measured one.

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.

Response: Thanks for your comment. We have deleted the expression "variable ecosystems" and listed the corresponding ecosystems of our study site in detail.

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.



Response: Thanks for this comment. The leaf area index is commonly defined as half the total all-sided developed area of green leaves per unit ground surface area (Chen and Black, 1992; Liu et al., 2012; Xiao et al., 2016). In the publications listed in **Table 1**, only Kohonen et al. (2022) specified that the all-sided leaf area index (LAI) of FI-Hyy was ca.  $8 \text{ m}^2 \text{ m}^{-2}$  during the measurement period (2013–2017). In this study, we followed the convention of using one-sided LAI (for broadleaves). We now have added “one-sided” (Line 99 and Line 1994) to account for this. In Sect. 2.4.3, we have specified positive values indicate COS uptake. Furthermore, we have corrected the inappropriate use of "significantly".

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

- Where is  $F_{\text{cos,leaf}}$  used in the model? It is not present in any other equations after Eq. 3

Response: In eq.3,  $F_{\text{cos,leaf}}$  represents the leaf-level COS uptake rate. For COS simulations, BEPS uses the leaf-level resistance analog model of COS (Berry et al., 2013) with a two-leaf upscaling scheme (Chen et al., 1999) from leaf to canopy.

- 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.

Thanks for your comment, we have detailed the coefficients relevant to COS plant flux modeling (Eq. 3-6). For the COS soil model, we have updated them and detailed the coefficients currently used (please see Table S2 and Table S3 for details).

In NUCAS, the resistance analog model of COS plant uptake (Berry et al., 2013) were used. Such a model utilizes the COS mole fraction in the bulk air and the series conductance (conductance = 1/resistance) of the leaf system for COS (the terms in parentheses in Eq. 3) to calculate the flux of COS uptake. In the series conductance of the leaf system for COS, the stomatal conductance and laminar boundary layer conductance of COS are framed in reference to that of H<sub>2</sub>O vapor. The greater mass and larger cross section of COS restricts its diffusion relative to H<sub>2</sub>O in the stomatal pore by a factor of 1.94 and in the laminar boundary layer by 1.56 (Seibt et al., 2010; Stimler et al., 2010).

As for Eq. 5, we followed the modelling scheme of COS in the SiB (version 4.2) (Haynes et al., 2020), and we have provided additional clarification on this.

- What is  $f_w$  (how it is defined, is there an equation, what unit does it have and what kind of variation does it have) exactly.

Response: Thanks for your comment, we renamed it to  $f_w$ . In sect. 2.1.3, we mentioned  $f_w$  is a soil moisture stress factor describing the sensitivity of  $g_{sw}$  to soil water availability. We have added the definition of  $f_w$  to the appendix and also citations to the relevant literature, i.e. Ju et al. (2006).

-  $V_{\text{cmax}}$ ; what is the unit and how do you get values (and which values) for it?

Response: The unit of  $V_{cmax}$  is  $\mu\text{mol m}^{-2} \text{s}^{-1}$ , we now added the detail calculation of  $V_{cmax}$  in the appendix.

-  $F_{cos,biotic}$  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  $\Theta g$ ?

Response: Thanks for this comment. To enhance readability, we have revised the manuscript to ensure consistency in terminology. In the soil COS model proposed by Whelan et al. (2016), The soil abiotic COS flux corresponding to a soil moisture of  $SWC_i$  can be calculated by Eq. 7 (Eq. 9 in the revised manuscript). In Eq. 7,  $SWC_{opt}$  denote the optimum soil moisture, at which soil abiotic COS flux reaches a maximum ( $F_{opt}$ ),  $SWC_g$  denote a certain soil moisture, which is greater than  $SWC_{opt}$  and whose corresponding soil abiotic emissions are known. The last constant (a) that needs to be known in Eq. 7 can be calculated by Eq. 8 (Eq. 10 in the revised manuscript).

- How is “optimum soil moisture” defined? Optimum in terms of what?

Response: According to Whelan et al. (2016) and Whelan et al. (2022), there exists an optimum soil moisture at which the simulated biotic COS flux is maximized, i.e. optimum in terms of COS soil biotic uptake.

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

Response: Thank for your suggestion. We have thoroughly reviewed our manuscript and made refinements to the text.

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.

Response: Thank for your suggestion. We now plotted the corresponding scatterplots and added them to the supplement.

Specific comments:

L19: “various processes” is too ambiguous

Response: Thanks for this comment. We have deleted the expression "variable ecosystems".

L25: “various ecosystems”; please specify which ecosystems

Response: we now specified the ecosystems, including evergreen needleleaf forest, deciduous broadleaf forest, C3 grass and C3 crop, respectively.

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

Response: Thanks for this comment. Now we rewrite this sentence.

**Comparing prior simulations with validation datasets, we found that the assimilation of COS can significantly improve the model performance in gross primary productivity,**

**sensible heat, latent heat and even soil moisture.** (L26-L27)

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

Response: Corrected.

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

Response: Thanks for this comment. We have revised the references in the manuscript.

**Recently, carbonyl sulfide (COS) has emerged as a promising proxy for understanding terrestrial carbon uptake and plant physiology (Montzka et al., 2007; Campbell et al., 2008) since it is taken up by plants through the same pathway of stomatal diffusion as CO<sub>2</sub> (Goldan et al., 1988; Sandoval-Soto et al., 2005; Seibt et al., 2010) and completely removed by hydrolysis without any back-flux in leaves under normal conditions (Protoschill-Krebs et al., 1996; Stimler et al., 2010).** (Line 47-51)

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

Response: Thanks for this comment. We now deleted these two references.

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

Please rephrase

Response: Thanks for this comment. As mentioned earlier, a crucial hypothesis in this study is that the assimilation of COS is expected to improve the modelling of LE, H and SWC due to the ability of COS to indicate transpiration and the mechanism of transpiration. Therefore, here we would like to emphasize the second half of the sentence, i.e., only few experiments were conducted to systematically assessed the ability of COS to simultaneously constrain photosynthesis, transpiration and other related processes in ecosystem models. Of course, We also mentioned COS observations here (in the first half of the sentence). That is because the lack of COS measurements is for sure an essential limiting factor in examining the ability of COS to constrain ecosystem processes, such as photosynthesis and transpiration. At the same time, we also believe that the mention of observations here can also serve to pave the way for the introduction of data assimilation below. Therefore, we have rewritten the sentence while retaining the main content. The revised sentence now reads as: **However, with the lack of ecosystem-scale measurements of the COS flux (Brühl et al., 2012; Wohlfahrt et al., 2012; Kooijmans et al., 2021), only few studies were conducted to systematically assess the ability of COS to simultaneously constrain photosynthesis, transpiration and other related processes in ecosystem models.** (Line 58-61)

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).

Response: Thank for this suggestion. We have split it in two:

**In this study, we present the newly developed adjoint-based Nanjing University Carbon**

**Assimilation System (NUCAS) v1.0. NUCAS v1.0 is designed to assimilate multiple observational data streams including COS flux data to improve the process-based Biosphere-atmosphere Exchange Process Simulator (BEPS) (Liu et al., 1997), which has been specifically extended for simulating the ecosystem COS flux with the advanced two-leaf model that is driven by satellite observations of leaf area index (LAI). (Line 72-76)**

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

Response: Corrected.

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.

Response: Thanks for your comment. We have reorganized and revised that question and question one " What are the main changes in the parameters through the assimilation of COS flux and which processes are constrained?" The revised sentence reads as follows: **What parameters are the COS simulation sensitive to and how do these parameters change in the assimilation of ecosystem scale COS flux data? (Line 78-79) Which processes are constrained by the assimilation of COS and what are the mechanisms leading to adjustments of the corresponding process parameters? (Line 82-83)**

Response: Thanks for your comment.

L81: List the ecosystems

Response: Corrected.

**To achieve these objectives, COS observations across a wide range of ecosystems (including evergreen needleleaf forest, deciduous broadleaf forest, C3 grass and C3 crop) are assimilated into NUCAS to optimize the model parameters using the four-dimensional variational (4D-Var) data assimilation approach, and the optimization results are evaluated against *in situ* observations. (Line 85-88)**

L96: all-sided or one-sided LAI?

Response: one-sided LAI.

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

Response: The BEPS model (Liu et al., 1997; Chen et al., 1999) used in this study is a process-based diagnostic model driven by remotely sensed leaf area index (Chen et al., 2019). In BEPS, LAI is used as an indicator of the current state of vegetation within an ecosystem, and the plant phenology is driven by LAI. In contrast, in prognostic models, LAI is used as a dynamic variable that evolves over time, and the prognostic models allow researchers to make predictions about how LAI will change in response to varying environmental conditions and disturbances.

L103: remove one "of the"

Response: Corrected.

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>

Response: Thank for this comment. we have corrected the units in this manuscript.

L153: “And the leaf-level” -> “The leaf-level”

Response: Corrected.

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

Uniform leaf laminar boundary layer conductance was applied to both shaded and sunlit leaves. However, BEPS takes into account radiation transmission processes (e.g., direction and scattering) within the canopy and calculates the amount of radiation received by the sunlit and shade leaves accordingly. Thus, the sunlit and shade leaves have different photosynthesis rates in theory due to the different radiation they receive, and in turn have different stomatal conductance (Ball et al., 1987; Ju et al., 2010).

L179: Do you perhaps mean Table S2?

Response: Yes, we have corrected the clerical error here.

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.

Response: Thanks for this comment. This arose from the fact that certain literature corresponding to the sites from which we obtained data lacked detailed site descriptions. We have addressed this by including references to the papers from which we sourced the data.

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

Response: Corrected.

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

Response: Corrected.

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.

Response: Thanks for this comment. Mean LAI during the campaign of DK-Sor (referred to DBL in Spielmann et al. (2019)) was presented in Table S1 of the supplement in Spielmann et al. (2019).

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

Thank you for your comment. We re-examined and collected the meteorological data of the

US-Ha1 site. As a FLUXNET site and an Ameriflux site, the meteorological data for the US-Ha1 can be found in both the Ameriflux and FLUXNET datasets, and both datasets does include some radiation data. However, the shortwave radiative data required by the BEPS model of US-Ha1 are only available at FLUXNET while only net radiation and PPFD data are available at Ameriflux. Considering the meteorological data of US-Ha1 provided by FLUXNET are only available in 1991-2012, we currently use FLUXNET data at US-Ha1 in 2012 and ERA5 shortwave radiation data with Ameriflux data in 2013 to drive the BEPS model.

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

Thanks for your comment. Measurement information on COS soil fluxes already included in the literature we listed in Table 1 except for FI-Hyy. The reason we did not cite literature on soil COS flux observations at FI-Hyy (Sun et al., 2018) is that we assimilated ecosystem scale COS fluxes (Vesala et al., 2022) in this study. However, soil texture derived from the harmonized world soil database (Wieder et al., 2014) was used before. Now, we have updated the soil texture with *in situ* data and added relevant references (including Sun et al. (2018)).

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!

Thanks for your comment. Currently, we kept both positive and negative values of COS fluxes and re-ran the assimilation experiments.

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

Response: Corrected.

L257: Cite Reichstein 2005 for the nighttime partitioning method

Response: Corrected.

L260: How is nighttime defined?

Response: In light of the extended daylight hours during the Northern Hemisphere summer and to prevent misclassification of actual daytime hours as nighttime due to discrepancies in local longitude and locally adopted time, we fit the equation for the relationship between respiration and temperature based only on data from 21:00 local time to 3:00 the following day.

L280: “And as a...” -> “As a..”

Response: Corrected.

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

Response: Thanks for your comment. We absolutely recognize that e.g.,  $V_{cmax}$  varies greatly from ecosystem to ecosystem. In this study, we take the PFT- and texture-dependence of

parameters into consideration, thus the parameter number of one set of accurate and generalized model parameters is 76. In other words, the only one set of model parameters mentioned here, includes parameters that are specific to a PFT or texture but not to the point on the global that is populated by this PFT and characterized by this texture.

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?

Response: The interdependence of parameters was considered in this study. Therefore, when counting the PFT-dependent parameters as well as the texture-dependent parameters, we multiply the number of PFTs and the number of textures considered in the BEPS model. This is how the number 76 is obtained.

L310: "correlation" -> "coefficient"

Response: Corrected.

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

Response: We have modified this sentence with specific instructions.

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

Response: Thanks for your comment. We have reorganized the sentence: **"Corresponding to the PFT and soil texture of the experimental site, some PFT-dependent and texture-dependent parameters as well as global parameters showed different adjustments from others as they can affect the simulation of COS to different degrees."**

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

Response: We detailed how these parameters affect the simulation of COS in the appendix.

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

Response: As shown in the Figure 3j of the original manuscript, it is because the prior simulated COS at IT-Soy is already very close to the corresponding observations.

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

Response: Corrected.

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?

Thanks for your comment. But according to Vesala et al. (2022), these months were not considered to be drought because the SWC remained at a normal level (well above  $0.1 \text{ m}^3 \text{ m}^{-3}$ ). However, the SWC observations as well as simulations in August 2014 are indeed noticeably lower than the other months, and are close to the optimum soil moisture for the COS abiotic flux modelling (see Figure S9 for details). As a result, the prior simulated COS for that month were significantly overestimated by 41.06 %, resulting in  $V_{cmax25}$  and VJ\_slope being

considerable downward adjustments by -42.44 % and -41.03 % in the single-site experiments. Thus, the simulated GPP were also markedly downgraded by 53.54 % in August 2014, ultimately resulting in the underestimation of the single-site posterior simulated GPP. Regarding this, we have added the text in the manuscript: **“However, with a low SWC in August 2014, the prior simulated COS were obviously overestimated by 41.06 %, which led to remarkable downward adjustments of  $V_{cmax25}$  as well as VJ\_slope. Thus, the simulated GPP were also markedly downgraded by 53.54 % in August 2014, ultimately resulting in the underestimation of the single-site posterior simulated GPP.”** (Line 478-481)

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

Response: Corrected.

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

Response: Yes, thus we say “ $R^2$  remained almost unchanged by the optimizations”.

L387: Why are the simulated nighttime fluxes unchanged?

Response: In the BEPS model, stomatal conductance was set to a constant value at night. Meanwhile, soil fluxes were small and less variable relative to the magnitude of plant COS flux.

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

Response: Could, of course, be either, but according to Kooijmans et al. (2021), the air depleted in COS can then suddenly be captured by the EC system when turbulence is enhanced in the morning.

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

Response: Now we changed our expression from 'multi-site' to 'two-site'.

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

Thanks for your comment. According to Ryu et al. (2018), the default  $f_{leaf}$  value in the BEPS model and the prior uncertainty of  $f_{leaf}$  in this study is overestimated. Thus, it tends to overshoot in the previous assimilation experiments. Now, we have computed the mean value of  $f_{leaf}$  with its standard deviation as an estimate of the error based on the MODIS PAR and SW data from 2012-2017 (Ryu et al., 2018) and re-ran the assimilation experiments.

L429: Either “In particular,” or “Particularly”

Response: Corrected.

L444: “underestimated (by 55.72%), ...”

Response: Corrected.

L444: “greatly increased”; how much?

Response: We have provided a quantitative description.

L445: “...simulations of COS flux at FI-Hyy..”



Response: Corrected.

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

Response: Corrected.

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

Response: Thanks for your comment. We know that GPP cannot be measured directly. In order to distinguish it from the modeled GPP of BEPS, we rephrase it to **GPP derived from EC measurements**.

L502: “excellent match” needs quantification

Response: Corrected.

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

Thanks for your comment. Due to the lack of *in situ* COS observation data of the same PFT, we only conducted a two-site assimilation experiment. Therefore, we admit that the results of our experiments are not very convincing. More multi-site or two-site assimilation experiments would have helped us to get more statistically significant and plausible results, however we are faced with the challenge of lack of COS data.

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

Response: the results be without COS assimilation, i.e., the prior simulation result can be found in Figure 4 and Figure 5 in the revised manuscript.

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.

Response: Thanks for your suggestion. We have reached out to the corresponding authors via email to kindly request assistance in obtaining the sensible and latent heat flux data. With their assistance, we have conducted a thorough comparison and evaluation of H and LE simulations at the AT-Neu and IT-Soy sites. For the help they provided, we have added a note in the acknowledgements.

L525: “And the assimilation..” -> “The assimilation..”

Response: Corrected.

L536 & L554-556: Refer to the supplement figs

Response: Corrected.

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

Response: Thanks for your comment. Actually, this sentence is not necessary. We have therefore deleted it to avoid confusion.

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

Response: Thanks for your comment. We rewrite the sentence.

**However, the simulated SWC exhibited a clear diurnal cycle whereas the observed SWC had almost no diurnal fluctuations.** (Line 534-535)

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

Response: Thanks for your comment. We rewrote the sentence.

L583-585: Refer to the supplement figs

Response: Corrected.

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

Response: Corrected.

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

Response: Thanks for the comment. Since  $V_{cmax25}$  and  $f_{leaf}$  have their physical significance, the optimized values of both should be within certain ranges, e.g., greater than zero. Currently, both are within their physical significance, despite the huge relative change of them. The magnitude of the adjustment of  $f_{leaf}$  is expected to be limited by improving the estimation of its prior uncertainty. However, the prior uncertainty we set of the parameter  $V_{cmax25}$  is comparable to the existing dataset Chen et al. (2022). Furthermore, we have indeed refined the prior uncertainty of  $f_{leaf}$  and re-run the assimilation experiments.

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

Response: Thanks for the comment. The optimized parameter values are the result of the trade-off between the two parts of the cost function. When the reduction in the discrepancy between observation and simulation resulting from the adjustment of the parameters is not sufficient to offset the increase in the discrepancy between the current and prior parameter values, the adjustment is not continued.

L652-655: Already mentioned in the previous section”

Response: Removed.

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

Thanks for your comment. As shown in Table 3 of the original manuscript,  $f_{leaf}$  has been greatly downregulated after the assimilation of COS. We believe that this inappropriate parameter value is the main reason for the underestimation of posterior simulation. Now, we have refined the prior parameter uncertainty and re-ran the assimilation experiment.

L691: Table 1 perhaps?

Response: Yes, now we corrected this error.

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

According to Kohonen et al. (2022), the all-sided leaf area index (LAI) of FI-Hyy was ca.  $8 \text{ m}^2 \text{ m}^{-2}$  during the measurement period (2013–2017). In this study, we followed the convention of using one-sided LAI, so the LAI at FI-Hyy is  $4 \text{ m}^2 \text{ m}^{-2}$ , as listed in **Table 1**.

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

Response: Corrected.

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

Thanks for your comment. We have currently referred to the relevant literature and refined the prior uncertainty of the parameters (as mentioned before). Specifically, as the COS data utilized in this study range from 2012-2017, only the Moderate Resolution Imaging Spectroradiometer (MODIS) PAR and shortwave radiation (SW) data ranging from 2012-2017 was used to calculate the mean and standard deviation of  $f_{\text{leaf}}$ , and the prior uncertainty of  $f_{\text{leaf}}$  was estimated as the calculated standard deviation. The MODIS PAR and SW datasets are publicly available at: <http://environment.snu.ac.kr>. L735-738: Given that this is already known, why is the COS concentration variation not already taken into account in this model?

Response: Continuous COS concentration data are a pre-condition for continuous COS flux simulations based on COS concentrations due to the linear relationship between the two (Stimler et al., 2011; Berry et al., 2013). However, similar to COS flux data, the *in situ* observed COS concentrations are not continuous in the whole assimilation windows. Therefore, in order to perform continuous simulations of COS flux based on a variable COS concentration, Kooijmans et al. (2021) used the surface COS mole fraction fields retrieved from an atmospheric transport inversion performed with TM5-4DVAR. We also think that modelling and assimilation of COS fluxes based on spatially and temporally varying COS concentrations is an aspect of the NUCAS system that can be further enhanced, and we will strive to combine the ecosystem model with atmospheric transport model to address this issue in our next steps. However, **with the lack of *in situ* COS mole fraction data**, COS mole fractions in the bulk air are currently assumed to be spatially invariant over the globe and to vary annually in NUCAS, which may introduce significant errors into the parameter calibration.

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

Response: Thanks for your comment. According to the summary of species information used in Yu et al. (2019), they do not include the crassulacean acid metabolism (CAM) plants in the study. However, the CAM plants are indeed commonly found in harsh environments such as arid and semi-arid regions (Amin et al., 2019), and the main feature of stomatal conductance patterns in CAM plants is nocturnal opening (Males and Griffiths, 2017). Data availability section: Please include also citations to all datasets used

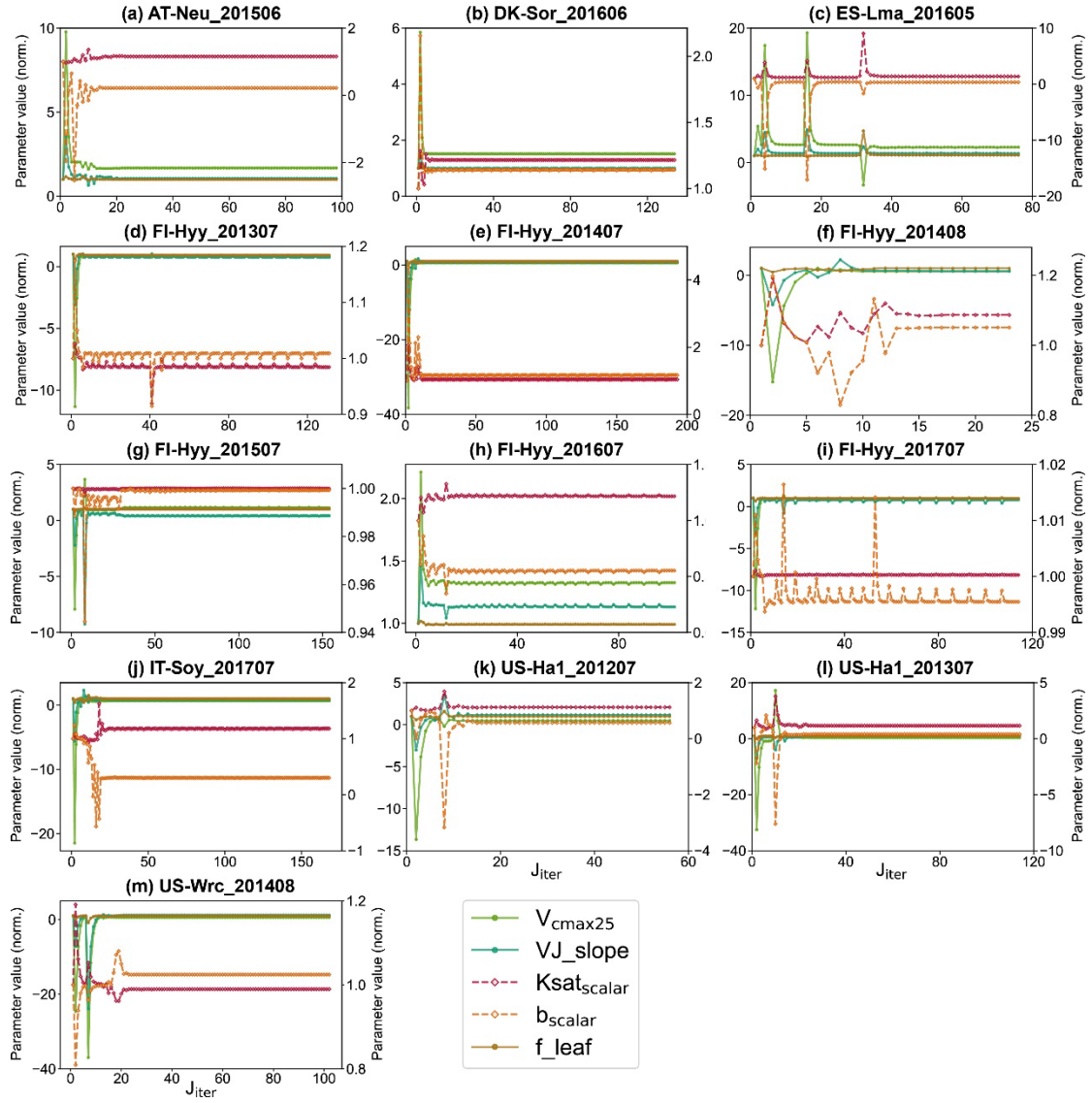
Response: Done.

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

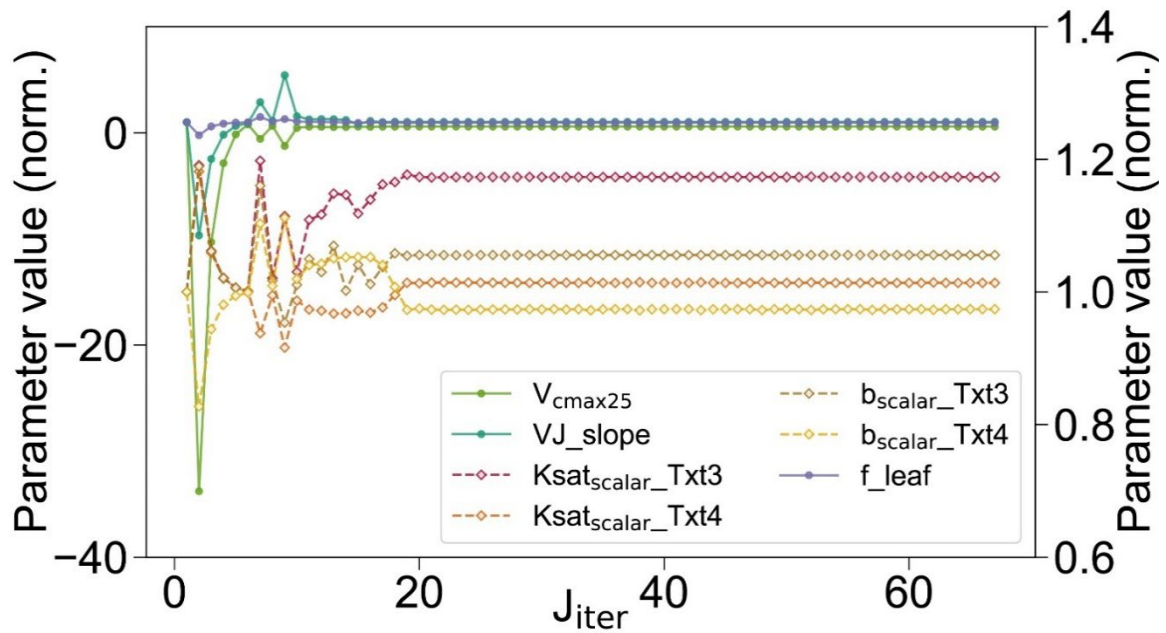
Response: Thanks for your comment. In the resistance analog model of COS plant uptake (Berry et al., 2013), the apparent conductance for COS uptake from the intercellular airspaces (include the mesophyll conductance and the biochemical reaction rate of COS and carbonic anhydrase) is represented by  $g_{COS}$ . The dashed box includes the driver data of BEPS, and those data were utilized in both diagnostic process and prognostic process.

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.

Response: We didn't set any boundary values for the parameters. Currently, they are normalized by their prior values. We have carefully considered showing the convergence trajectory through the parameter space from the starting point of the iterative procedure to the final point. In fact, this trajectory is to a large extent arbitrary, because branches depend on specifics of the floating-point arithmetic/rounding, which depend in turn on aspects like computing platform, compiler, or even compiler flags. What both technically and scientifically matters are the values of parameters, cost function and its gradient at the starting and end points of the minimization. These are now provided in Tables S5 for the twin experiments and S4 and 2 for the experiments with real data. We thus refrain from including the trajectory plots into the manuscript or its supplement, but provide the corresponding graphs and their presentation (requested by the reviewer) here:



**Figure 1.** The evolution of model parameters with the number of iterations of cost function ( $J_{iter}$ ) during the single-site experiments. Evolution (open carats and dashed lines) of soil texture dependent parameters is plotted on the right-hand y axis, evolution (filled circles and solid lines) of PFT-dependent parameters and global parameter is plotted on the left-hand y axis. Parameters are normalized by their prior values.



**Figure 2.** The evolution of model parameters with the number of iterations of cost function ( $J_{iter}$ ) during the two-site experiment. Evolution (open carats and dashed lines) of soil texture (abbreviated as Txt) dependent parameters is plotted on the right-hand y axis, evolution (filled circles and solid lines) of PFT-dependent parameters and global parameter is plotted on the left-hand y axis. The texture-dependent parameters for FI-Hyy are denoted by “Txt3” and that of US-Wrc are denoted by “Txt4”. Parameters are normalized by their prior values.

Corresponding to the PFT and soil texture of the experimental site, some PFT-dependent and texture-dependent parameters as well as global parameters showed different adjustments from others as they can affect the simulation of COS to different degrees. Those parameters are the maximum carboxylation rate at 25 °C ( $V_{cmax25}$ ), the ratio of  $V_{cmax}$  to maximum electron transport rate  $J_{max}$  ( $VJ\_slope$ ), the scaling factors ( $Ksat_{scalar}$  and  $b_{scalar}$ ) of saturated hydraulic conductivity (Ksat) and Campbell parameter (b), and the ratio of photosynthetically active radiation (PAR) to shortwave radiation ( $f\_leaf$ ). Particularly, as the soil textures at the FI-Hyy and US-Wrc are different,  $Ksat_{scalar}$  and  $b_{scalar}$  corresponding to these two soil textures were both optimized in the two-site twin experiment.

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?

Response: Thanks for your suggestion. We have modified the color scheme of our figures to make them easier to read for the color-blind. Certainly, the times presented here are local time. We have included the variability of the circle size in the legend in the revised manuscript. We use the mean because it is sensitive to all values.

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

Response: Thanks for your suggestion. For a detailed explanation of the need for two-site experiments we as well, refer to the previous section. Therefore, we’ve left the experiment in the main manuscript but changed to "two-site". Additionally, we also added the explanation of the need for two-site experiment in the revised manuscript. (Line 744-751)

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

Response: Corrected.

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

Response: Thanks for your suggestion. We have combined these two figures in one as two different rows.

Figure 7: same comments as for Figure 3.

Response: Thanks for your suggestion. We will modify the color scheme of our figures to make them easier to read for the color-blind. Certainly, the times presented here are local time. We will include the variability of the circle size. We use the mean because it is sensitive to all values

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.

Response: Thanks for this comment. The less effective simulation of H by the BEPS model compared to other variables, i.e. LE has been confirmed in previous studies (Ju et al., 2006). We acknowledge that the different direction of the simulated sensible heat and the measured one was observed at FI-Hyy. However, the optimization of H was demonstrated successfully, including at the FI-Hyy site. The connection between COS and latent and sensible heat, and the hypotheses of this paper have already been explained in the previous section and we have put the corresponding figures in the supplement.

Figure 9: Suggest to remove or move to supplement.

Response: Thanks for this comment. The connection between COS and SWC, and the hypotheses of this paper have already been carefully explained in the previous section, and we have put the corresponding figures in the supplement.

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

Response: Thanks for this comment. We have cited this figure in the results section and specified these four types of 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.

Response: Thanks for this comment. We've changed the reference.

Table 4: Suggest to remove.

Response: Thanks for this suggestion. The necessity of conducting two-site experiment, we have already explained in detail above in this response and now also provide the explanation in the revised manuscript on lines 744-751.

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

Response: Thanks for your comment. This is due to the fact that we take into account the interdependence of parameters, and we actually optimize the scaling factor of  $K_{sat}$  and  $b$  in this study. Regarding this, we have modified the table (**Table S4** in the revised supplement) and restated the description of the parameters.

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