# Response to the comments of Reviewer #2

The authors have modelled vegetation and soil COS fluxes within the "two-leaf" version of the BEPS (Boreal Ecosystem Productivity Simulator) model. Then, they used observations of COS fluxes at seven sites and a Monte-Carlo approach to reduce parameter uncertainty in BEPS. They further evaluate the impact on GPP, and discuss parameter identifiability.

The paper is well built and very neat, the results are clearly presented. Some further explanations are however needed, and a few outlooks would be welcome.

We are truly grateful to the positive comments and thoughtful suggestions. These comments are all valuable and very helpful for revising and improving our manuscript. In response, we have made changes according to the referee's suggestions. 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.

## **Main comments**

## Abstract

L14-15: "However, most of the current modeling approaches for COS and CO<sub>2</sub> did not explicitly consider the vegetation structural impacts, i.e. the differences between the sun-shade and sunlit leaves in COS uptake" -> It is a bit misleading that the authors bring forward such an argument, because they did not demonstrate in this paper the advantage of distinguishing between sunlit and shaded leaves. Why did not they show the impact of having a two-leaf model compared to a one flux model, as they were the first ones (to my knowledge) to use such a model? This would indeed have been a great achievement.

Response: Thanks for the valuable comments. In order to quantify the effect of changes in the quality of incoming radiation on photosynthesis, land surface models (LSMs) need to stratify the canopy into sunlit and shaded leaves and consider the differences in the transfer of direct and diffuse beams within the canopy (Mercado et al., 2009; He et al., 2013). The advantage of distinguishing between sunlit and shaded leaves in LSMs have been demonstrated in a number of studies (Wang and Leuning, 1998; Luo et al., 2018; Guan et al., 2022; Bao et al., 2022). Specifically, the performance of BL (big leaf), TBL (two big leaf), and TL (two leaf) upscaling scheme in estimating Evapotranspiration (ET) and gross primary productivity (GPP) using the Biosphere-atmosphere Exchange Process Simulator (BEPS) are evaluated with flux measurements from nine eddy covariance towers in Luo et al. (2018). They demonstrated that BL underestimates ET and GPP across all sites because the radiation gradient calculated based on Beer's law fails to describe the instantaneous radiation distribution in the canopy. As most current process-based plant COS uptake simulations are predominantly based on the Berry's stomatal conductance model of COS and the Ball-Barry model, the underestimation of GPP by the BL model ultimately impacts plant COS flux simulations.

As the advantages of the two-leaf model over both the big-leaf model and the two big-leaf model in terms of canopy radiation distribution, GPP, and stomatal conductance have been extensively discussed, we adopted the two-leaf model to simulate COS in this study. The reason

for not further comparing the results of the two-leaf COS model with those of other models based on COS observations is primarily twofold: the lack of accurate BEPS model driving data, and the absence of in-situ COS concentration and flux observation data.

- (1) The lack of accurate BEPS model driving data. For sunlit and shaded leaf stratification, we need accurate description of the canopy structure with at least two structural parameters (Chen et al., 2012). One is the leaf area index (LAI), defined as one half the total (all sided) leaf area per unit ground surface area (Chen and Black, 1992). The other is the foliage clumping index characterizing the way that leaves in a canopy are spatially organized. Thus, In Luo et al. (2018), nine sites in Canada are selected mainly because they have some measured LAI, clumping index, and soil moisture data. The measured soil moisture data were utilized in Luo et al. (2018) to minimize the possible deviations in stomatal conductance modeling caused by the soil moisture simulation. Unfortunately, among the seven sites in this study, no continuous in-situ LAI or clumping index data were provided along with the COS data (Wehr et al., 2017; Rastogi et al., 2018; Spielmann et al., 2019; Vesala et al., 2022). The measured soil moisture data were also not available at US-Ha1. Furthermore, as mentioned in the manuscript, even continuous in-situ meteorological data were lacking at the IT-Soy site.
- (2) The lack of COS concentration and flux observation data. Unlike CO<sub>2</sub>, the concentration of COS exhibits strong seasonal variations, with seasonal amplitudes reaching up to 100-200 parts per trillion (Montzka et al., 2007; Kooijmans et al., 2021; Hu et al., 2021; Ma et al., 2021). Given the linear relationship between plant COS uptake and COS concentration (Stimler et al., 2010), these variations can significantly impact the simulation of COS plant fluxes. Unfortunately, continuous in-site COS concentration data are lacking at the sites. Moreover, for the majority (5/7) of sites in this study, the COS observation sequences are very short, lasting only about one month. As a contrast, observed sequences of GPP and ET at measurement sites all span over five years in Luo et al. (2018).

Overall, due to the lack of accurate BEPS model driving data and continuous in-site COS concentration data, the simulated COS flux subject to great uncertainty, whether it is based on the two-leaf model or other models. Furthermore, the majority of sites used in this study lack long time series of COS observations, and COS flux observations also exhibit considerable uncertainty (Kohonen et al., 2020). Therefore, we have refrained from comparing the COS simulation performance of the two-leaf model and other models. However, we do agree with your opinion and we also believe that comparing the COS simulation performance of the two-leaf model with other models (i.e., BL and TBL model) is an objective we should pursue, given the conceptual scientificity and practical robustness of the two-leaf model (Chen et al., 2012). We anticipate that the simulation of plant COS uptake based on the two-leaf model will outperform other models (i.e., BL and TBL model), and the global vegetation COS flux estimated based on the two-leaf model will exceed that estimated by other models. This will provide insights into both the accurate simulation of plant COS uptake and the magnitude and distribution of global COS vegetation sink.

# 2.4.1 Parameter selection and sampling strategy

L154-155: "9 parameters were selected to be calibrated in this study" -> Why didn't the authors perform a sensitivity analysis to select the most important parameters for COS and GPP? We are left with the impression that the selection was arbitrary, and we may fear that they have missed some important parameter.

Response: Thanks for the valuable comments. As mentioned in the manuscript, currently, numerous studies on parameter sensitivity in COS and GPP simulations have been conducted, laying the foundation for the parameter selection in this study. Specifically, the Morris method and RS-HDMR method were employed to identified that the sensitive parameters in simulating GPP by BEPS for 10 sites covering 7 plant functional types (PFT) over China in Xing et al. (2023). In this study, 21 model parameters were screened, encompassing not only photosynthesis-related parameters but also those associated with energy and water balance, heterotrophic respiration, and autotrophic respiration. The results highlighted that  $V_{cmax25}$ ,  $N_{leaf}$ ,  $r_{decay}$ ,  $b_{H_2O}$ ,  $m_{H_2O}$  and  $f_{leaf}$  as the most crucial parameters for GPP simulation by BEPS. In another related manuscript (Zhu et al., 2023), we identified the model parameters sensitive to COS for BEPS. Therefore, the 9 parameters were selected to be calibrated in this study. Certainly, other literature listed in **Section 2.4.1** also provided references for our parameter selection.

We would like to highlight that the references listed in Section 2.4.1 have been updated. Specifically, the recently manuscript by **Abadie et al. (2023)** and **Zhu et al. (2023)** have been incorporated into the section. (line 216-217)

L155: Table B1 should be placed in the main manuscript, it's important to see here the detailed description of the parameters.

Response: Thanks for the comments. We have moved the Table into the main manuscript (renamed as **Table 2**).

# 2.4.2 Selection of behavioral simulations

"Behavioral simulation" is not an expression I've seen before. Could the authors use simpler terms like "selected" and "rejected" (for "non-behavioral")?

Thanks for your comment. The terms "behavioral" and "non-behavioral" have been extensively employed in the domain of Monte Carlo-based calibration, as evidenced by Beven and Binley (1992), Beven and Freer (2001) and Houska et al. (2014). Hence, we have maintained the usage of "behavioral" and "non-behavioral" in this context. In response, we have added introductions for "behavioral parameter sets" and "non-behavioral parameter sets". "Subsequently, model realizations are grouped into behavioral and non-behavioral model runs and associated parameter sets based on the values of the single or multiple performance measures and the predefined threshold value (Houska et al., 2014). The former describes acceptable model realizations conditioned on the available observational data (Blasone et al., 2008; Beven and Binley, 2014). The latter describes parameter sets that produce behavior inconsistent with observed behavior."(line 199-203).

L168-169: "Thus, the deterministic model prediction is given by the ensemble mean of the 100 behavioral simulations." -> The authors could explain that the "100" comes from 0.5%\*20,000.

Response: Thank you for your comments. Now we rewrite this sentence: "Specifically, here we chose an ASR of 0.5%, i.e., the top 100 model runs with the lowest RMSE values for COS as behavioral simulations." (line 234-235)

# 2.6 Parameter uncertainty

L183: "Due to the complexity of ecosystem" -> Could the authors be more specific: "Due to the functional and structural complexity of ecosystems"?

Response: Thanks for your comment. We have made the modification to the sentence accordingly. (line 247)

L193-194: "Taking into account the influence of the prior distribution to the behavioral parameter sets, the PI is defined as the reduction of the parameter range width. -> This means that if the initial range is overestimated, the PI may be artificially high. This could be the case for the  $b_{\rm H2O}$  parameter, where the max value (1) is 57 times larger than the initial value. Plus, the authors later write, citing Miner et al. (2017), that "83 % of the  $b_{\rm H2O}$  values are located between 0 and 0.15 mol m<sup>-2</sup> s<sup>-1</sup>, and about half are located between 0 and 0.04 mol m<sup>-2</sup> s<sup>-1</sup>" (L236-237).

Response: Thank you for your comments. As we mentioned in the manuscript, the default values and prior ranges for these selected parameters were chosen based on literature and default model settings. For  $b_{H_2O}$ , the default value of it in BEPS is 0.0175 mol m<sup>-2</sup> s<sup>-1</sup>, and we assigned the prior range of it according to Miner et al. (2017). We also highlighted that "literature-documented values of  $b_{H_2O}$  are highly variable". Actually, in the compilation provided by Miner et al. (2017), a number of documented values of  $b_{H_2O}$  are already several tens of times greater than the prior value, for example, reaching as high as 0.57 mol m<sup>-2</sup> s<sup>-1</sup> in Bunce (2004) and 0.69 mol m<sup>-2</sup> s<sup>-1</sup> in Leuning (1995). Specifically, the value of 0.69 mol m<sup>-2</sup> s<sup>-1</sup> was provided alongside a corresponding standard deviation of 0.10 mol m<sup>-2</sup> s<sup>-1</sup>. Considering the wide range of literature values of  $b_{H_2O}$ , we thus opted for a broad prior range (0-1 mol m<sup>-2</sup> s<sup>-1</sup>) and performed the Monte Carlo simulations. Certainly, we acknowledge that the setting of prior ranges for parameters involves subjective decisions, and the prior range of  $b_{H_2O}$  may be overestimated. Indeed, the involvement of subjective decisions is the primary reason for the controversy surrounding GLUE (Beven and Binley, 2014). In response, we have provided clarification regarding the subjectivity controversy surrounding Monte Carlo-based model calibration method. "However, the Monte Carlobased parameter optimization approach subject to controversy (Sambridge and Mosegaard, 2002) due to the numerous subjective decisions involved in its implementation, such as the selection of parameter range, sample size and performance metric, etc. Further research is needed to investigate the impact of these factors on the parameter optimization results related to COS and the assessment of model prediction uncertainty." (line 571-575)

## 3.2 Posterior parameter distributions

L252: The authors should explain what they call "the grouping value".

Response: Thank you for your comments. In Miner et al. (2017), the literature-documented values of  $m_{H_2O}$  were grouped by plant function type (PFT). Thus, we reorganized the sentences as: "Nevertheless, the optimization of  $m_{H_2O}$  is generally achievable through COS assimilation, as supported by our results in good agreement with the compilation of Miner et al. (2017), in which the average historical values of  $m_{H_2O}$  grouped by PFT (referred to as the PFT-grouping values below) are provided." (line 314-316).

Figure 2. The authors should add 'COS' somewhere in the legend, document the boxplot (say it describes the posterior distribution), and explain axes, colours, title (PI).

Response: Thanks for your comment. We have revised the legend, as follows: "Figure 3. Cumulative frequency distributions and boxplots for the posterior model parameters obtained by COS assimilation. The grey area represents uniform parameter distributions, while the colored areas denote posterior CDF distributions, with parameters for different sites represented using different colors. The box extends from the first quartile to the third quartile of the parameter values, with a line at the median. "×" markers denote outliers, and the whiskers represent the lowest or highest parameter values excluding any outliers. The black square represents the prior parameter value, and the axis ranges denote the prior ranges of the parameters. PI denote parameter identifiability, defined as the reduction of the parameter range width." (line 333-348)

# 3.3 The optimization performance in COS fluxes

L300-301: "despite remarkable improvement is attached by the posterior simulations" -> This is a weird formulation, to be rephrased.

Response: Thanks for your comment. The revised sentence reads as: "Particularly, significant underestimation is found in the posterior simulations in 2017 for FI-Hyy, despite the posterior simulations shows a remarkable improvement in reproducing COS fluxes over the entire period (2013-2017)." (line 364-376)

Figure 3/Figure 4: "The means and uncertainties of these observations and simulations are calculated and plotted on a daily or monthly scale" -> Do the authors compute the standard deviation of hourly values for daily means and over daily means for monthly means? Do they compute the standard error of the mean (SEM), defined as the standard deviation (SD) divided by the square root of the number of observations, and which would be more appropriate than SD to estimate the uncertainty of the mean?

Response: Thanks for your comments. Here the standard deviation of hourly values for daily means or monthly means were calculated.

The standard error of the mean (SEM) quantifies uncertainty in the estimate of the mean (Barde and Barde, 2012). However, our intention here is to quantify the uncertainties of the hourly observations on a daily or monthly scale, which does not align with the definition of SEM. Certainly, standard deviation (SD) quantifies the variability, which is also distinct with

uncertainty. Therefore, we have modified the corresponding sentence to clarify this. "The mean observed COS and its uncertainty (estimated by the standard deviation) are represented by black dots with error bars. The means and uncertainties of these hourly observations and simulations are calculated and plotted on a daily or monthly scale." (line 386-388 and line 418-420)

#### 4.2 Parameter interactions

L407: "their weak equivalence" -> What do the authors mean? Equivalence to what?

Response: Thanks for your comment. The sentence is unnecessary, and we have deleted it.

Figure 6 is a bit difficult to interpret, I'm not sure it brings something, could it be moved to the Supplementary part?

Response: Thanks for your comments. The design of this figure is inspired by Figure 4 from Beven and Binley (2014). Similar to Beven and Binley (2014), we employ 3D plots to further explore, visually, the parameter space. Following your suggestion, we have relocated this figure to the appendix.

# 4.3 Parameter identifiability

L442: "the sensitivity of the input data to the parameter" -> This should rather be "the sensitivity of the modeled output to the parameter".

Response: Thanks for your comments. As you mentioned, it should rather be "the sensitivity of the modeled output to the parameter". More specifically, "modeled output" here refers to COS simulation. Therefore, we have revised the original sentence accordingly, and the modified sentence is as follows: "In this study, the identifiability of a parameter closely related to the sensitivity of COS simulations to the parameter, although it is known to be influenced by model over-parameterization and parameter interactions (Gan et al., 2014)." (line 497-498)

L446-447: "However, our findings indicate that the sensitivity of Vcmax25, Nleaf is much greater than that of bH2O, yet the latter is much more identifiable" -> An alternative explanation is once again the overestimated prior range of bH2O.

Response: Thanks for your comment. We acknowledge that the prior range of  $b_{H_2O}$  may be overestimated and the overestimation of the prior range of  $b_{H_2O}$  can be an alternative explanation of  $b_{H_2O}$  being more identifiable (having larger PIs) as PI is defined as the reduction of the parameter range width. A detailed explanation of why we chose such a broad prior range for  $b_{H_2O}$  has been provided previously, along with clarification of the drawback (i.e., involving subjective decisions) of the Monte Carlo-based parameter optimization approach.

L448: "as parameter interaction is a primary contributor to parameter unidentifiability" -> But then, this should also apply to bH2O, as it is highly correlated to fleaf and mH2O, as shown in Figure 5.

Response: Thanks for your comment. As shown in **Figure 5** and **Figure C1** of the original manuscript, there are complex correlations between the 9 pre-selected parameters, and  $b_{H_2O}$  is indeed highly correlated to  $f_{leaf}$  and  $m_{H_2O}$  at AT-Neu. But as mentioned in the original manuscript,  $N_{leaf}$  and  $VJ_{slope}$  is the only parameter combination that is significantly correlated at all sites.

L456-457: "It has been previously demonstrated that soil hydrology-related parameters exert a minimal impact on COS simulations and cannot be effectively constrained through COS assimilation" -> That would depend on whether soil water stress conditions are present or not.

Response: Thanks for your comment. We agree with your point that the impact of soil hydrology-related parameters on COS simulations may vary depending on the presence of soil water stress conditions. We have revised the sentence as follows: "It has been previously demonstrated that soil hydrology-related parameters exert a minimal impact on COS simulations (Figure 2) and cannot be effectively constrained through COS assimilation in general (Figure 3)" (line 514-515)

# 4.4 Relationship between COS and GPP simulation performance -> performances

Response: Corrected

L464: "respond to RMSE" -> This seems awkward, to be rephrased.

Response: Thank you for your comment. We have revised the sentence as follows: "Therefore, it is necessary to investigate the distribution of RMSEs for COS simulations and GPP simulations, and to understand the relationship between the model performance of COS and that of GPP." (line 517-519)

Figure 7: "Each data point represents a parameter set, with color indicating data density" -> That does not seem possible, some binning has to be made to get a density.

Response: Thank you for your comment. At each site, we actually obtained 20,000 discrete points distributed in a two-dimensional space of RMSE for COS (RMSE<sub>COS</sub>) and GPP (RMSE<sub>GPP</sub>), and some binning has to be made to get a density. In this study, we utilized kernel density estimation (<a href="https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.gaussian\_kde.html">https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.gaussian\_kde.html</a>) to estimate the probability density of each scatter point. Subsequently, we assigned colors to each scatter based on the estimated density, and plotted the scatter plots.

## 5 Conclusions

L485-486: "within the Monte Carlo-based methodology base on the coupling of COS modeling and the BEPS model" -> "with a Monte Carlo approach using COS modeling within BEPS"

Response: Thanks for your comment. We have revised the sentence accordingly. (line 577-578)

L486-487: "Global parameter sensitivity analysis was conducted to identify the sensitive parameters" -> "A global parameter sensitivity analysis was conducted to identify the most sensitive ones among a set of 9 pre-selected parameters."

Response: Thanks for your comment. We have revised the sentence accordingly. (line 578-579)

The conclusion is a bit abrupt. The authors should develop some outlooks. What are the consequences of this study? Is there a need to acquire more COS fluxes observations, or a need to improve the COS vegetation model? What will be the next steps with BEPS?

Response: Thank you for your valuable comment. As you mentioned, conducting more observations, developing advanced COS models (as done by Cho et al. (2023)), and utilizing varying COS concentrations for COS simulations are indeed our goals. Inevitably, this study was constrained by these factors. Regarding this, we have added a new section (Section 4.5 Caveats and implication) to discuss these issues and provide an outlook for our future work. Specifically, we have conducted COS simulations based on the two-leaf model at the site scale and utilized COS to optimized GPP. However, at the global scale, the scientific community is grappling with the COS missing sink issue, and the two-leaf model holds promise for addressing this problem. Thus, global COS simulations within two-leaf model are the next step awaiting our investigation. For a more detailed discussion on this aspect, please refer to Section 4.5 in the revised manuscript.

# A2 BEPS leaf COS modeling approach

L568: "where COSa represents the COS mole fraction in the bulk air" -> Did the authors use a variable atmospheric COS mole fraction as it has been shown important (Kooijmans et al., 2021; Abadie et al., 2022)?

Response: Thank you for your valuable comment. We have revised the manuscript to include a more detailed description of the data used in this study. The revised sentence reads as follows: "Data used in this study include LAI, land cover type, meteorological and soil data, as well as CO2 and COS mole fraction data. The CO2 and COS mole fractions in the bulk air were assumed to be spatially invariant over the globe but to vary annually. The CO2 mole fraction data in this study are taken from the Global Monitoring Laboratory (https://gml.noaa.gov/ccgg/trends/global.html). For the COS mole fraction, we utilized the average of observations from sites SPO (South Pole) and MLO (Mauna Loa, United States) drive the model. **These** data are publicly available online at: https://gml.noaa.gov/hats/gases/OCS.html," (line 153-158)

L572: How did the authors derive the empirical relationship expressed in equation (A19)?

Response: Thanks for your comment. Here we adapted the COS leaf uptake modeling approach from SiB4 (Equation 175 in Haynes et al. (2020)). Now, a more detailed description of the modeling approach is provided in the main manuscript (line 122-139):

The leaf-level COS uptake rate  $F_{cos_{deaf}}$  is determined by the formula (Berry et al., 2013):

$$F_{cos,leaf} = COS_a \left( \frac{1.94}{g_{sw}} + \frac{1.56}{g_{bw}} + \frac{1}{g_{cos}} \right)^{-1}$$
 (5)

where  $COS_a$  represents the COS mole fraction in the bulk air.  $g_{sw}$  and  $g_{bw}$  are the stomatal conductance and leaf laminar boundary layer conductance to water vapor (H<sub>2</sub>O). The factors 1.94 and 1.56 account for the smaller diffusivity of COS with respect to H<sub>2</sub>O.  $g_{COS}$  indicates the apparent conductance for COS uptake from the intercellular airspaces, which combined the mesophyll conductance (Evans et al., 1994) and the biochemical

reaction rate of COS and carbonic anhydrase (Badger and Price, 1994). It can be calculated as:

$$g_{COS} = \alpha V_{cmax} \tag{6}$$

Where  $\alpha$  is a parameter that is calibrated to observations of simultaneous measurements of COS and CO<sub>2</sub> uptake (Stimler et al., 2012).  $V_{cmax}$  is the maximum carboxylation rate of Rubisco. Analysis of these measurements yield estimates of  $\alpha$  of ~1400 for C3 and ~7500 for C4 species. With reference the COS modelling scheme of the Simple biosphere model (version 4.2) (Haynes et al., 2020),  $g_{cos}$  can be calculated as

$$g_{COS} = 1.4 * 10^{3} * (1.0 + 5.33 * F_{C4}) * 10^{-6} F_{APAR} f_{w} V_{cmax}$$
 (7)

where  $F_{C4}$  denotes the C4 plant flag, taking the value of 1 for C4 plants and 0 otherwise.  $f_w$  is a soil moisture stress factor describing the sensitivity of  $g_{sw}$  to soil water availability (Ju et al., 2006).  $F_{APAR}$  is the scaling factor for leaf radiation (Smith et al., 2008), calculated as:

$$F_{APAR} = 1 - e^{(-0.45 \, LAI)} \tag{8}$$

## **Minor comments**

L15: "i.e." -> "i.e.,"

Response: Corrected.

L15: I could not find information on the "sun-shade" expression, would not the simpler "shaded" be more appropriate?

Response: Thanks for your comment. Here "shaded" indeed is more appropriate and we have revised the sentence.

L31: "(GPP), is" -> "(GPP) is"

Response: Corrected.

L33: "the modeling of GPP are affected" -> "the modeling of GPP is affected"

Response: Corrected.

L60: "Ecosystem carbon, water and energy processes are interacted" -> "Ecosystem carbon, water and energy processes are interacting"

Response: Corrected.

L64: "e.g." -> "e.g.,"

Response: Corrected.

L67: "Which parameters the COS simulation is sensitive to" -> "To which parameters is the COS simulation sensitive"

Response: Corrected.

L84: "calculated" -> "calculates" (harmonize verb tenses.)

Response: Thanks for your comment. We have reviewed the verb tenses in the manuscript.

L111: "locations" -> "Locations" (capital letter L)

Response: Corrected.

L116: "three" -> "two" (I see only GLOBMAP and GLASS.)

Response: Thanks for your comment. We have revised the manuscript to include a more detailed description of the LAI data used in this study. "The LAI dataset used here are the GLOBMAP global leaf area index product (Version 3) (see GLOBMAP global Leaf Area Index since 1981 | Zenodo) and the Global Land Surface Satellite (GLASS) LAI product (Version 3) (acquired from <a href="ftp://ftp.glcf.umd.edu/">ftp://ftp.glcf.umd.edu/</a>). They represent Leaf area index at a spatial resolution of 8 km (Liu et al., 2012) and 1 km (Xiao et al., 2016) respectively, and a temporal resolution of 8-day. With reference to the observed LAI at these sites (Wehr et al., 2017; Rastogi et al., 2018; Spielmann et al., 2019; Kohonen et al., 2022), we used GLOBMAP products to drive the BEPS model at most sites (5/7) duo to its good agreement with the observed LAI. Specifically, as the GLOBMAP product had considerably underestimated LAI at DK-Sor and was not consistent with the vegetation phenology at ES-Lma during the measurement campaign (Spielmann et al., 2019), GLASS LAI was used at these two sites. In addition, these LAI products were interpolated into daily values by the nearest neighbor method for the simulation." (line 160-168)

L163: "in in" -> "in"

Response: Corrected.

L168, 387: "In specific" -> "Specifically"

Response: Corrected.

L181: "if all model parameters is considered" -> "if all model parameters are considered"

Response: Corrected.

L184: "compensating with each other" -> "compensating each other"

Response: Corrected.

L193-194: "Taking into account the influence of the prior distribution to the behavioral parameter sets" -> "Taking into account the influence of the prior distribution of the behavioral parameter sets"

Response: Corrected.

L220 (twice): Fig. 1 -> Fig. 2

Response: Thanks for your comment. We have thoroughly reviewed the manuscript to ensure accurate referencing of figures and tables.

L225: "parameters related energy balance" -> "parameters related to energy balance"

Response: Corrected.

L281: "Fig. 2" -> "Fig. 3"

Response: Corrected.

L287: "e.g. Fig. 2d" -> "e.g., Fig. 3d"

Response: Corrected.

L297: "a further underestimate of the" -> "a further underestimation of the"

Response: Corrected.

L307: "the ensemble mean deviate remarkable from observations" -> "the ensemble mean strongly deviates from the observations"

Response: Corrected.

L320, 352: "posterior (green)" ->

Response: Thanks for your comment. We have rechecked the manuscript to avoid any errors in color representation.

L322, 354: "blue dots" -> -> It seems gray.

Response: Corrected.

L334: "Fig. 3" -> "Fig. 4"

Response: Corrected.

L363-364: "by influence the modeling of stomatal conductance" -> "by influencing the modeling of the stomatal conductance"

Response: Corrected.

L384: "in photosynthetic machinery" -> "in the photosynthetic machinery"

Response: Corrected.

L397: "confident levels" -> "confidence levels"

Response: Corrected.

L399: "A total of 14 parameter combinations demonstrate significantly correlated" -> "A total of 14 parameter combinations demonstrate significant correlations"

Response: Corrected.

L411, 596: The red font looks weird, like mixed with a black one, could the authors improve that?

Response: Of course. Now we have changed the font color and redrawn the figure.

L419: "e.g." -> "e.g.,"

Response: Corrected.

L450: "exhibits low sensitivity" -> "exhibits a low sensitivity"

Response: Corrected.

L468: "for COS simulation" -> "for COS simulations"

Response: Corrected.

L475: "such as that" -> "for example considering that"

Response: Thanks for your valuable comment. We have modified the sentence accordingly.

L478: "e.g." -> "e.g.,"

Response: Corrected.

L495: "interactions exists" -> "interactions exist"

Response: Corrected.

L495-496: "In particularly" -> "Particularly" or "In particular"

Response: Corrected.

L519: "according the" -> "according to the"

Response: Corrected.

L525: In the first exponential of equation (A7), "Kn" should be "kn".

Response: Corrected. Thank you for your detailed comment.

L530: "is the is the" -> "is the"

Response: Corrected.

L535: "(gsw in)" -> The unit is missing.

Response: Thanks for your comment. Now the unit  $(\text{mol m}^{-2}\text{s}^{-1})$  of the leaf stomatal conductance for water vapor  $(g_{sw})$  has been added.

L538: "is intercept" -> "is the intercept"

Response: Corrected.

L549: "the number of soil layer" -> "the number of soil layers"

Response: Corrected.

L572: In equation (A19), shouldn't "LAI" be "L" as in equations (A6/7)?

Response: Thanks for your valuable comment. According to Chen et al. (2012), here "L" actually denote the canopy depth (m), and we have corrected the error accordingly.

L590: "of the 9 parameters were" -> "of the 9 parameters that were"

Response: Corrected.

L591: "to the parameter dependent" -> "to the parameter dependency"

Response: Corrected.

L620: "Reference" -> "References"

Response: Corrected.

## **References:**

Abadie, C., Maignan, F., Remaud, M., Kohonen, K. M., Sun, W., Kooijmans, L., Vesala, T., Seibt, U., Raoult, N., and Bastrikov, V.: Carbon and water fluxes of the boreal evergreen needleleaf forest biome constrained by assimilating ecosystem carbonyl sulfide flux observations, Journal of Geophysical Research: Biogeosciences, e2023JG007407, 2023.

Badger, M. R. and Price, G. D.: The role of carbonic anhydrase in photosynthesis, Annual review of plant biology, 45, 369-392, 1994.

Bao, S., Ibrom, A., Wohlfahrt, G., Koirala, S., Migliavacca, M., Zhang, Q., and Carvalhais, N.:

- Narrow but robust advantages in two-big-leaf light use efficiency models over big-leaf light use efficiency models at ecosystem level, Agricultural and Forest Meteorology, 326, 109185, 2022.
- Barde, M. P. and Barde, P. J.: What to use to express the variability of data: Standard deviation or standard error of mean?, Perspectives in clinical research, 3, 113-116, 2012.
- Berry, J., Wolf, A., Campbell, J. E., Baker, I., Blake, N., Blake, D., Denning, A. S., Kawa, S. R., Montzka, S. A., and Seibt, U.: A coupled model of the global cycles of carbonyl sulfide and CO2: A possible new window on the carbon cycle, Journal of Geophysical Research: Biogeosciences, 118, 842-852, 2013.
- Beven, K. and Binley, A.: The future of distributed models: model calibration and uncertainty prediction, Hydrological processes, 6, 279-298, 1992.
- Beven, K. and Binley, A.: GLUE: 20 years on, Hydrological processes, 28, 5897-5918, 2014.
- Beven, K. and Freer, J.: Equifinality, data assimilation, and uncertainty estimation in mechanistic modelling of complex environmental systems using the GLUE methodology, Journal of hydrology, 249, 11-29, 2001.
- Blasone, R.-S., Vrugt, J. A., Madsen, H., Rosbjerg, D., Robinson, B. A., and Zyvoloski, G. A.: Generalized likelihood uncertainty estimation (GLUE) using adaptive Markov Chain Monte Carlo sampling, Advances in Water Resources, 31, 630-648, 2008.
- Bunce, J. A.: Carbon dioxide effects on stomatal responses to the environment and water use by crops under field conditions, Oecologia, 140, 1-10, 2004.
- Chen, J. M. and Black, T.: Defining leaf area index for non flat leaves, Plant, Cell & Environment, 15, 421-429, 1992.
- Chen, J. M., Mo, G., Pisek, J., Liu, J., Deng, F., Ishizawa, M., and Chan, D.: Effects of foliage clumping on the estimation of global terrestrial gross primary productivity, Global Biogeochemical Cycles, 26, 2012.
- Cho, A., Kooijmans, L. M., 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, 2023.
- Evans, J. R., Caemmerer, S., Setchell, B. A., and Hudson, G. S.: The relationship between CO2 transfer conductance and leaf anatomy in transgenic tobacco with a reduced content of Rubisco, Functional Plant Biology, 21, 475-495, 1994.
- Gan, Y., Duan, Q., Gong, W., Tong, C., Sun, Y., Chu, W., Ye, A., Miao, C., and Di, Z.: A comprehensive evaluation of various sensitivity analysis methods: A case study with a hydrological model, Environmental modelling & software, 51, 269-285, 2014.
- Guan, X., Chen, J. M., Shen, H., Xie, X., and Tan, J.: Comparison of big-leaf and two-leaf light use efficiency models for GPP simulation after considering a radiation scalar, Agricultural and Forest Meteorology, 313, 108761, 2022.
- Haynes, K., Baker, I., and Denning, S.: Simple biosphere model version 4.2 (SiB4) technical description, Colorado State University: Fort Collins, CO, USA, 2020.
- He, M., Ju, W., Zhou, Y., Chen, J., He, H., Wang, S., Wang, H., Guan, D., Yan, J., and Li, Y.: Development of a two-leaf light use efficiency model for improving the calculation of terrestrial gross primary productivity, Agricultural and forest meteorology, 173, 28-39, 2013.
- Houska, T., Multsch, S., Kraft, P., Frede, H.-G., and Breuer, L.: Monte Carlo-based calibration

- and uncertainty analysis of a coupled plant growth and hydrological model, Biogeosciences, 11, 2069-2082, 2014.
- Hu, L., Montzka, S. A., Kaushik, A., Andrews, A. E., Sweeney, C., Miller, J., Baker, I. T., Denning, S., Campbell, E., and Shiga, Y. P.: COS-derived GPP relationships with temperature and light help explain high-latitude atmospheric CO2 seasonal cycle amplification, Proceedings of the National Academy of Sciences, 118, e2103423118, 2021.
- Ju, W., Chen, J. M., Black, T. A., Barr, A. G., Liu, J., and Chen, B.: Modelling multi-year coupled carbon and water fluxes in a boreal aspen forest, Agricultural and Forest Meteorology, 140, 136-151, 2006.
- Kohonen, K.-M., Kolari, P., Kooijmans, L. M., Chen, H., Seibt, U., Sun, W., and Mammarella, I.: Towards standardized processing of eddy covariance flux measurements of carbonyl sulfide, Atmospheric Measurement Techniques, 13, 3957-3975, 2020.
- Kohonen, K.-M., Dewar, R., Tramontana, G., Mauranen, A., Kolari, P., Kooijmans, L. M., Papale, D., Vesala, T., and Mammarella, I.: Intercomparison of methods to estimate gross primary production based on CO 2 and COS flux measurements, Biogeosciences, 19, 4067-4088, 2022.
- Kooijmans, L. M. J., Cho, A., Ma, J., Kaushik, A., Haynes, K. D., Baker, I., Luijkx, I. T., Groenink, M., Peters, W., Miller, J. B., Berry, J. A., Ogée, J., Meredith, L. K., Sun, W., Kohonen, K. M., Vesala, T., Mammarella, I., Chen, H., Spielmann, F. M., Wohlfahrt, G., Berkelhammer, M., Whelan, M. E., Maseyk, K., Seibt, U., Commane, R., Wehr, R., and Krol, M.: Evaluation of carbonyl sulfide biosphere exchange in the Simple Biosphere Model (SiB4), Biogeosciences, 18, 6547-6565, 10.5194/bg-18-6547-2021, 2021.
- Leuning, R.: A critical appraisal of a combined stomatal photosynthesis model for C3 plants, Plant, Cell & Environment, 18, 339-355, 1995.
- Liu, Y., Liu, R., and Chen, J. M.: Retrospective retrieval of long term consistent global leaf area index (1981–2011) from combined AVHRR and MODIS data, Journal of Geophysical Research: Biogeosciences, 117, 2012.
- Luo, X., Chen, J. M., Liu, J., Black, T. A., Croft, H., Staebler, R., He, L., Arain, M. A., Chen, B., and Mo, G.: Comparison of big leaf, two big leaf, and two leaf upscaling schemes for evapotranspiration estimation using coupled carbon water modeling, Journal of Geophysical Research: Biogeosciences, 123, 207-225, 2018.
- Ma, J., Kooijmans, L. M., Cho, A., Montzka, S. A., Glatthor, N., Worden, J. R., Kuai, L., Atlas, E. L., and Krol, M. C.: Inverse modelling of carbonyl sulfide: implementation, evaluation and implications for the global budget, Atmospheric Chemistry and Physics, 21, 3507-3529, 2021.
- Mercado, L. M., Bellouin, N., Sitch, S., Boucher, O., Huntingford, C., Wild, M., and Cox, P. M.: Impact of changes in diffuse radiation on the global land carbon sink, Nature, 458, 1014-1017, 2009.
- Miner, G. L., Bauerle, W. L., and Baldocchi, D. D.: Estimating the sensitivity of stomatal conductance to photosynthesis: a review, Plant, Cell & Environment, 40, 1214-1238, 2017.
- Montzka, S., Calvert, P., Hall, B., Elkins, J., Conway, T., Tans, P., and Sweeney, C.: On the global distribution, seasonality, and budget of atmospheric carbonyl sulfide (COS) and some similarities to CO2, Journal of Geophysical Research: Atmospheres, 112, 2007.
- Rastogi, B., Berkelhammer, M., Wharton, S., Whelan, M. E., Itter, M. S., Leen, J. B., Gupta,

- M. X., Noone, D., and Still, C. J.: Large uptake of atmospheric OCS observed at a moist old growth forest: Controls and implications for carbon cycle applications, Journal of Geophysical Research: Biogeosciences, 123, 3424-3438, 2018.
- Sambridge, M. and Mosegaard, K.: Monte Carlo methods in geophysical inverse problems, Reviews of Geophysics, 40, 3-1-3-29, 2002.
- Smith, B., Knorr, W., Widlowski, J.-L., Pinty, B., and Gobron, N.: Combining remote sensing data with process modelling to monitor boreal conifer forest carbon balances, Forest Ecology and Management, 255, 3985-3994, 2008.
- Spielmann, F., Wohlfahrt, G., Hammerle, A., Kitz, F., Migliavacca, M., Alberti, G., Ibrom, A., El - Madany, T. S., Gerdel, K., and Moreno, G.: Gross primary productivity of four European ecosystems constrained by joint CO2 and COS flux measurements, Geophysical research letters, 46, 5284-5293, 2019.
- Stimler, K., Berry, J. A., and Yakir, D.: Effects of carbonyl sulfide and carbonic anhydrase on stomatal conductance, Plant Physiology, 158, 524-530, 2012.
- Stimler, K., Montzka, S. A., Berry, J. A., Rudich, Y., and Yakir, D.: Relationships between carbonyl sulfide (COS) and CO2 during leaf gas exchange, New Phytologist, 186, 869-878, 2010.
- Vesala, T., Kohonen, K.-M., Kooijmans, L. M., Praplan, A. P., Foltýnová, L., Kolari, P., Kulmala, M., Bäck, J., Nelson, D., and Yakir, D.: Long-term fluxes of carbonyl sulfide and their seasonality and interannual variability in a boreal forest, Atmospheric Chemistry and Physics, 22, 2569-2584, 2022.
- Wang, Y.-P. and Leuning, R.: A two-leaf model for canopy conductance, photosynthesis and partitioning of available energy I:: Model description and comparison with a multi-layered model, Agricultural and Forest Meteorology, 91, 89-111, 1998.
- Wehr, R., Commane, R., Munger, J. W., McManus, J. B., Nelson, D. D., Zahniser, M. S., Saleska, S. R., and Wofsy, S. C.: Dynamics of canopy stomatal conductance, transpiration, and evaporation in a temperate deciduous forest, validated by carbonyl sulfide uptake, Biogeosciences, 14, 389-401, 2017.
- Xiao, Z., Liang, S., Wang, J., Xiang, Y., Zhao, X., and Song, J.: Long-time-series global land surface satellite leaf area index product derived from MODIS and AVHRR surface reflectance, IEEE Transactions on Geoscience and Remote Sensing, 54, 5301-5318, 2016.
- Xing, X., Wu, M., Zhang, W., Ju, W., Tagesson, T., He, W., Wang, S., Wang, J., Hu, L., and Yuan, S.: Modeling China's terrestrial ecosystem gross primary productivity with BEPS model: Parameter sensitivity analysis and model calibration, Agricultural and Forest Meteorology, 343, 109789, 2023.
- Zhu, H., Wu, M., Jiang, F., Vossbeck, M., Kaminski, T., Xing, X., Wang, J., Ju, W., and Chen, J. M.: Assimilation of Carbonyl Sulfide (COS) fluxes within the adjoint-based data assimilation system—Nanjing University Carbon Assimilation System (NUCAS v1. 0), EGUsphere, 2023, 1-35, 2023.