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.

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?

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.

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.

Other minor comments:
Line 142: “For NUCAS, we use the same soil texture” to “we used the same soil texture.”
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.
Line 197: “the CO_2 and COS mole fractions in the bulk air were assumed to be spatially invariant.” What is the value of CO_2 and COS mole fractions in your case?
Line 227: “in situ” to “*in situ*”, and all elsewhere.
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.
Line 425: “transpiration and soil water transport, and therefore provide an indirect constraint for improving the simulation of GPP, LE, H”. Please specify LE and H, at the first place giving full names.
Line 440: “very reasonable”. Is there another way to say “very”?
Line 450: “very similar”. The same as Line 440. And check 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.
Line 1165: Figure 4, it is not easy to see clearly the green and gray shading. Please consider better visualization.

Ling 1170 and 1175: Figure 5 and 6, why there are error bars for some sites but no error bars for other sites?
Line 1185: Figure 8. It is hard to see difference between green and gray. The dots in c and f are maybe too big.