

Biogeosciences Discuss., referee comment RC1 https://doi.org/10.5194/bg-2021-281-RC1, 2021 © Author(s) 2021. This work is distributed under the Creative Commons Attribution 4.0 License.



Comment on bg-2021-281

Anonymous Referee #1

Referee comment on "Global modelling of soil carbonyl sulfide exchange" by Camille Abadie et al., Biogeosciences Discuss., https://doi.org/10.5194/bg-2021-281-RC1, 2021

Abadie et al. implemented a mechanistic and empirical soil model of COS exchange into the ORCHIDEE land surface model and compare those with observations of soil COS fluxes at several sites, representing different soil types. Through a sensitivity study they find the most important parameters for the soil COS flux and optimize those parameters with observations at two sites to improve the COS soil flux simulations. Finally, the authors provide an updated global soil COS budget, including both oxic and anoxic (wetland) soils. This is a very complete and thorough study that I find very well readable. My comments are hence minor.

Answer: The authors thank the Referee for the overall positive answer to this study and for the very helpful comments to improve the manuscript.

Abstract:

P1, L44: -576 Gg S yr-1 for vegetation+soil, or only the vegetation?

Answer: -576 GgS yr-1 corresponds to the revised budget for vegetation only. We replaced "which helped reduce the imbalance of the atmospheric COS budget by lowering COS uptake by soils and vegetation globally (-10% for soil, and -8% for vegetation with a revised mean estimate of -576 GgS y-r1 over 2009-2016)" by "which helped reduce the imbalance of the atmospheric COS budget by lowering **soil COS uptake by 10% and plant COS uptake by 8% globally (with a revised mean vegetation budget of -576 GgS yr⁻¹ over 2009-2016)".**

Introduction:

P2, L62-63: This sentence reads weird.

Answer: We rephrased this sentence as shown in the answer of the next comment.

P2, L63-64: The numbers 700-1100 GgS yr-1 sound like a very large gap. If I'm correct, Berry et al. (2013) added an additional ocean flux of 600 to close the gap, and Kuai et al. (2015) added 559 Gg S yr-1. Do the values 700-1100 GgS yr-1 represent the total ocean emissions? So not only the emission gap? A reference to a more recent inversion could be added (Ma et al. (2021) with a total gap of 432Gg S yr⁻¹).

Answer: Indeed, the values 700-1100 GgS yr-1 represent the total COS oceanic emission

estimates (Berry et al., 2013; Kuai et al., 2015; Launois et al, 2015). We modified the sentence as follows "Several atmospheric transport inversion studies have suggested that an unidentified COS source located over the tropics, of the order of 400-600 GgS yr⁻¹, was needed to close the contemporary COS budget (Berry et al., 2013; Glatthor et al., 2015; Kuai et al., 2015; Ma et al., 2021; Remaud et al., 2022)."

P2, L78: better say something like: "they have usually not been considered in atmospheric COS budgets".

Answer: We replaced the sentence as suggested by the Referee "Although such COS emissions can be large in some conditions, **they have usually not been considered in atmospheric COS budgets**."

P3, L87: form = from

Answer: Thank you, this error was corrected.

P3, L113: For clarification, consider adding something like: "at the different sites **that will be used for evaluation in this study**".

Answer: We completed the sentence as suggested "To better represent the observed soil conditions at the different sites **that will be used for evaluation in this study**, we substituted the soil textures initially assigned in ORCHIDEE from the USDA texture global map with the observed soil textures corresponding to the USDA texture classes (Table S2)."

P3, L119: More important to the mechanistic model than to the empirical model?

Answer: Yes, this precision was added to the sentence "The move from the coarse Zobler classes to the finer USDA classes is found to be more important to the mechanistic model **than to the empirical model**."

P8, anoxic soil COS production: Did you consider to use the formulations of Meredith et al., 2018? These are similar to that of Whelan et al., 2016, but then with the alfa and beta parameters specific for peatland/wetland soils. That is, fca = 3700 for boreal peatland (Meredith et al., 2019) and alfa and beta for peatland from Meredith et al., (2018,). It would be interesting to compare those COS production estimates for wetland soils.

Answer: In the mechanistic approach, the f_{CA} parameter is related to COS uptake by oxic soils only, as we consider anoxic soils as COS sources (equation 18). We did not use the formulation of Meredith et al. (2018) to represent soil COS flux for boreal peatlands as we decided to use the same formulation adapted from Ogée et al. (2016) for all anoxic soils. Indeed, soil COS emissions from peatlands are difficult to characterize as they can vary by an order of magnitude depending on the observation site (see Figure 1 in Meredith et al., 2018). This large variability shows that factors other than soil temperature could be important to include to represent and parametrize soil COS emissions from peatlands. Moreover, the wetland map from Tootchi et al. (2019) used in ORCHIDEE does not distinguish between the different wetland types. Therefore, improving soil COS flux modeling for the different types of anoxic soils should be the focus of future work as adapting the parameters to each wetland type might not be sufficient to improve their representation. However, as the approach to estimate soil COS fluxes from wetlands could be refined by distinguishing boreal peatland as suggested, we added this in section 4.3. as a future improvement. We completed the sentence as follows "We could also refine our approach by distinguishing between the different types of wetlands and define a P_{ref} value for each wetland type instead of a global value of 10 pmol COS $m^{-2} s^{-1}$. Then, a distinction could also be made for anoxic soil COS fluxes from boreal peatlands,

as Meredith et al. (2019) give a value of f_{CA} specific to this biome."

P10, L330: "....the same training method than the one used in Spielmann et al." should be "....the same training method **as** *the one used in Spielmann et al."*

Answer: Thank you, this error was corrected.

P10, L333: If I understand the description in Wehr et al. (2017) right, the soil COS fluxes at US-HA are not based on eddy-covariance fluxes. It can be better described as flux-profile measurements, connected to CO2 soil chamber measurements and profiles.

Answer: The Referee is right, we clarified the description of US-HA measurement methods for soil COS fluxes "At US-HA, soil COS fluxes in 2012 and 2013 were not directly measured but derived from **flux-profile measurements**, **connected to CO2 soil chamber measurements and profiles.** A sub-canopy flux gradient approach was used to partition canopy uptake from soil COS fluxes. For more information on this approach and its limitations, see Wehr et al. (2017)."

P10,L350-351:" The stations located in the northern Hemisphere sample air masses coming from the entire northern hemisphere domain above 30 degrees." The stations cover mainly North-America and actually Eurasia is hardly covered, so I would not agree with this statement.

Answer: The stations located in the Northern hemisphere cover mainly North America, however they are sensitive to air masses coming from the entire Northern hemisphere domain above 30 degrees based on atmospheric modeling, as shown in Remaud et al. (2022; Figure 1 and part 2.2.1).

P11, L384: what does "d" stand for?

Answer: The abbreviation "80 or 667 d" was replaced by "80 or 667 days".

P12, L412: spell out "DA".

Answer: The abbreviation "DA" was replaced by "Data assimilation".

Results:

P13, section 3.1.1. I think the authors could put more emphasis on the potential role of nitrogen fertilization on soil fluxes. E.g. the results of IT-CRO, an agricultural site, could be emphasized in this context. Also the overestimated COS uptake at AT-NEU and ES-LMA could be discussed in light of nitrogen fertilization.

Answer: Thank you, we emphasized the importance of nitrogen inputs at AT-NEU, ES-LMA and IT-CRO in the description of figure 2. "Besides, AT-NEU and ES-LMA are managed grassland sites with nitrogen inputs. Then, soil COS production could also be enhanced by a high nitrogen content as suggested by several studies (Kaisermann et al., 2018; Kitz et al., 2020; Spielmann et al., 2020), which is not represented in our models. The mechanistic model is able to represent a net COS production at IT-CRO but overestimates it. This might highlight the importance of adapting the production parameters (α and β) in this model to adequately represent a net COS production. In this model, the net soil COS production is related to an increase in soil temperature. However, it is to be noted that IT-CRO is an agricultural site with nitrogen fertilization. Therefore, soil COS production in the observations could also be enhanced by nitrogen inputs."

P13, L468 (Table 3): I would consider showing Table 3 as a figure. The same also for Table 4, which could even be combined with a Fig. from Table 3.

Answer: We inserted the RMSD values in Table 3 and Table 4 in Figure 2 and Figure 3, respectively.



Figure 1: Seasonal cycle of weekly average net soil COS fluxes (pmol m⁻² s⁻¹) at: AT-NEU, ES-LMA, IT-CRO, DK-SOR, ET-JA, FI-HYY and US-HA. The shaded areas around the observation and simulation curves represent the standard-deviation over a week for each site. Soil COS fluxes are computed with a variable atmospheric COS concentration. RMSD values between the simulated and observed fluxes are given with the respective model color at each site, and for both soil chambers at FI-HYY (ch1 and ch2).



Figure 2: Mean diel cycle of net soil COS fluxes (pmol m⁻² s⁻¹) over a month at: AT-NEU (08/2015), ES-LMA (05/2016), IT-CRO (07/2017), DK-SOR (06/2016), ET-JA (08/2016), FI-HYY (08/2015) and US-HA (07/2012). Soil COS fluxes are computed with a variable atmospheric COS concentration. The observation-based diel cycles (dots) are computed using Random Forest models at At-NEU, ES-LMA, IT-CRO, DK-SOR and ET-JA. At AT-NEU and ES-LMA. RMSD values between the simulated and observed fluxes are given with the respective model color at each site, and for both soil chambers at FI-HYY (ch1 and ch2).

P14, L486-488: Or the division by PFT is not sufficient, and more specific information on e.g. nitrogen content is needed.

Answer: Indeed, the mismatch between the observed and simulated fluxes could also be due to the PFT fractions attributed at each site, or to missing processes in the models. These assumptions were added to the one made on the need to adapt the PFT-specific parameters on site. We completed the sentence as follows **"The mismatch between the model and the observations could be due to several factors including: i) an insufficient representation of the vegetation complexity by the division in PFTs; ii) a poor calibration of the PFT-specific parameters (f_{CA}, \alpha, \beta); or iii) missing processes in the model, such as considering the effect of nitrogen content on soil COS fluxes."**

P14, L496: globally = generally?

Answer: "Globally" was corrected by "generally".

P14, L503-505: This seems to be a repetition of line 500-501.

Answer: Lines 500-501 refer to the soil moisture optimum while lines 503-505 refer to the temperature optimum, both described in Ogée et al. (2016). This was clarified as follows "Furthermore, an optimum soil water content for net soil COS uptake is found between 10% and 15%, which was also observed in Ogée et al. (2016) and in several field studies to be around 12% (Kesselmeier et al., 1999; Liu et al., 2010; van Diest and Kesselmeier, 2008). This optimum soil water content for soil COS uptake is related to a site-specific temperature optimum, which is found between 13°C and 15°C at US-HA for example. Indeed, Ogée et al. (2016) also describe a temperature optimum with a value that depends on the studied site (Kesselmeier et al., 1999; Liu et al., 2010; van Diest and Kesselmeier, 2008)."

Fig 4: Can you show the same plots for observations?

Answer: We represented below a version of Figure 4 for the observed soil COS flux. The comparison between the observed and modelled soil temperature and water content response of soil COS flux is limited by the observation periods. However, the observations do not show a net increase in soil COS uptake with soil temperature as seen at all sites for the empirical model in Figure 4. The increasing trend in net soil COS emissions with soil temperature at ES-LMA and IT-CRO represented for the mechanistic model is also found in the observations. At ET-JA, the net soil COS uptake increases with lower soil water content, which is also shown in Figure 4 for the mechanistic model. However, at AT-NEU the response of soil COS fluxes to soil temperature differs between the simulation and the observations.



Figure RC1_1: Observed net soil COS flux (pmol m² s⁻¹) versus soil temperature (°C) and soil water content (SWC) (m³.m⁻ ³) at AT-NEU, ES-LMA, IT-CRO, DK-SOR, ET-JA, US-HA and FI-HYY.

This figure was added to the supplement as Figure S1 and part 3.1.3. was completed as follows "At IT-CRO and ES-LMA where a strong net soil COS production is simulated by the mechanistic model, the main driver of soil COS fluxes becomes soil temperature. At these sites, the net soil COS production increases with soil temperature, due to the exponential response of soil COS production term to soil temperature. **The increase in soil COS production with soil temperature at IT-CRO and ES-LMA is supported by the observations (Figure S1).**

Contrary to the mechanistic model, soil COS uptake computed with the empirical model is mainly driven by soil temperature, with a soil COS uptake that increases with increasing soil temperature. This response of the empirical model to soil temperature is due to its relation to soil respiration, which is enhanced by strong soil temperature. **However, this net increase in soil COS uptake with soil temperature at all sites is not found in the observations (Figure S1).**"

Fig 5: Can the numbers at the end of the parameter names be replaced with an abbreviation? It is not entirely clear to me what the numbers represent, are they a PFT ánd soil texture number?

Answer: Yes, we changed the parameter names to avoid confusion. The numbers at the end of the parameter names were kept only for PFTs and removed for soil texture as the same soil texture was imposed at the two sites (texture 3 "sandy loam"). We also reminded the PFT numbers in the legend of the figure.



Figure 5: Morris sensitivity scores of the key parameters to which soil COS fluxes are sensitive, for the empirical (left) and the mechanistic (right) models. The two studied sites are FI-HYY (top) and US-HA (bottom). Full descriptions of each tested parameter can be found in Tables S3 and S4 in the supporting information. The PFT is indicated at the end of the parameter names for the PFT-dependent parameters (at FI-HYY: PFT7 = boreal needleleaf evergreen and PFT 15 = boreal natural C3 grassland, at US-HA: PFT6 = temperate broadleaf summergreen and PFT10 = temperate natural C3 grassland). The first-order parameters are shown in the frames.

P16, L555: Can you remind the reader what PFT 15 is?

Answer: Yes, we reminded the name of PFT 15 (boreal C_3 grass) in the sentence L555 "However, at FI-HYY the most influential uptake parameter is for PFT 15 (**boreal C**₃ grass) that only represents 20% of the PFTs at this site while PFT 7 (boreal needleleaf evergreen forest) is the dominant PFT."

Figure E1: Can you explain the green and blue points, which are prior and which are posterior?

Answer: We added the description of the prior and post optimization parameter values in the figure legend:

Figure E1: Comparison between prior and posterior optimization parameter values at FI-HYY and US-HA. The y-axis represents the normalization between the edges of the range of variation for each parameter. Prior values of the parameters are represented in blue and post optimization values are in green.

P17, L600-605: It is very interesting to read that the optimized parameters not only improve the simulated soil COS flux, but also the soil hydrology! Can you give some more details on the improvement of the soil moisture, e.g. with a figure or numbers?

Answer: Yes, we added information on the RMSD value change for soil water content prior and post optimization for both models to this sentence "However, while it improves the simulated water content compared to the observations for the mechanistic model at the two sites (RMSD decreases by 28% at FI-HYY and 22% at US-HA), it leads to a degradation at FI-HYY for the empirical model (RMSD increases by more than 3 times)."

P17, L612-613: It may be worth discussing the resemblance of the global distribution of COS soil fluxes of oxic soils with that presented by Kooijmans et al. (2021) (see their supplementary material). It is nice to see that the implementations of both the empirical and mechanical models show very similar global distributions in ORCHIDEE and SiB4.

Answer: Indeed, we added a comparison of the empirical and mechanistic models between SiB4 and ORCHIDEE in this section. The empirical approach shows a similar distribution in SiB4 and ORCHIDEE. However, as explained in this section the authors do not completely agree on the resemblance of SiB4 and ORCHIDEE distributions for the mechanistic model concerning the regions with a net COS uptake by oxic soils. We added this comparison to section 3.2.1: "The distribution and magnitude of soil COS flux from the empirical approach is similar to the one presented in Kooijmans et al. (2021) (see Figure S15 in the supplementary material of Kooijmans et al., 2021), when implemented in SiB4. For the mechanistic model, the comparison of oxic soil COS flux distribution with the one in SiB4 shows a net soil COS flux is about 60 pmol m⁻² s⁻¹ higher in ORCHIDEE than in SiB4. The regions with the strongest net oxic soil COS uptake also differ between SiB4 and ORCHIDEE as it is concentrated in the tropics in SiB4 and in Western North and South America, and in China for ORCHIDEE."

P19, L683-684: So the soils do not seem to explain the biases at high latitudes, so can we conclude that the vegetation sink is underestimated at the higher latitudes?

Answer: Yes, this point was mentioned in section 4.1 ("This positive net global budget could be due to an underestimation of vegetation COS uptake in the northern hemisphere, participating in the underestimation of the COS concentration drawdown (Figure 9), but the absence of anthropogenic emission seasonality could also play a role.").

We completed the reference to inversion studies in section 3.3 to support the argument that the mismatch in the high latitudes was related to an underestimation of vegetation uptake "These model-observation mismatches have led top-down studies to identify **vegetation as an underestimated sink in the high latitudes (Ma et al., 2021; Remaud et al., 2022)**, and the tropical oceanic emissions as being the missing source (Berry et al., 2013; Launois et al., 2015; Le Kuai et al. 2015; Ma et al. 2021; Remaud et al., 2022)."

P19, L699-702: But at the same time it is inconsistent with comparisons at AT-NEU, ES-LMA, IT-CRO and US-HA, and the marginal model-observation biases can not explain the too high atmospheric concentrations, so I find this sentence out of place and would remove it.

Answer: Thank you, this sentence was removed.

P19, L709-710: Instead of showing the Launois et al. results in Fig. 10 you could consider to include that of Maignan et al. (2021), which to me seems to be a more fair comparison.

Answer: We clarified the difference between the simulated atmospheric COS concentrations in Figure 10. Maignan et al. (2021) used the soil fluxes from Launois et al. (2015) when transporting the surface fluxes. In Figure 10, the contribution from all components (described in Table 2) other than soils is the same for the simulated concentrations. This clarification was added in the legend figure:

Figure 10. Detrended temporal evolution of simulated and observed COS concentrations at two selected sites, simulated with LMDZ6 transport between 2011 and 2015. The simulated concentrations are obtained by transporting the surface fluxes described in Table 2, and changing only the contribution from soils, with mechanistic (Oxic soils alone, and Oxic + Anoxic soils) and empirical approaches (Berry et al., 2013; Launois et al., 2015). Top: Alert station (ALT, Canada), bottom: Harvard Forest station (HFM, USA). The curves have been detrended beforehand and filtered to remove the synoptic variability (see Sect. 2.3.3).

Discussion:

P20, L717: It would be relevant to compare also with recent global soil COS sink estimates of Kooijmans et al. (2021) and to include those in Table 5.

Answer: Indeed, we added the results from Kooijmans et al. (2021) to the comparison in Table 5 (which became Table 3 after the removal of Table 3 and Table 4). We completed section 4.1. of the discussion "According to the mechanistic approach of this study, the COS budget for oxic soil is a net sink of -126 GgS yr-1 over 2009-2016, which is close to the value of -130 GgS yr-1 found by Kettle et al. (2002) (Table 3). **This net COS uptake by oxic soils is higher than the one found in SiB4 by Kooijmans et al. (2021) with -89 GgS yr⁻¹, also based on the mechanistic model described in Ogée et al. (2016). In SiB4 and in ORCHIDEE, the mechanistic model gives the lowest oxic soil COS net uptake compared to all previous studies using empirical approaches."**

Table 3: Comparison of soil COS budget per year (GgS yr⁻¹). The net total COS budget is computed by adding all sources and sinks of COS (anthropogenic, ocean, biomass burning, soils, vegetation, atmospheric OH oxidation, photolysis in the atmosphere) used to transport COS fluxes (Table 2).

	Kettle et al.	Berry et al.	Launois et al. (2015)			Kooijmans et al. (2021)	This study	
	(2002)	(2013)	OPCHIDEE	IDI	CI M4	SiB4 (modified)	Empirical	Mechanistic
			OKCIIIDEE	LIJ	CLIVI4		soil model	soil model
Period	2002	2002–2005	2006-2009		2000-2020	2009-2016		
Plants	-238	-738	-1335	-1069	-930	-664	-576	
Soil oxic	-130	-355	-510		-89	-214	-126	
Soil anoxic	+26	Neglected		+101		Neglected	Neglected	+96

Soil total	-104	-355	-409			-89	-214	-30
Net total	+64	+1	-566	-300	-161	(-)	-165	+19

A correction of the net total COS budget was made for the estimates of this study as the contribution from atmospheric sinks was previously omitted (OH oxidation that accounts for -100 GqS y^{-1} and COS photolysis in the troposphere representing -30 GqS y^{-1} as explained in section 2.1.3). Therefore, the net total COS budgets using the empirical or the mechanistic approach for soil contribution were corrected to -165 GgS y^{-1} and $+19 \text{ GgS y}^{-1}$, respectively. The net total COS budget computed using the mechanistic model for soils is of the same order of magnitude as the uncertainty on the COS budget components (Table 2). We added in section 4.1 "When computing the net total COS budget considering all sources and sinks of COS (Table 2) with the empirical soil model, we found that neglecting the potential COS production of oxic soils and COS emissions from anoxic soils leads to an overestimation of COS sink or an underestimation of COS source to close the budget (-165 GgS yr^{-1}). On the contrary, the total COS budget computed with the mechanistic soil model is closed given the uncertainties on each component (Table 2). However, despite a closed budget, the mismatch between the observed and simulated latitudinal gradients of atmospheric COS concentration highlights errors in COS flux component distributions (Figure 9)."

P20, L738: Please, specify that this is about the lack of seasonality in the COS soil flux.

Answer: We added this clarification as suggested by the Referee "It is also to be noted that the mechanistic model better simulates the lack of seasonality **in the soil COS flux** at US-HA compared to the empirical model (Figure 2)."

P21, L759-772: The authors here talk about under- or overestimations, but it does not read as if this is compared to actual observations. So I do not think under- or overestimations are the right term here, they are simply higher or lower than other estimates.

Answer: The Referee is right, this is not a comparison with observations but between simulations. We replaced all the comparison terms as suggested in this section.

P22, The authors briefly touch upon the role of nitrogen fertilization in the discussion of section 4.3, but I think the authors could (and should) put more emphasis on the potential role of nitrogen fertilization in this manuscript.

Answer: We agree and we developed the discussion on the role of nitrogen and the importance of including its effect in future developments of the model in this section. "Several studies also found that soil COS production could be related to nitrogen content, which increases with nitrogen fertilizer application (Kaisermann et al., 2018; Meredith et al. 2018, 2019). At the sites where soil is enriched with nitrogen inputs, such as agricultural fields, managed and fertilized grasslands and forests, the fertilization practices would also need to be included when representing the dynamics of soil COS fluxes. However, the soil nitrogen content and soil microbial nitrogen biomass vary not only with fertilization, but also with location. Then, in addition to indications on land use, information on the total soil nitrogen content should be included in the model to consider nitrogen impact on soil COS flux."

P22, L788-789: More recent references such as Kaisermann et al. (2018) would be appropriate here.

Kaisermann, A., Jones, S. P., Wohl, S., Ogée, J. and Wingate, L.: Nitrogen Fertilization Reduces the Capacity of Soils to Take up Atmospheric Carbonyl Sulphide, Soil Syst., 2(4), doi:10.3390/soilsystems2040062, 2018. 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 Discuss. [accepted], https://doi.org/10.5194/bg-2021-192, 2021.

Meredith, L. K., Boye, K., Youngerman, C., Whelan, M., Ogée, J., Sauze, J. and Wingate, L.: Coupled Biological and Abiotic Mechanisms Driving Carbonyl Sulfide Production in Soils, Soil Syst., 2(3), doi:10.3390/soilsystems2030037, 2018.

Meredith, L. K., Ogée, J., Boye, K., Singer, E., Wingate, L., von Sperber, C., Sengupta, A., Whelan, M., Pang, E., Keiluweit, M., Brüggemann, N., Berry, J. A. and Welander, P. V: Soil exchange rates of COS and CO18O differ with the diversity of microbial communities and their carbonic anhydrase enzymes, ISME J., 13(2), 290–300, doi:10.1038/s41396-018-0270-2, 2019.

Answer: These references were added as suggested.