

Feedback from the reviewer is written in italic face, while our responses are written in normal font in green.

Reviewer 1

The article is devoted to the urgent challenges of microbially-driven SOC models. The authors created numeric microbially-driven and depth explicit model of SOC dynamics using R code. They used different scenarios based on isotopic constraints to optimize model parameters, assessed parameter equifinality and checked model sensitivity related to uncertainties of input parameters. The authors revealed that numerical simulations of depth profiles of $\delta^{13}\text{C}$ are prone to uncertainties connected with data availability, wide range of $\delta^{13}\text{C}$ values of C3 vegetation, challenges in estimation of $\delta^{13}\text{C}$ value of root exudates. One more important findings is that despite the including data on the $\delta^{13}\text{C}$ and/or $\Delta^{14}\text{C}$ values of SOC to constrain parameter values during calibration did not substantially reduce equifinality of the most parameters, $\Delta^{14}\text{C}$ data needs to be incorporated to the model calibration for correct simulation of the turnover time of SOC (models without this data substantially overestimated SOC turnover rate). To include additional data during the parameter calibration process is one way forward to improve microbially-driven SOC models. However, they advise avoiding overparametrisation which lead to behavioural models. Defining the optimal structure of soil biogeochemical models and finding a balance between model complexity and available data is an important prerequisite to increase confidence in global projections of the soil carbon - climate feedback. Also, the authors suggests to create and use global databases with data related to SOC cycling to better constrain model parameters.

This article spotlights the biogeochemical modeling challenges and can help to improve simulation of SOC dynamics. But I have several questions concerning modeling methodology and I would appreciate if the authors explain some of the details. I have also added suggestions to improve the quality of the illustrations in the article and in the Supplementary information file. See attached files with comments.

We thank the reviewer for taking the time to read our manuscript and for providing detailed and constructive feedback. Please find our responses to the feedback below.

Specific comments

Title: M.b. "to reduce parameter equifinality" or "to reduce model equifinlity"

We thank the reviewer for this suggestion, we changed the title to "[...] parameter equifinality", so it's clear to the reader that it's this aspect of equifinality the manuscript is about.

Line 97: See the comments and questions in the Supplementary Information file

Thanks for having a detailed look at the supplement, we address this feedback below.

Line 152: As I saw in Supplementary Information user can choose any other year.

This should indeed be the last simulated year, this has been changed in the supplement: “[...] $\delta^{13}\text{C}$ value of atmospheric CO_2 for the last simulation year:”

Line 157-158: Please explain why this is so

As explained in a handbook on radiocarbon in the environment by Schuur et al. (2016, section 3.3.2, p 54; doi.org/10.1007/978-3-319-25643-6), the fractionation against $^{14}\text{CO}_2$ is roughly twice of that against $^{13}\text{CO}_2$, compared to $^{12}\text{CO}_2$, because the mass difference between $^{12}\text{CO}_2$ and $^{14}\text{CO}_2$ is twice than that between $^{12}\text{CO}_2$ and $^{13}\text{CO}_2$ (the atomic mass of $^{12}\text{CO}_2$, $^{13}\text{CO}_2$ and $^{14}\text{CO}_2$ is approximately 44.01 g/mol, 45.01 g/mol and 46.01 g/mol).

This has been clarified in the manuscript: “*It was assumed that during photosynthesis, the fractionation against $^{14}\text{CO}_2$ is twice that of against $^{13}\text{CO}_2$, as the mass difference between $^{14}\text{CO}_2$ and $^{12}\text{CO}_2$ is twice than that between $^{13}\text{CO}_2$ and $^{12}\text{CO}_2$ (Schuur et al., 2016).*”

Line 189: But if you excluded occluded light fraction it is not total OC...

That’s correct. To make this clear to the reader, and avoid having to indicate this every time total SOC is mentioned, we now added the following: “*As SOILcarb does not simulate aggregate dynamics, the total amount of measured OC was reduced by the amount of OC in the occluded light fraction, which constituted 8.4% of total SOC down to 60 cm. Therefore, when referring to total SOC in this manuscript, we refer to the sum of POC and MAOC.*”

Line 209: Do you mean you analysed root exudates?

No, we did not do this. Since we had no information on the $\delta^{13}\text{C}$ value of root exudates, or data from other studies to fall back to, we ran the model with a range of reasonable values of the $\delta^{13}\text{C}$ of root exudates, and choose the value that resulted in the $\delta^{13}\text{C}$ value of SOC closest replicating the measurements. This resulted in the value for the $\delta^{13}\text{C}$ of root exudates used in the simulations of -28.9 ‰.

To clarify this for the reader, we changed these sentences to: “*As measurements of the $\delta^{13}\text{C}$ value of root exudates were not available, a range of reasonable values was tested and the resulting $\delta^{13}\text{C}$ values of SOC and MAOC depth profiles were compared to measured values. The tested $\delta^{13}\text{C}$ of root exudates that resulted in the closest fit of measured and modelled depth profiles of $\delta^{13}\text{C}$ was -28.9 ‰, which was used for all subsequent simulations.*” We hope that this clarifies this strategy for the reader.

Line 210: Please explain in more details. [Resulting in an optimal $\delta^{13}\text{C}$ value for root exudates of -28.9 per mil]

Please see the response to the previous question.

Line 223: Why? [33 % as DOC, 66 % as POC and 1 % as microbial C]

The choice for this distribution was made based on our expectations of reasonable values. As we did not have any data on this, and the focus of the study is on soil OC, our aim was to calibrate the litter compartment of the model to result in reasonable values, which could be used as C inputs to the soil.

To make this more clear for the reader, we changed this to: “*No information on the distribution of the total amount of litter C between the simulated model pools ($C_{\text{POC-l}}$, $C_{\text{DOC-l}}$ and $C_{\text{mic-l}}$) was present. As the focus of the present study is on OC dynamics in the soil, the amount of measured OC in the litter layer was assumed to be distributed as follows: 33 % as DOC, 66 % as POC and 1 % as microbial C. We note that these portions were not based on data, but on our best estimates of a reasonable distribution of OC in the litter layer of a temperate forest.*”

Figure 2: May be black? [(open circles)]

This should indeed be “black circles”, thanks for noticing this.

Figure 2: Please give the error bars in the color of circles to which they are corresponded.

Thanks for this suggestion, this has been changed.

Line 334: behavioural

Thanks for noticing this mistake, this has been corrected.

Line 360-362: For which three parameters did the inclusion of OC, 13C, and 14C data result in a significant increase in constraints? $K_{m,ads}$, $K_{m,DOC-b}$, and what is third one?

Also $K_{deprotect}(0)$. This is indeed not easy to see in Figure 4, but the difference in values, and better constraints, has a large effect on the simulated $\Delta^{14}C$ values (Figure 3). To make this clear to the reader, we now explicitly mention these 3 parameter names in the sentence: *“The most notable observation from these results is that for six out of the nine calibrated model parameters (all except $K_{m,ads}$, $K_{m,DOC-b}$ and $k_{deprotect}(0)$) [...]”*

Line 384: Why did you miss in this section absorption as a mechanism influencing 13C depth profile?

The reason for not including absorption in the sensitivity analysis is that in the model, ^{12}C and ^{13}C are absorbed on minerals at the same rate. As a result, the $\delta^{13}C$ value of mineral-associated OC is determined by the $\delta^{13}C$ value of DOC and microbial residues, which are in their turn influenced by the factors included in the sensitivity analysis (such as the $\delta^{13}C$ value of roots, exudates and aboveground biomass). For this reason, absorption as a process was not included in the sensitivity analysis.

As this may not be clear to the reader, we included the following sentence in section 2.5.2 (which describes the methods of the sensitivity analysis): *“We note that the process of absorption was not included in this sensitivity analysis, as there is no preferential absorption of ^{12}C , ^{13}C or ^{14}C on minerals in the model.”*

Figure 4: Please show all labels in black. And it would be better you enlarge the labels

Thanks for this suggestion, we gave all labels a black color. It would indeed have been better to increase the size of the labels, but in that case the labels on the x-axis overlap. Therefore, we have to keep the original size of the labels.

Line 386-387: It seems like collinearity can exist between this parameter and $\delta^{13}\text{C}$ of leaves. Have you checked correlation between these parameters?

That is correct, the parameter S (representing the effect of the atmospheric CO_2 concentration on the discrimination against ^{13}C during photosynthesis) directly affects the $\delta^{13}\text{C}$ value of leaves, so their values will be correlated (the larger the value of S , the lower the $\delta^{13}\text{C}$ value). As the parameter of S is fixed and the effect is unidirectional (S affects the $\delta^{13}\text{C}$ value of biomass), this should not be a problem for, e.g., equifinality.

As this effect is generally not included in models simulating the $\delta^{13}\text{C}$ value of SOC, we included this separately in the sensitivity analysis (on top of changing the $\delta^{13}\text{C}$ value of leaves and roots), to make the magnitude of this effect clear to the reader.

Figure 5: Please enlarge these figures (labels are illegible).

Thanks for this suggestion, we enlarged the labels.

Line 406-408: As for me this effect is reflected in $\delta^{13}\text{C}$ composition of leaves. So, as I have already mentioned above, this parameter can be collinear.

As mentioned above, both parameters (the simulated $\delta^{13}\text{C}$ value and the value of the parameter S) are probably collinear. The two processes mentioned in these lines are, however, different, and affect the $\delta^{13}\text{C}$ value of vegetation over different timescales:

- The first parameter (changes in the $\delta^{13}\text{C}$ value of vegetation due to temporal changes in the $\delta^{13}\text{C}$ value of atmospheric CO_2 , mainly due to fossil fuel burning) affected the $\delta^{13}\text{C}$ value of vegetation mainly since the 1950s
- The second parameter (changes in the $\delta^{13}\text{C}$ value of vegetation due to differences in the concentration of atmospheric CO_2) affects the $\delta^{13}\text{C}$ of vegetation over 10,000s of years, as the CO_2 concentration of the atmosphere has not been consistently stable over this period.

Therefore, we would like to keep this differentiation in the manuscript.

Line 502-504: What about combination of OC, $\delta^{13}\text{C}$ and $\Delta^{14}\text{C}$?

That was indeed missing here, thanks for pointing this out. We now added: “Adding a combination of $\delta^{13}\text{C}$ and $\Delta^{14}\text{C}$ data improved the simulation of the $\delta^{13}\text{C}$ value in the topsoil, and the rate of sorption and desorption of OC on minerals along the soil profile, and thus the turnover rate of SOC along the soil profile.”

Feedback on supplementary information

Line 44: plant-derived OC adsorbed onto soil minerals? Unclear how

The reason for this simulated flux is to account for the fact that a significant portion of mineral-associated OC has a plant origin (opposed to microbial origin), as shown by recent review articles (Wang et al., 2021 (<https://doi.org/10.1016/j.soilbio.2021.108422>, 2021); Angst et al., 2021 (<https://doi.org/10.1016/j.soilbio.2021.108189>, 2021)). Therefore, the simulated bioavailable C pool (consisting of root exudates and depolymerised POC) can be directly associated with soil minerals.

Line 64: $V_{\text{max_POC_I}}$?

That's correct, thanks for pointing this out.

Line 64: $V_{\text{max_DOC_I}}$?

That's correct, thanks for pointing this out.

Line 106: This is unclear. You have told about transferring of the litter POC pool to the rhizosphere POC pool before the formula, but after that you tell that the litter POC pool is transferred to the soil POC pool.

You are right, “soil POC pool” has been changed to the “rhizosphere POC pool”

Line 174: Is it right? May be $(1-f_{\text{sol}})$?

Yes, it is correctly formulated. The soluble part of microbial necromass (e.g. the cytoplasm) is transferred to the bio-available C pool, as the assumption in the model is

that this C can be taken up readily by microbes. The non-soluble part (e.g. the cell wall) is transferred to the DOC pool, which needs to be depolymerized before being taken up by microbes (although depolymerisation and uptake are simulated as a single-step process in the bulk soil).

Line 175: Is it right? May be fsol?

See the previous response

Line 195: double brackets

Thanks for pointing this out

Line 331-336: It is better to shift this part to previous paragraph (325)

Thanks for this suggestion. We followed this, and made some other small changes to this paragraph.

Line 363-364: Have you checked if the "diff_fixed" values are different for other years? If so, how much do the values change?

The values of *diff_fixed* is the same for every simulation year, it's a measure for the difference in $\delta^{13}\text{C}$ between atmospheric CO_2 and plant biomass. The variable part is added to account for additional fractionation against $^{13}\text{CO}_2$ due to differences in the concentration of CO_2 in the atmosphere for every simulated year.

Line 376: Why have you taken double discrimination?

Please see our response to the same question above.

Line 388: I think that you'd better give the value you choose in this section (not only in the Table S3). And for "diff13C_leaf-exudates" too.

Thanks for this suggestion, we added these values to the text in this section

Figure S5: (7)

Thanks for noticing this, this has been changed.

Figure S9: Please enlarge these figures (labels are illegible).

The size of the labels has been enlarged.

Figure S10: Please label each figure (A, B, C) in the figure caption.

This has been added.

Figure S11: Please label each figure (A, B, C) in the figure caption.

This has been added.

Figure S11: What about $\delta^{13}\text{C}$ of atmospheric CO_2 ?

The temporal variation in the $\delta^{13}\text{C}$ of atmospheric CO_2 is what drives the temporal changes in the $\delta^{13}\text{C}$ of vegetation (the process being simulated). To make this clear to the reader, this has been added to the caption: “[*(ii) temporal changes in the $\delta^{13}\text{C}$ of vegetation (due to temporal variations in the $\delta^{13}\text{C}$ value of atmospheric CO_2)*]”.

Table S6: Can you add references for fixed values (where it is possible)?

Where possible, references for the fixed parameter values are provided in the detailed model description in the supplement. Other fixed parameter values were fixed to realistic values, to not further complicate the model calibration process. To make the reader clear where references can be found, the following sentence was added to the caption: “*Where possible, references to fixed values are provided in the detailed model description above.*”.

Table S6: “?”

This parameter is used to create simulated soil layers which increase in thickness with depth. This is explained in section 1.1, and is used in equation (1).

Table S6: You missed parameter "surf" in this section.

This is not a parameter but is used as a state variable in the model. This should thus be added to table S5 (thanks for noticing this). We did so, and added a note stating that this parameter is calculated by subtracting the actual amount of MAOC from the total potential amount of MAOC.

Table S6: I did not see "m" in this section. And the discription of "m" is the same with "a".

The parameter m is used in equation (43). To make the difference between m and alpha more clear to the reader, their description has been changed. For m this is now "Coefficient to calculate the effective gas diffusivity", and for alpha "Coefficient to calculate gas diffusivity of CO₂ in free air".