



Colorado State University

Department of Soil and Crop Sciences,  
Colorado State University,  
Fort Collins,  
Colorado 80523-1170  
USA

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Cover Letter and Responses to Reviewer Comments to accompany the manuscript:  
**“Unifying soil organic matter formation and persistence frameworks: the MEMS model”**

**Authors:** Andy Robertson, Keith Paustian, Stephen Ogle, Matthew Wallenstein, Emanuele Lugato, and Francesca Cotrufo

Thank you for your correspondence concerning our manuscript and for giving us the opportunity to resubmit a revised version. All comments from the reviewers have been carefully considered and appropriate responses are made below.

Sincerely,

Andy Robertson

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## **Responses to comments from Thomas Wutzler on “Unifying soil organic matter formation and persistence frameworks: the MEMS model” by Andy D. Robertson *et al.***

Reviewer comments in bold and our responses in normal text. Selected new text in the revised manuscript is pasted here in italics. Reference to the manuscript is given as new line number (L).

### General comments

**The study of Robertson *et al.* presents a first version of the MEMS model, a parsimonious dynamical model of soil organic carbon (SOC) development at ecosystem scale, together with a validation across many sites. I enjoyed reading the manuscript, which is well structured and succeeds in getting the fundamental ideas across in a concise way and provides the details in the appendix.**

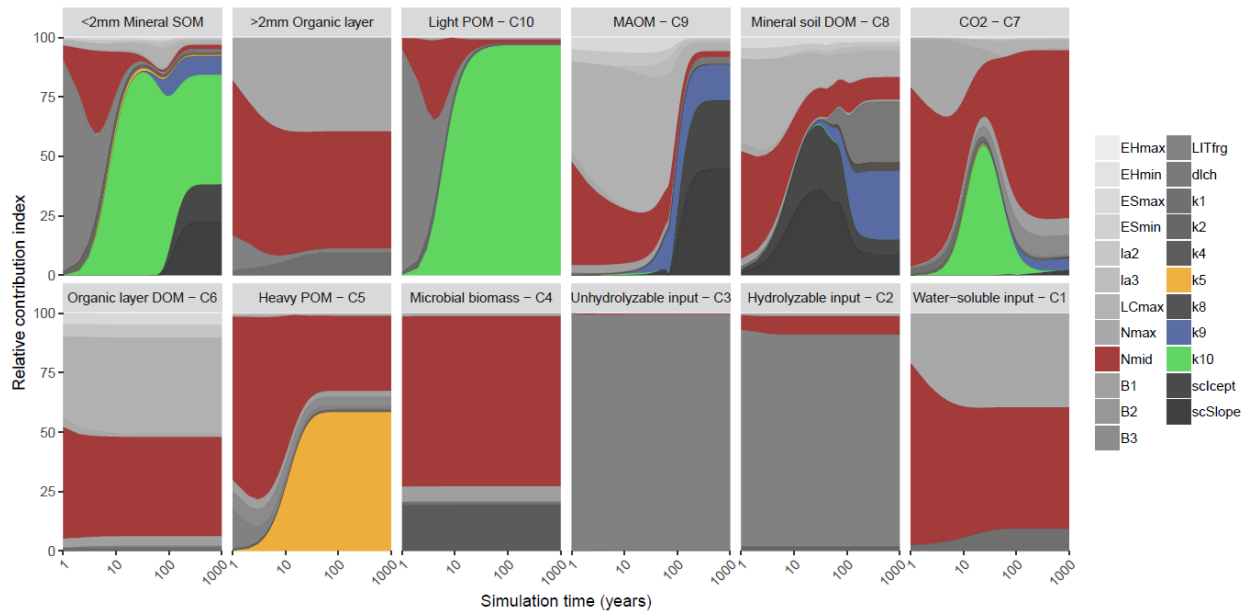
**The proposed model is of similar complexity as classical pool-based models but better incorporates recent mechanistic understanding and is better comparable to measurable pools. Hence, it is of great interest to soil science, ecosystem research, and potentially also global change communities. It adds a complementary alternative in the suite of simple to much more detailed SOC models and the study should be published after revisions.**

Many thanks for your comments and time spent reviewing our manuscript. We appreciate the detail and clarity of your suggested revisions – this certainly helps us to improve our manuscript. We are glad you enjoyed reading it and are excited to have an opportunity to publish the MEMS model. It is our hope that it can do just as you say and add to the suite of SOC models already available and stimulate discussion of how to advance this field.

Through the revisions described in detail below we hope to have addressed all your comments.

**I liked the approach of directly modeling relevant quantities at the scale model purpose, the management scale. I liked the simulation time dependent sensitivity analysis, although Fig. 2 is hard to read.**

I suspect part of the difficulty in reading the figure is because the submission guidelines are to embed the picture as a low-quality jpg. The original vectorized PDF is much clearer. However, we have also now hopefully made the figure easier to read by increasing the size of the text and limiting the colours to only the 4 most influential parameters. All other parameters are coloured in greyscale in order from top to bottom. The ‘full colour’ figure version is included as in a supplementary zipped file attached to these responses (Figure S5 is a lossless vector PDF for detailed inspection if the reader wishes). For your reference we show the new figure below (due to the odd submission process the figure may be repeated in higher quality at the end of this file).



**The supplementary is complicated by already anticipating several mineral soil layers and sometimes is inconsistent with the main text. For example, there is explicit microbial assimilation in mineral layers in the supplementary, but the main text states that microbes are implicit there. Please, provide a version that matches the main text and the presented model structure.**

We apologise for this confusion – the microbial assimilation, as a process, is indeed ‘explicit’ in that it is represented by fluxes into a microbial pool. However, in this inaugural version of the model the use of a microbial pool is more one to help differentiate the direct *versus* microbially-processed flux of organic matter inputs (pools C1-C3) to the soil C pools, *sensu* Liang *et al.*, 2017. Once these inputs are added to the soil pools belowground, then the microbial biomass and associated metabolic processes are implicit (i.e., we assume there is microbial activity and mineralization of the carbon within these soil pools, but we do not represent these processes with discrete pools or fluxes). We certainly appreciate the comment because on review this is an important point that needed to be made clearer. At different points in the main manuscript, we have added additional points as to why we have a distinct microbial pool at the point of entry of the C input, but not after it is processed and transformed into the SOC pools, which have microbes within them.

A large part of the confusion likely resulted from the ‘microbial assimilation from litter’ section of the supplementary and we can indeed understand why. The use of the layer superscript certainly made our descriptions less clear. Consequently, we have also removed the superscript notations for soil layers that created unnecessary confusion in the supplementary model description. There should now be no inconsistency between the main text and the supplementary materials.

Liang, C., *et al.* (2017). "The importance of anabolism in microbial control over soil carbon storage." *Nature Microbiology* 2: 17105.

L197-217:

*Many of the biogeochemical processes represented by MEMS v1.0 are assumed to be microbially mediated (and therefore result in exo-enzyme breakdown and CO<sub>2</sub> production), but only two lead to C assimilation into a distinct microbial biomass pool – from the water-soluble and acid-soluble litter pools (C1 and C2, respectively). In the mineral soil (i.e., pools C5, C8, C9 and C10), microbial anabolism and catabolism are implicit and considered part of the turnover of each pool. This ensures parsimony and allows model parameters to represent the differences in microbial community for each pool, as opposed to the alternative of explicit microbial pools. The C transferred from the C1 and C2 litter pools into microbial biomass is defined by a dynamic CUE parameter controlled by the N content of the input material and the lignocellulose index (LCI; defined as the ratio between acid-insoluble to the sum of acid-soluble + acid-insoluble) of the litter layer (i.e., lower CUE results when a higher proportion of the litter is acid-*

*insoluble). Including microbially-explicit processes in the litter layer helps to determine the proportion of C inputs that result in MAOM vs POM formation (see Liang et al., 2017) and allows for future model versions to account for distinctions between different points of entry for inputs (Sokol et al., 2018). The lack of C transferred from other pools (e.g., C3) into microbial biomass implies their decay from co-metabolism with the more labile C sources (i.e., Klotzbucher et al., 2011; Moorhead et al., 2013). Once assimilated within microbial biomass, the anabolism of microbial activity results in generation of microbial products (i.e., necromass) that form tightly bound aggregates of biofilms and small litter fragments around sand-sized soil particles (Huang et al., 2006; Buks and Kaupenjohann, 2016), and dissolved organic matter (DOM). These contribute to the heavy POM (C5) and litter DOM (C6) pools, respectively. While these specific processes are well supported by relevant literature, to retain parsimony and the generalizable structure required by an ecosystem scale model MEMS v1.0 represents microbial metabolism processes more generally (i.e., by linking them to a dynamic microbial CUE rather than specific community traits).*

**The wording of “litter layer” and “mineral soil” are used in a fuzzy way. Also it did not become clear to me, how model-data comparison dealt with organic layers, which are neither part of the litter (in the model lacking particulate organic matter (POM) pools) nor the mineral soil (in the model simulating sorption to minerals). Maybe this partly causes the large model-data discrepancies for broadleaved sites with large POM stocks.**

Thank you for raising this. Our categorization of the aboveground and belowground pools as litter layer and mineral soil, respectively, appear to have led to some confusion. We have changed the terminology throughout the manuscript to make clear that all belowground pools (all POM, pools C5 and C10; MAOM, pool C9 and soil DOC, pool C8) are operationally defined as < 2mm in size and sum to what we refer to as *total soil* (i.e., **not** that ‘mineral soil’ only refers to MAOM and that we are using the terms to differentiate between mineral and organic soil layers).

It is our intention that the sum of the C1/2/3 pools equal all the carbon inputs as above and below ground litter. However, we do not have any ‘litter layer’ measurements to provide us model-data comparisons. In fact, both above- and below-ground litter was removed during the LUCAS soil sampling and post-processing. We agree with you that the current model does not have the ability to simulate a specific organic horizon, and this is why we removed all organic soils (> 12% OC) from our analysis. Initially, simulating organic soil layers was not our initial priority but now after seeing the current model’s results it has become a priority for our next steps in development. As a result, we are working to fractionate several soils with high OC content, so we can help parameterize a new model version that has a finer resolution of soil layers to depth. We are also adding an explicit hydrological submodel that will help to improve the model’s capability to vary decomposition processes in different environmental conditions. Both should help reduce some of the large model-data discrepancies from this first version.

It is our belief that the model structure should not need to change to better represent an organic horizon (which will be dominated by litter and POM pools), but rather parameter values may differ to help represent how decomposer communities differ with depth/access to fresh inputs. Additionally, we are aware that if future model versions are to represent an organic horizon we would need to implement a mechanism that reduces sorption to mineral surfaces accordingly to account for large POM accrual (for example in anaerobic conditions). This will be a key feature when we look to test the model in peaty soils where the ‘mineral layer’ is moved further from the surface while POM (and associated organic layer) accumulates.

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#### Detailed comments for model structure:

**Could you, please, elaborate a bit more why you (as well as the LIDEL model) choose microbes to not consume DOM?**

This fundamentally comes down to the way we are ‘feeding’ the microbial pool (in both models). Our assumption is that the microbes consume fresh inputs from the water- and acid- soluble, coarse organic matter (pools C1/C2) and the aboveground DOM (pool C6) that exists is, in fact, what is left over and

available to move to the soil. We decided to use this formulation to enable the C6 pool to be measurable as, for example, using the approach described in Soong *et al.*, 2015. Belowground, microbes are assumed to be consuming soil DOM (pool C8) but those processes are implicit to the mineralization equations of those pools, and not related to the microbial assimilation pathways aboveground.

To help clarify this in the manuscript we have revised our descriptions and justification of why we have a microbial pool in MEMS – the primary purpose (at least in this initial model version) is to clearly differentiate between an “ex-vivo” more physical path to SOM formation and an in-vivo microbial processing one (*sensu* Cotrufo *et al.*, 2015 and Liang *et al.*, 2017). This formulation will be very helpful when trying to match real-world observations of the stoichiometry of different fractions with their corresponding pools in the model.

Cotrufo, M. F., *et al.* (2015). "Soil organic matter formation from biochemical and physical pathways of litter mass loss." *Nature Geosciences*.

Liang, C., *et al.* (2017). "The importance of anabolism in microbial control over soil carbon storage." *Nature Microbiology* **2**: 17105.

*See quoted text shown above lines around 201 in the main manuscript and L163-174 in the supplementary:*

Where  ${}_jC x_{in}^{Cy}$  refers to DOM leaching from pool y to pool x on day j. The parameters used are detailed in Table 2 in the main manuscript, and/or defined in previous equation in this section. Note that pool C6 is not the DOM consumed by microbial biomass but rather the amount leftover after microbial activity. In this initial model version, the litter layer only refers to the aboveground component, but the same structure can equally apply to belowground C inputs such as root death. However, measurably, the DOM in the C6 pool is directly equivalent to the belowground soil DOM (C8). In MEMS v1.0, DOM enters the soil through the C6 pool only. When explicit inputs from belowground litter (e.g., roots) are simulated in future versions Eqs. **Error! Reference source not found.-Error! Reference source not found.** can apply for each soil layer adding the DOM that is in excess of microbial activity directly to pool C8 instead of the ‘C6’ shown in the equations above.

**In the LIDEL model there is a C5 microbial products pool also in the litter layer, why do you assume in MEMS that all microbial turnover is transferred to the mineral soil?**

The LIDEL model doesn’t represent soil, thus there was the need for a microbial product pool in it. The main reason why the C5 pool in MEMS v1 is a SOC pool is because there is little added value (or sense) and the downside of increased complexity if we were to include a specific microbial products pool in soil – heavy SOC pools are made mostly of microbial products. Furthermore, microbial turnover in SOC pools is implicit and thus the microbial products generated by these processes is captured only by the mineralization of each of these pools.

**You choose decomposition to be independent of the size of biomass pool to avoid some problematic feedback. Then I suggest to simplify the model even more by replacing microbial biomass turnover by the sum of inputs to the biomass pool. Then you do not need to simulate this pool, save one state variable and several model parameters. If microbial biomass is required for data comparison, you can still compute it assuming near steady state with inputs (e.g. Wutzler 2013).**

We discussed at length the possibilities of removing the microbial biomass pool and came to the conclusion that it is required to help us differentiate SOM formation pathways (as mentioned above) and in future versions the “point of entry” *sensu* Sokol *et al.* 2018. We acknowledge that your suggestion would likely work for this simple first version of the MEMS model, but in the next stages of model development the fresh organic matter inputs will come from above- and below-ground sources and we will need to be able to differentiate between different rhizosphere inputs, different root types and the aboveground litter. From this, it is our intention to be able to vary parameter values associated with the microbial pool of each point of entry (e.g., aboveground, topsoil, subsoil) so as to represent variability in microbial traits. We also require an explicit microbial pool for the next stages in model development regarding N-immobilization. Since our submission of the manuscript, the Sokol *et al.*, 2018 paper was published and discusses some of

the details around our assumptions regarding the split between plant- and microbe-derived SOM, and the importance of getting this right.

Sokol, N. W., Sanderman, J., & Bradford, M. A. (2018). Pathways of mineral-associated soil organic matter formation: Integrating the role of plant carbon source, chemistry, and point of entry. *Global change biology*.

#### Detailed comments for model-data integration:

**It should be clarified better also in the discussion, that the model performance was judged by comparing steady state MAOM pools to observations. I am still looking forward to a comparison where a model successfully simulated dynamics compared to observed changes decadal stock changes across many sites.**

We agree – we’re excited to test the model’s ability to replicate ‘short-term’ changes in soil organic matter dynamics. We have now made it clear that model-data comparisons are against steady-state systems.

**L376: averaging parameters is dangerous, because of nonlinearities. I suggest to use only one non-averaged parameter combination. You may pick the fold randomly.**

We have made this change and chosen parameter values from a single fold (values were only very slightly different from the averages – see Table S2).

*L417-425*

*To determine the optimized parameter values, a single fold was chosen at random from those that reported the lowest RMSE for each subset of training sites (i.e., each fold). Optimized values differ depending on which measured fraction is compared to model predictions (whether comparing pool C9 to measured MAOM-C, the sum of pools C5 and C10 to measured total POM-C, or the sum of pools C5, C8, C9 and C10 to measured bulk SOC). The new, optimized parameter values (Table S2) were derived from a randomly chosen fold that minimized RMSE when compared to the MAOM fraction.*

**L376: You can avoid the choice of one criterion among three data streams of MAOM-C, POM-C and bulk SOC by using a cost function based on the sum of squared residuals of all the data streams.**

This is a good point. Thanks for the suggestion which we will apply for the next stage of calibration. For this initial parameter estimation, we performed the full optimization procedure on all data streams. While parameter values did vary, the results and general fit was similar regardless of which criterion we chose. Consequently, we do not feel that this change would make considerable difference to the results we are presenting and hope you will agree it would not be worth redoing the entire analysis for this change. An additional factor to consider is that our ongoing development of the MEMS model is already revising some of the parameters (many are being adjusted to accommodate nitrogen effects on carbon transfers) and therefore the values themselves may have little application beyond this initial version.

We do agree with your suggestion though and have added this to the discussion.

*L422-428*

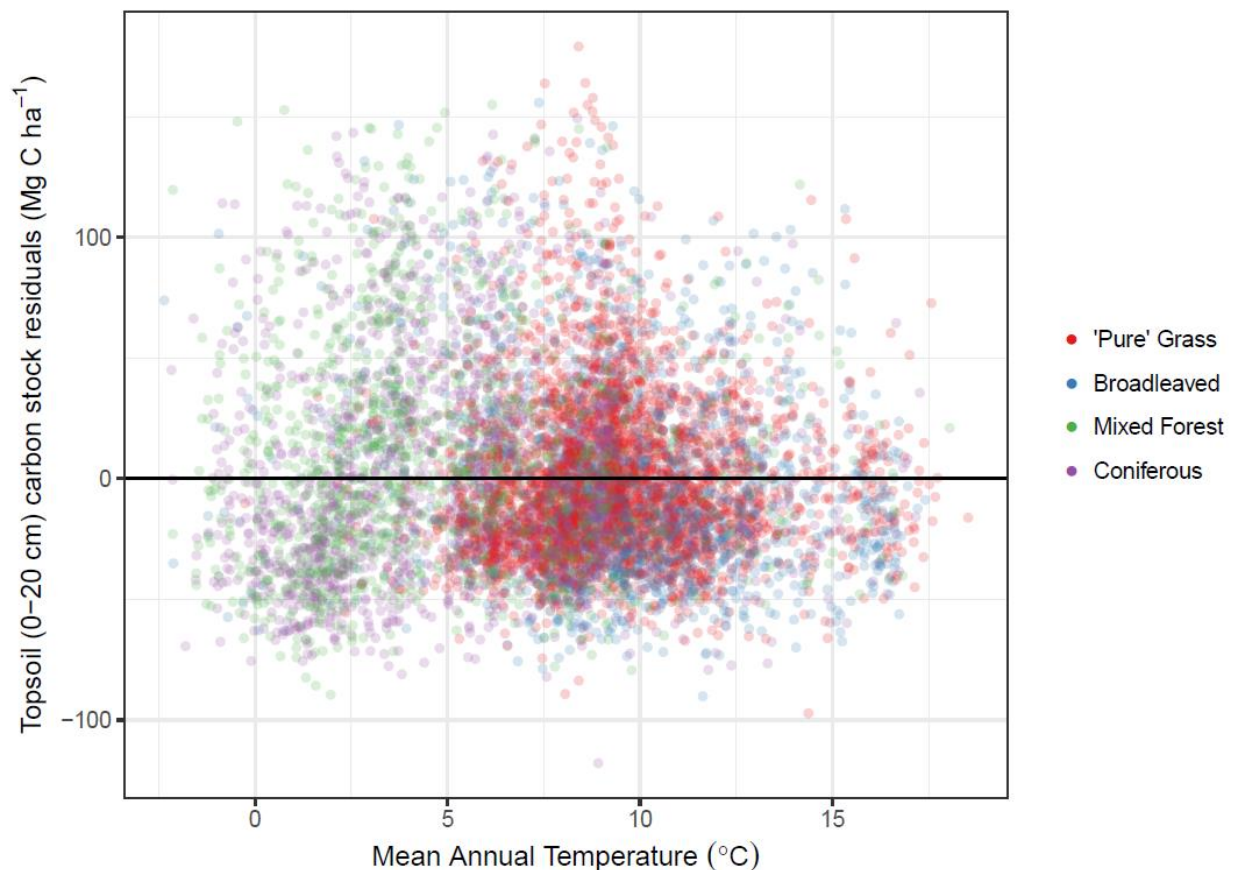
*The new, optimized parameter values (Table S2) were derived from a randomly chosen fold that minimized RMSE when compared to the MAOM fraction. This was chosen (instead of those optimized for POM or bulk SOC) since the MAOM fraction is typically the largest single soil C pool and using this approach led to the biggest overall decrease in RMSE when compared to all available data (Table S2). In future analyses, a more rigorous approach may be to apply a cost function regarding all available measured pool data (e.g., including litter pool data when it is also measured) but for our initial model evaluation we random choice is deemed sufficient*

**Fig 5: The classification to land use not particularly helpful, because variables are very similar with a high range across these classes, including the mentioned significant different of MAOM:POM (L 485). Furthermore, plotting the distribution of observations and distribution of predictions separately does not help to judge model performance (L488).**

**I suggest instead inspecting and plotting the distribution of model-data residuals of several variables and relating these differences to classes and other environmental conditions. This would indicate which variables and processes are most urgent to extend MEMS v1, as done with the discussing Fig 7.**

We understand your point and have in fact plotted these all residuals against the full range of environmental conditions. Unfortunately, these tend to make the results seem worse than they are because the dense number of points near the 0-residual line cannot be shown well. However, to address your concern we have added a residual plot to the supplementary to illustrate individual residual points (new Figure S6 – see attached in the associated zipped supplementary file). This figure does make an important point, but it is hard to determine clear recommendations of where to focus next developments purely from these figures.

Below we attach an overall summary of individual residuals against mean annual temperature of the sites and in the supplementary we show a similar figure but split by different environmental divisions (new Figure S6).



Other detailed comments main text:

**Text in Figs 2 and 6 are hard to read. Can you provide a vector graphics of this figure? There are too many classes to distinguish by color, but I have no suggestion how to improve.**

We did provide vector graphics versions with the manuscript but unfortunately as part of the peer review process they do not include them and instead choose to embed them in the file. We have tried to address

this as described above. The full colour version of figure 2 (new Figure S5) is in the supplementary zipped file and we have replaced the main text figure with a one that is easier to interpret, as described above. We have also increased the font size and changed the resolution slightly of figure 6 to make it clearer. This is also obviously much clearer when viewed on the vectorized file (also attached separately – see Figure 6 in the zipped supplementary file with these responses).

**Fig 4: Suddenly, pH is popping up, but was never introduced as a driving variable. I suggest to shortly state that sorption rate is pH dependent, and refer to the eq. 35 in the Appendix.**

We have now made this change.

See L266:

*This parameter can be very difficult to generalise without requiring exhaustive information on soil physiochemical conditions (e.g., clay type, Fe/Al concentration, etc.), but the work of Mayes et al. (2012) presented an empirical relationship between  $K_{lm}$  and native soil pH, with pH acting as a proxy for mineralogical conditions. As a result, sorption rates to mineral surfaces are dependent on pH (see Equation 35 in supplementary). This relationship (derived from isotherms calculated for 138 soils of varying taxonomies) provides a good starting point for estimating  $K_{lm}$  and is also used by the MILLENNIAL model (Abramoff et al., 2017).*

**L 529: These are interesting effect of N in a C-only based model. While the microbially detailed models of Perveen 2014 and Wutzler 2017 attribute low litter N effects to N mining in older usually N-rich pool and accumulation of less processed material, MEMS attributes this to reduced microbial accessibility and reduced DOM production. Do you think that chemical and stoichiometric effects are two sides of the same coin, or are these competing hypotheses? I am looking forward to the version that explicitly simulates N fluxes.**

Thanks, we are excited to be working on simulating N fluxes, which indeed are complex depending on the microbial N demand (stoichiometry), as well as on the energetic (chemistry) and accessibility (physics) of soil organic C pools. Rather than competing, in our opinion these are all simultaneously at play. We follow the LIDEL model (Campbell *et al.*, 2016), according to which both N limitation and C chemistry (i.e., Lignocellulose index) drive microbial decomposition and DOM production, with the most limiting factor being the actual driver of the process. We find the recent model of N input effects on SOC dynamics proposed by Averill and Waring (2018) to be particularly effective at capturing this complexity and may follow their logic in our new model version which will include N.

Averill, C. and B. Waring (2018). "Nitrogen limitation of decomposition and decay: How can it occur?" *Global Change Biology* **24**(4): 1417-1427.

Campbell, E. E., *et al.* (2016). "Tracking the fate of litter carbon using the Litter DEcomposition and Leaching (LIDEL) model." *Soil Biology and Biochemistry* **100**: 160-174

Other detailed comments appendix:

**To me its difficult to always keep a list of meaning of pool 1 to 10 in my head. Could you come up with more expressive pool names?**

We are aware of this issue. The initial development of this first MEMS v1 model was intended to be an advancement from the LIDEL model and therefore we kept the same names to ease reference to that model. However, we now know that this approach won't be effective as the model grows. For our MEMS v2.0 we are making this change.



**L 70: I do not find more information on  $u_B$  and  $u_K$  in Table 2 in the main text. I suggest referring to eqs. 19-22.**

Apologies for this omission. We have made this change.

L80

*More information of the parameters  $u_B$ ,  $u_K$ ,  $B_x$ ,  $la_x$  and  $k_x$  can be found in Campbell et al. (2016) and in the equations below, but briefly:*

*$\mu_B$  and  $\mu_K$  are rate modifiers to represent the litter chemistry controls (LCI and available nitrogen) on microbial use efficiency, on day  $j$*

**L 110-112: The long sentence did not become clear to me. Is  $L_{j\_C5\_C4\_gen}$  really a combined flux of bioturbation, . . . , and DOC leaching? I thought the latter one is covered by eq. 33.**

You are right that this was confusing. The C4 to C5 flux was inherited from the LIDEL model to represent microbial turnover and you are right in saying that DOC generation from this process is represented elsewhere. We have adjusted the text accordingly and hopefully it is now clearer.

L120

*Where  $\mu_{C5_{gen}^{C4}}$  refers to the fraction of carbon that is transferred from C4 to C5 (i.e., microbial products transported belowground when physical and hydrological processes mix between the input layer [aboveground litter only in MEMS v1.0] and soil layer) on day  $j$ .*

**eq 47:  $k_8$  does not match the text before that states  $k_5$ .**

We have made this change.

L256

*While the maximum decay rates ( $k_x$ ) for most pools are fixed constants, Campbell et al. (2016) suggested that  $k_3$  is best estimated in relation to the maximum decay rate of the microbially-accessible litter (C2) pool ( $k_2$ ).*

**Thanks for this work. I suspect MEMS to be included in further model comparisons as a complementary model.**

Thank you for your insightful review. We hope the MEMS model can help to stimulate a discussion that advances SOM modelling in the coming years. It is our intention to participate in model comparisons with MEMS v2.0.