Final response to reviewer's comments on "Dynamic upscaling of decomposition kinetics for carbon cycling models"

We would like to thank the three reviewers for their comments. In this brief summary, we highlight the comments that in our view are most important to address should a revision of our manuscript be encouraged. In general, the reviewers commented favourably regarding the potential interest of the proposed work, but raised concerns about its applicability. We agree with this general concern and had already openly acknowledged the limitations of our approach in the original manuscript. However, we also think that a theoretical approach to link different scales in soil carbon cycling models is missing and this contribution provides a way to start bridging this gap that complements ongoing efforts by other groups.

Reviewer 1: the main concerns regard the interpretation of results (oscillations, convergence to equilibrium, sensitivity to changes in parameter values), and the establishment of a closed-form solution that can be applicable in biogeochemical models. In our response, we provide additional analyses and explanations of the results that can be included in an extended Discussion in the revised manuscript. In particular, we extended our analysis to a fourth type of decomposition kinetics used in soil C cycling models (inverse Michaelis-Menten).

Reviewer 2: the main concerns regard the validation of the proposed approach, its high level of abstraction, and the lack of representation of some physical processes known to determine heterogeneous distributions of soil substrates and microorganisms. In our response, we argue in favour of a theoretical framework, while acknowledging its limitation. A 'standard' model calibration/validation is not possible due to lack of fine-scale data, but the theoretical insights provided by our approach can still be useful. It is correct that some physical processes had not been represented, but our goal is to establish a link between macro- and micro-scale dynamics starting from an idealized system. In a revised manuscript, we would further highlight approach limitations; moreover, also in response to reviewer 3, we can include a simple representation of mass transfer as a proxy for physical transport processes that we had initially neglected.

Reviewer 3: the main concerns regard the applicability of the approach, the assumption of negligible cell-to-cell connectivity, and our interpretation of averaging and mean-field approximations. As explained in the responses above, our approach is still admittedly far from being readily applicable and we acknowledge this limitation in the manuscript. We can, however, improve the model by including mass transfer, thus addressing the second concern (new results are presented in the detailed response). Finally, we clarify our interpretations of the terms 'mean field approximation' and 'well-mixed' conditions, which might have created some ambiguities.

Detailed responses are attached below.

Response to reviewer 1 (Thomas Wutzler):

We would like to thank Thomas Wutzler for an encouraging and detailed review of our manuscript. In the following, we address the points raised by Dr. Wutzler (denoted by italic font). Our responses are highlighted in blue font.

General comments

1. *Methodology description: the way of providing spatial moments to analytic equations did not become clear to me (P17L11). I assume, you computed the quantities for sufficiently close time points from the distributed model, and provided a smoothing function depending on time as input to the solver for the analytic equation system.*

There are two ways to illustrate how heterogeneities affect soil organic matter kinetics. One is to solve directly the upscaled equations (assuming the second order terms are known); the other is to numerically solve the micro-scale equations and aggregate (=average) results at the macro-scale. In the first approach, solving the upscaled differential equation would require transferring information on the second order moments (either via closure equations or using moments calculated by the distributed model) to the upscaled differential equation – this issue of 'model closure' is presented in the Discussion. Here we followed the second approach and instead of solving the upscaled differential equations (Eq. (9) and (10), P8L15), we used the averaged dynamics as simulated from the distributed model (explained in the manuscript in P13L4 and P30L22). The average dynamics are then compared to those obtained under homogeneous conditions.

This choice might seem to counter the purpose of this work – i.e., propose an analytical approach to the upscaling problem. However, the lack of model closure (admittedly the main limitation of our approach, as acknowledged in the Discussion) does not allow a full solution of the upscaled analytical model. Thus we used numerical solutions to illustrate the effect of heterogeneities, and the analytical equations to provide a theoretical framework for studying the problem.

It should be pointed out that the numerical averaging approach yields exactly the same solution of the upscaled analytical equations. We tested this for the case of biophysical heterogeneity with multiplicative kinetics because the upscaled equation are exact and only the covariance of substrate and biomass is needed as additional information (the second order moments only involve the covariance). As expected, results were exactly the same from the upscaled differential equation and the distributed model.

In a revised manuscript, we would further emphasize this rationale.

2. *An overview of the approach would be helpful: 1) Express each equation of state variable change of each individual location based on the spatial mean of the pool sizes and the deviations from it at local scale. And 2) Apply a spatial averaging over the obtained equations, resulting in an equation composed of terms of the mean pool sizes and the spatial covariance of the pools and heterogeneously distributed parameters.*

   This is indeed our approach. We start with a micro-scale model i.e. Eq. (2) and (3) and apply spatial averaging to obtain the upscaled (or macro-scale) equation i.e. Eq. (9) and (10). However, instead of writing the averaged rates ($\bar{D}$) explicitly in Eq. (9) and (10), we derive $\bar{D}$ for different micro-scale kinetics. The upscaled expression of $\bar{D}$ are shown in Table 2 of manuscript. We will provide a better roadmap as suggested at the beginning of the theory section.

3. *I tried to check the math, but did not always come to the same results (see detailed comments, eq. A7)*

   There was a typing mistake. The incorrect term in Eq. A7 should read $-\frac{2\,k_{s,mm}K_M\,\bar{C}_B}{(K_M+\bar{C}s)^3}$. Numerical code and results are correct.

In the discussion I would like to read about several points:

4. *Slowdown of decomposition: To my opinion the slowdown of decomposition despite plenty of available substrate (Fig 7d) is a very important feature/insight of the model. A very simple model (albeit still required input of time series of heterogeneity variances) can explain why we can find very old potentially quickly decomposable SOM. The reasons should be explained in more detail (right skewed distribution of decomposition rate, low probability of co-occurrence of high substrate concentration, …)*

   A paragraph at the end of section 4.1 Predicted effects of spatial heterogeneity on decomposition will be added to address this comment:

   "Our analysis suggests that the persistence of SOM in heterogeneous systems is a consequence of the micro-scale heterogeneity in soil carbon cycling. In the transient simulations with biophysical heterogeneity, persistence is a result of spatial disconnection between substrate and microorganism, captured in our framework by a low probability of co-location at the beginning of the simulation. In the transient simulations for the fully heterogeneous systems, persistence is a result of the combined effects of low probability of co-location and high probability of low decomposition rate constant at the beginning of the simulation. The heterogeneity in substrate quality explains the higher persistence of SOM in the fully heterogeneous system compared to the biophysically heterogeneous system."

5. *Oscillations at multi-annual time scale: Observations of such a phenomenon are very rare. I once argued that we do not see such modelled oscillations with microbial explicit models because of superposition of dynamics across many pores. Here, such spatial heterogeneity is the cause of fluctuations.*

   In short, yes, we find that heterogeneous initial placement of substrates can trigger fluctuations around the steady state, and in the case of chemical heterogeneity can actually alter the steady state. Any perturbation from the steady state would lead to fluctuations, and not only a re-arrangement of substrates and microbes in space. When decomposition rate is a nonlinear function of substrate concentration in simple C cycling models like the one used here oscillations tend to appear in a wide region of the parameter space (Manzoni and Porporato, 2007; Sierra and Mueller, 2015). We elaborate on this in our reply to comment 8 below.

6. *Development of the heterogeneity / damping of oscillations (Fig 4): The systems develops to a steady state without any more oscillations. Is the initial heterogeneity developing in direction of homogeneity? Probably not because the simulated SOM stocks differ from the homogeneous system. What is the spatial distribution and covariance between substrate, biomass, and quality after 60 years? Is there a covariance pattern that is stable? I suggest putting another two panels to Fig. 2 showing microbial and substrate distribution at year 60.*

   Yes, in the case of biophysical heterogeneity, the covariance and the sum of the higher order terms are stable in the long term, after the steady state has been reached. Also in the case of full heterogeneity these moments stabilize, but now the steady state is different. We ran the simulation for 100 years and a figure similar to our original Figure 4 is shown below, which confirm that higher order terms are indeed stable.

Because C input is homogeneously distributed, the microbial and substrate concentration spatial distributions are also homogeneous at steady state. However, these compartments attained a different concentration value at steady state compared to the homogeneous system (shown in Figure 4). Adding panels showing a spatially homogeneous distribution might not add much information, but we can better explain this pattern in a revised manuscript.

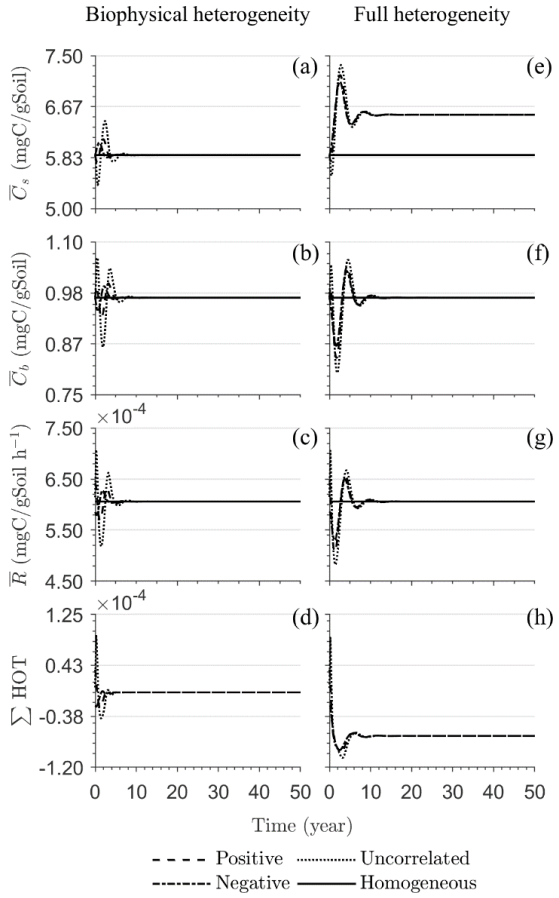

Figure R1: Substrate and microbial biomass C (top rows), respiration and higher order terms (bottom rows) as a function of time, for different scenarios of initial spatial heterogeneity. This figure is the same as Figure 4 in the manuscript but for 100 years of simulation period, aiming to highlight the long-term behaviors of C pools and fluxes.

7. *Role of disturbances: What happens if you simulate a disturbance (homogenization) after the system is near steady state? Does this start the oscillating pattern again?*

Homogenizing the system when it reaches the steady state will not change the spatial distribution of substrates and microbes because with spatially homogeneous inputs at steady state they are homogeneously distributed. Thus, oscillations would not start again after the system has reached a steady state, regardless of whether the system has only biophysical heterogeneities or is fully heterogeneous.

8. *Magnitude of the heterogeneity effects: In Figure 4, the effects look large, because the axis ranges from 5 to 7, but aside from the initial disturbance, the effect is only about 1/10 of the steady state. Are there reasonable parameter combinations where the effect is larger? Or do we not need to are this much about heterogeneity at steady state?*

   To answer, we ran two scenarios in which we changed the kinetic constant parameter $k_{s,mult}$: 1) decreasing $k_{s,mult}$ in the biophysical heterogeneity (Figure R2 and Figure R3) and 2) increasing the heterogeneity of $k_{s,mult}$ (by increasing its standard deviation) in the full heterogeneity case (Figure R4). From Fig. R3 and R4, it is clear that decreasing the rate constant increases the amplitude and wavelength of the oscillations. As shown in Figure R4, increasing the heterogeneity of the rate constant (right column) increases the amount of undecomposed substrate C compared to a lower degree of heterogeneity (middle column). This pattern can be explained using the analytical expression of the steady state substrate C (see Eq. (A13) in Appendix A2, P36L5). For the increased heterogeneity case shown in the right column, we used values of $a = -10.1$ and $b = -8.56$, where a and b have the same meaning as in Eq. (A13). The analytical expression for the steady state, evaluated with these values of a and b, results in exactly the same steady state of substrate C as simulated by the distributed model (i.e. 15 $\mathrm{mgC/gSoil}$).

   These fluctuations are similar to those noted in earlier papers using spatially lumped models (Manzoni and Porporato, 2007; Sierra and Mueller, 2015). These papers showed that the occurrence and amplitude of the fluctuations depends on the kinetic parameter values, as is the case here.

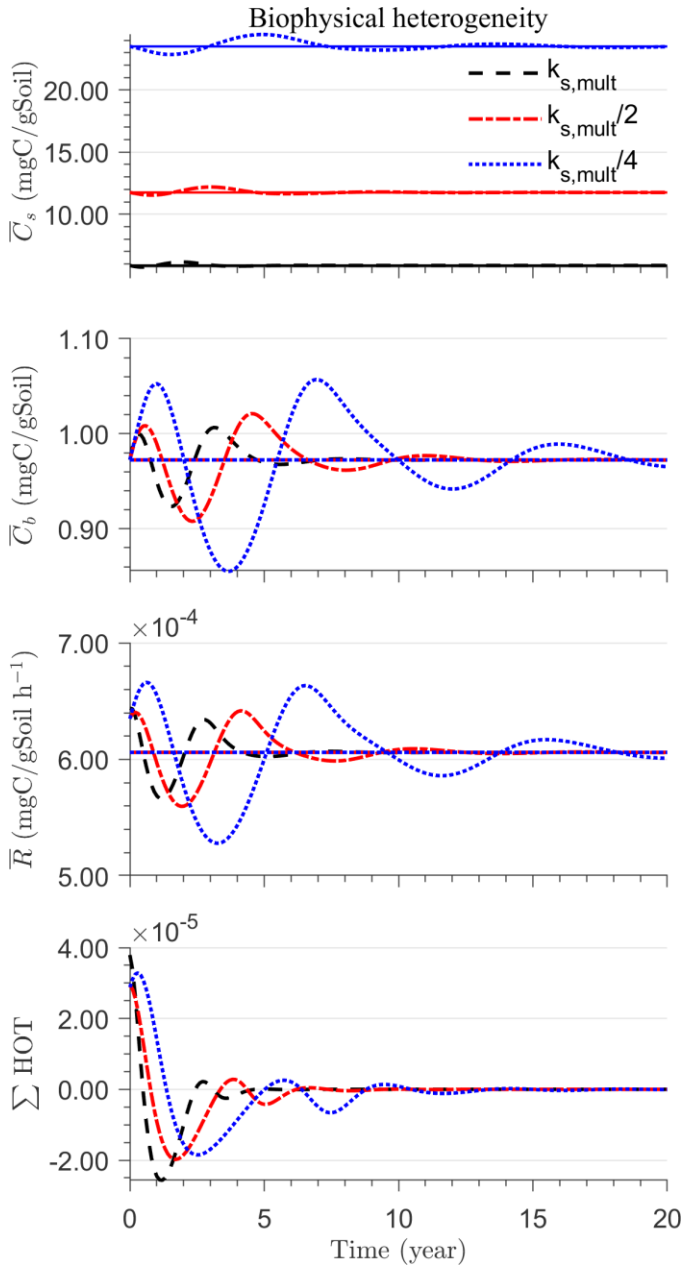

Figure R2: (a) mean substrate C ($\overline{C}_S$), (b) mean microbial C ($\overline{C}_B$), (c) mean respiration rate ($\overline{R}$), and (d) sum of second and third order terms (∑HOT) are shown as a function of time, for different scenarios of initial spatial heterogeneity. This figure is similar to Figure 4 left column in the manuscript (initial substrate is distributed randomly around the steady state). Different line colors represent varying levels of rate constant $k_{s,mult}$ with base case same as in Figure 4 of manuscript.

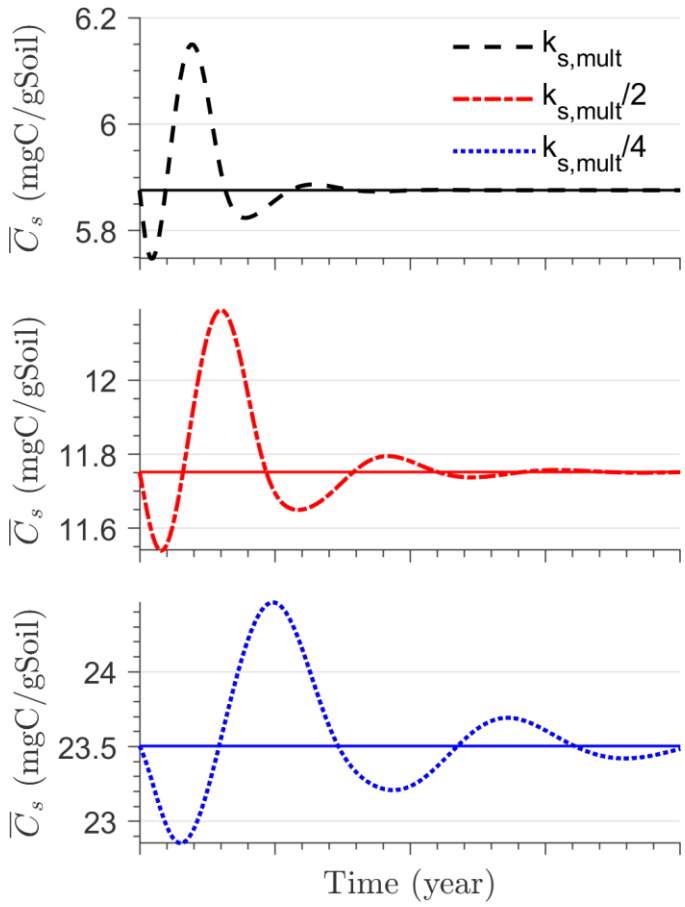

Figure R3: Enlarged view of the time trajectories of the mean substrate C concentration extracted from figure R2.

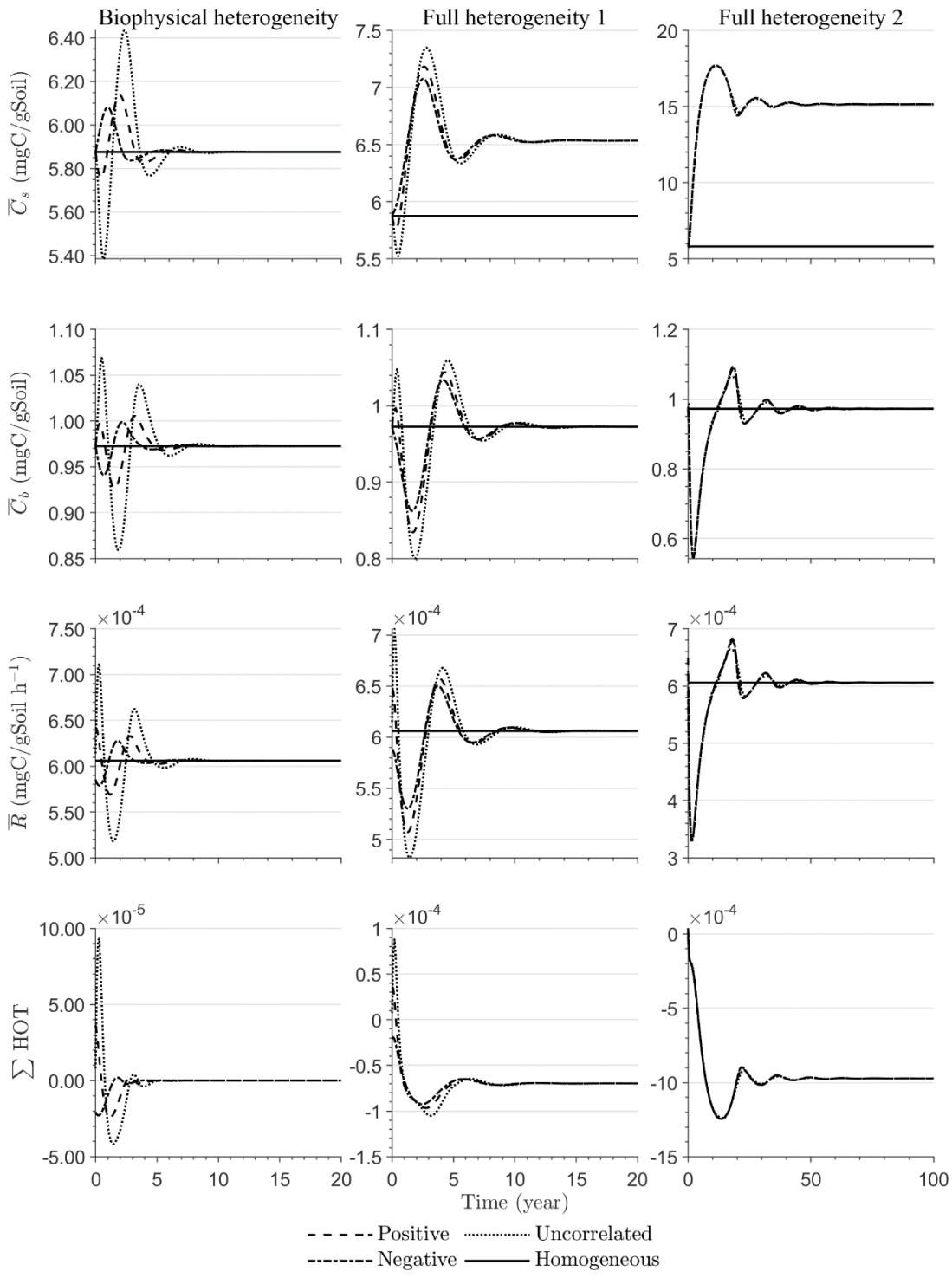

Figure R4: Substrate and microbial biomass C (top rows), respiration and higher order terms (bottom rows) as a function of time, for different scenarios of initial spatial heterogeneity. This figure is similar to Figure 4 in the manuscript, except for the right column, where we added trajectories for the full heterogeneity case, with increased heterogeneity of the rate constant ($k_{s,mult}$).

9. *2D system: Are the insights transferable to a 3D system. What would you expect to change? Since, there is currently no transport and interaction between the cells, I infer that aside from maybe slightly different development of the initial correlations, the dynamics should stay the same. The macro-scale equations are not affected, as I understood.*

   Yes, the approach should be applicable to a 3D system as long as the cells are not connected. In a revision, we would however include connectivity as described in our responses to comments by other reviewers.

10. *More complex systems: The analytical scale transition approach worked nicely with the basic simple model. With more complex models that include many more heterogeneous parameters it will be difficult to impossible to close the model with all the combination covariances (the factorial grows very fast). Can you describe a strategy to determine which combinations are important and which combinations can be neglected? When have we sufficiently including more and more heterogeneities?*

    This is an excellent point. We hope that this work will stimulate discussion precisely in this direction. At a large enough scale, most likely some of the higher order moments will not matter as much, possibly leading to model simplifications.

    Which higher order moments can be neglected would depend upon the kinetics and type of heterogeneity studied. If the kinetics of decomposition at microscale is known, then one could use the upscaling procedure provided in the manuscript and get a second order approximation of upscaled decomposition rate. Afterwards, depending upon the nature of heterogeneity (i.e., biophysical, biochemical or a combination of the two), one could start eliminating the unnecessary covariances and variance terms to arrive at a manageable upscaled decomposition rate.

    When have we included enough heterogeneities? This is more difficult question to answer. From a modeling perspective, the Taylor expansion could be truncated when results from distributed model and upscaled equation start to converge (or differ less than a preset error). To give an example, for a fully heterogeneous system simulated with multiplicative kinetics, $\bar{R} \neq (1-Y)\left(\bar{k}_{s,mult}\bar{C}_s\bar{C}_b + \bar{C}_s\overline{k'_{s.mult}C'_b} + \bar{C}_b\,\overline{k'_{s.mult}C'_s} + \bar{k}_{s,mult}\overline{C'_sC'_b}\right)$ because the third order moment $\overline{k'_{s.mult}C'_sC'_b}$ is missing in the summation. However, it is possible that the dynamics at the micro scale lead to low values of higher order moments, because substrate consumption, mortality of the microorganisms, and transport (not explicitly modelled here, through mass transfer between neighboring cells can be included as discussed in responses to other reviewers' comments) contribute to smoothing spatial gradients.

    In a revised version, we would include these points in the Discussion.

11. *Time scale: I am especially interested in modelling decadal to longer-term SOM dynamics. Are the multi-annual oscillations important for the longer term dynamics? Do you expect heterogeneity to change with global change in the longer term? What is the advantage of describing the changed steady state with heterogeneity*

(Fig 7d) with heterogeneity inputs compared to effective model parameters? I see some advantages, but it would be nice to clarify them in the paper.

Yes, multi-annual oscillations are important in our simulations, despite the rate of C inputs to the simulated system being time and space invariant. As our results suggest, in the fully heterogeneous system, organic carbon reaches a new steady state that is dependent upon the micro-scale features (see Eq. A13, P36L5); i.e., heterogeneity in the kinetic parameters affects the steady state soil organic C value.

The linkages between these predictions with global change are not clear at this stage. We know that environmental conditions (soil moisture, temperature) affect the dynamic behavior of lumped microbial-explicit models (Manzoni and Porporato, 2007), but we now also show that standard nonlinear kinetics might not be able to describe macro-scale dynamics in heterogeneous systems. We do not know if climatic changes alter the spatial or chemical heterogeneity of organic substrates. However, land management does. Based on our results we could speculate that less heterogeneous litter input – as for example in agricultural fields compared to a forest – could lead to less soil organic carbon in the long term for a given C input rate. In a revised manuscript, we will elaborate on this possibility.

Specific comments:

12. *eq. 4 ..6: Your simple basic model refers to the Schimel and Weintraub 2003, who actually used and suggested an inverse MM kinetics D = ks Cs Cb / (kM + Cb). It would be nice to amend your work by this decomposition equation.*

Upscaling of the inverse Michaelis-Menten (MM) kinetics could be easily done following our framework to approximate the mean decomposition rate. For example, in the biophysically heterogeneous system, the mean decomposition rate $\bar{D}$ is given by the following equation.

$$\bar{D} = \frac{k_s\,\bar{C}_s\,\bar{C}_b}{\bar{C}_b + K_M} + \frac{1}{2}\left[\frac{-2\,k_s\,K_m\bar{C}_s}{(\bar{C}_b + K_M)^3}\right]\sigma_b^2 + \left[\frac{k_s\,K_M}{(\bar{C}_b + K_M)^2}\right]\mathrm{Cov}(C_s, C_b)$$

Numerical implementation of the inverse MM is performed similarly to MM kinetics. The parameters of the inverse MM are chosen (by trial and error) in a way that respiration rate in the homogeneous system is comparable to that in the heterogeneous system. In Fig. R5, we show the dynamics of the state variables and of the sum of second order terms; this figure is similar to Fig. 7 in manuscript. The effect of heterogeneity on the specific growth rate as function of substrate for the inverse MM kinetics was also investigated, and extra panels were added to Fig 9, shown here for convenience as Fig. R6.

Both Fig. R5 and R6 can be added to revised manuscript.

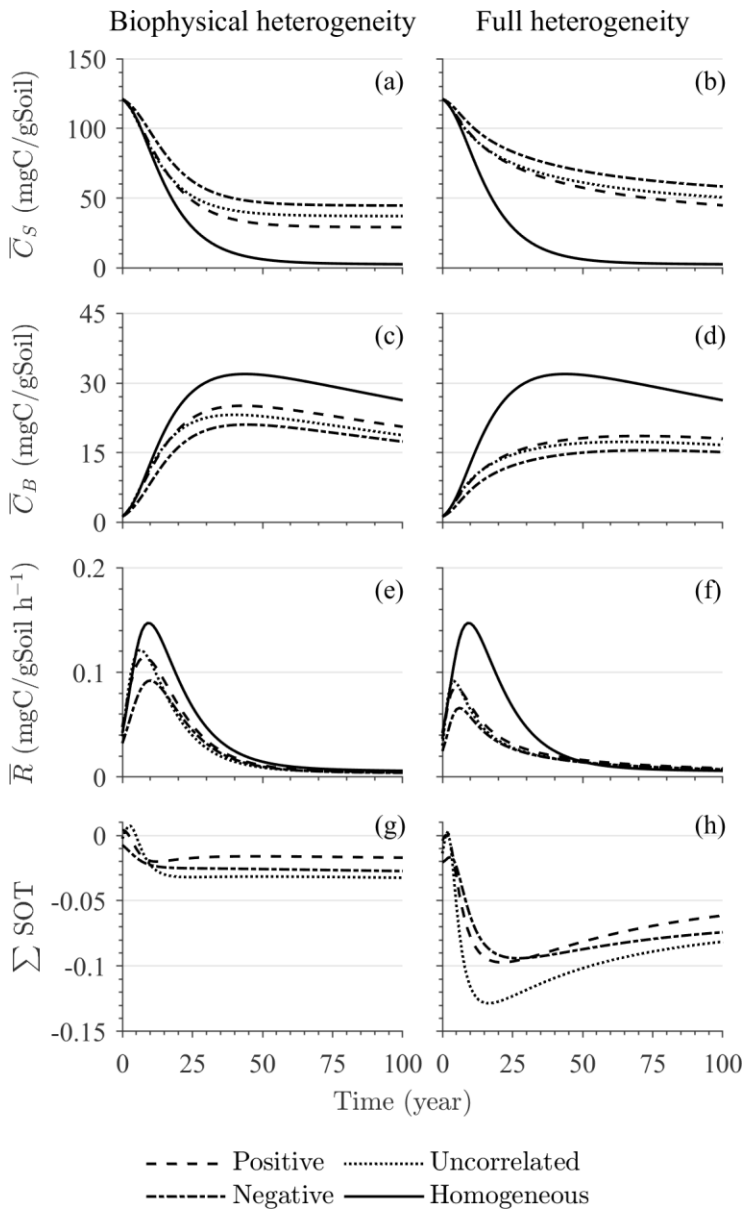

Figure R5: (a,b) mean substrate C ($\overline{C}_S$), (c,d) mean microbial C ($\overline{C}_B$), (e,f) mean respiration rate ($\overline{R}$), and (g,h) sum of second and third order terms ($\sum SOT$), shown as a function of time, for different scenarios of initial spatial heterogeneity. This figure is similar to Figure 7 in the manuscript and depicts Scenario 2 (transient dynamics with inverse Michaelis-Menten kinetics): effect of biophysical heterogeneity (left panel) and full heterogeneity (right panel) on the macroscopic decomposition dynamics when the substrate is distributed around a value higher than the steady state of the homogeneous system.

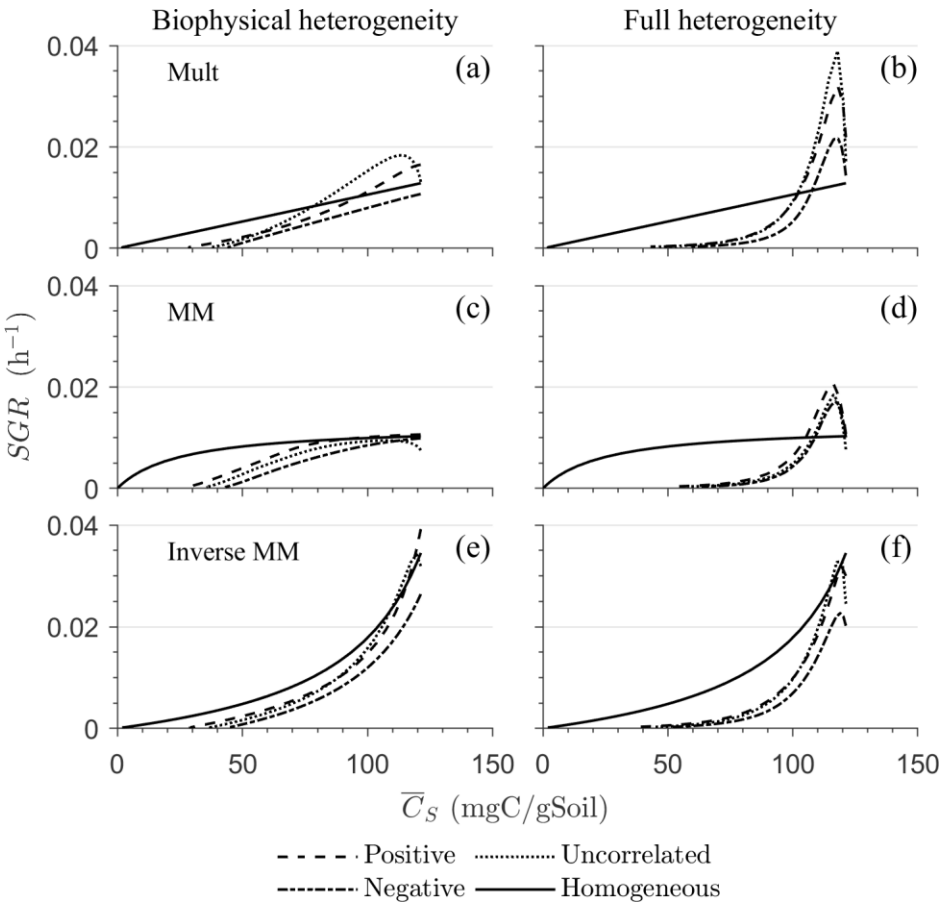

Figure R6: Effect of biophysical (left column) and full (right column) heterogeneity on the mean specific growth rate (SGR) as a function of mean substrate C ($\overline{C}_S$) for the heterogeneous system for (a,b) multiplicative, (c,d) Michaelis-Menten and (e,f) Inverse Michaelis-Menten kinetics. Time progresses from right to left, as substrate C is depleted.

13. *P11L11: The sentence does not make sense to me. The variance itself is not always negative. Probably you meant: "This term is always negative because the variance of the spatial substrate distribution is a positive quantity and ..."*

    This line will be changed to

    "The spatial variance term is always negative because the variance of the spatial substrate distribution is a positive quantity and"

14. *P12L15ff: May state that therefore the mean field approximation is exact and spatial variance of this parameter has no effect on the macro-scale dynamics.*

    Original paragraph was:

Similar derivations can be done for the microbial mortality rate ($F = T$). The Taylor expansion of microbial mortality is simpler because we assume T to follow first order kinetics. This implies that all the second order terms are equal to zero, and ($\overline{T}$) is obtained as

It can be changed to:

"Similar derivations can be done for the microbial mortality rate ($F = T$). The Taylor expansion of microbial mortality is simpler because we assume T to follow first order kinetics implying that all the second order terms are equal to zero. Therefore, the mean field approximation is exact and spatial variance of this parameter has no effect on the macro-scale dynamics, ($\overline{T}$) is obtained as"

15. *P12L19: This paragraph comes a bit surprising without context. Why do you look at SGR?*

    Original paragraph was:

    The rate of decomposition at macro-scale can be used to calculate the specific growth rate (SGR) of the microorganisms - i.e., the respiration rate divided by the mean microbial C,

    It can be changed to:

    "To understand how the decomposition kinetics if affect by the spatial heterogeneity, we define a macro-scale specific growth rate (SGR), which is calculated diving the mean respiration rate by the mean microbial C in the system."

16. *P14L11ff: Potential for moving to appendix. Only the information starting from P15L5 is important*

    P14L11-P15L7 can indeed be moved to the appendix.

    The starting paragraph of section 2.4 Initial 2D random fields of SOM and kinetic parameters will be changed as follows:

    "Two-dimensional spatially heterogeneous distributions of substrates and microbial C were generated to run the distributed model. The obtained distributions were based on following constraints: i) the total amount of organic C is set, ii) the total amount of microbial C is 1% of total organic C, iii) the maximum amount of C in a cell is set (Eq. (A11)), and iv) some grid cells have no microbial biomass. For details of field generation procedure, see Appendix A2."

17. *P14L19: What is (fg)? I could not find the explanation. It is used several times in the text eq. 26, 27 and appendix figure and table captions.*

    $fg = 10^{-15}g$. It is explained at P14L9.

18. *P16L10ff: I suggest to give more meaningful names to the scenarios instead of numbers. E.g "Steady simulation" and "High Substrate Simulation" (also update Fig 3).*

Labelling the scenarios in this way would make reading easier and it is easy to implement in a revised version. Thanks for the suggestion.

19. *P17L11: It did not*

    This comment was truncated and we could not address it

20. *P18L14: The equation is not understandable here (what is a and b). I suggest just referring to the appendix equation*

    Done.

References

Manzoni, S. and Porporato, A.: A theoretical analysis of nonlinearities and feedbacks in soil carbon and nitrogen cycles, Soil Biology and Biochemistry, 39(7), 1542–1556, doi:10.1016/j.soilbio.2007.01.006, 2007.

Sierra, C. A., and Mueller, M.: A general mathematical framework for representing soil organic matter dynamics, Ecological Monographs, 85, 505-524, 10.1890/15-0361.1, 2015.