

We would like to thank Thomas Wutzler for an encouraging and detailed review of our manuscript. This response is intended to be short and part of the full response which would be submitted after the other reviews become available as well. In the following, we address the most conceptually important points raised by Dr. Wutzler (denoted by italic font). Our responses are highlighted in blue (normal font).

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; the other is to numerically solve the micro-scale equations and aggregate (=average) results at the macro-scale. Solving the upscaled differential equation would require some mechanism of transferring second order moments calculated from distributed model to the upscaled differential equation – this issue of ‘model closure’ is presented in the Discussion. Here we followed the second approach and did not solve the upscaled differential equations (Eq. (9) and (10), P8L15), as explained in the manuscript (P13L4 and P30L22). We only used the averaged dynamics as simulated from distributed model and compared that with the homogeneous equivalent.

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. As expected, results were exactly the same from the upscaled differential equation and the distributed model.

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

It is a typing mistake. Eq. A7 should be $-\frac{2 k_{s,mm} K_M \bar{C}_B}{(K_M + \bar{C}_s)^3}$. Numerical code and results are correct.

3. *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, the covariance pattern for biophysical heterogeneity and the sum of the higher order terms are stable in the long term, after new steady state has been reached. We ran the simulation for 100 years and a similar figure to 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 would be also homogeneous. However, they attained a different concentration value at steady state. This concentration value is 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.

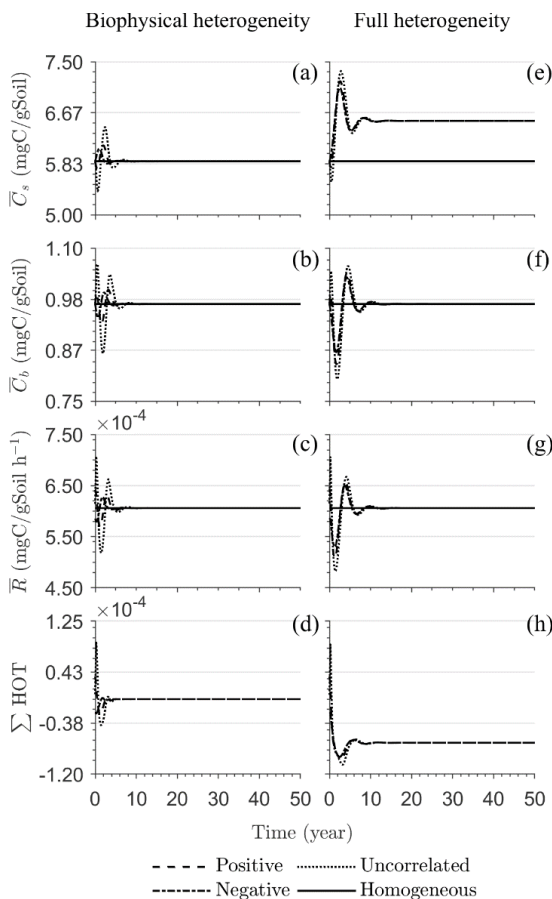


Figure R1: This figure is same as to Figure 4 in the manuscript but for 100 years simulation period.

4. *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?*

No, oscillations would not start again after the system has reached a steady state, because with spatially homogeneous inputs the steady state will also be spatially homogeneous. Thus, no oscillations would occur whether the system has only biophysical heterogeneities or is fully heterogeneous.

5. *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 care 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 (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 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.

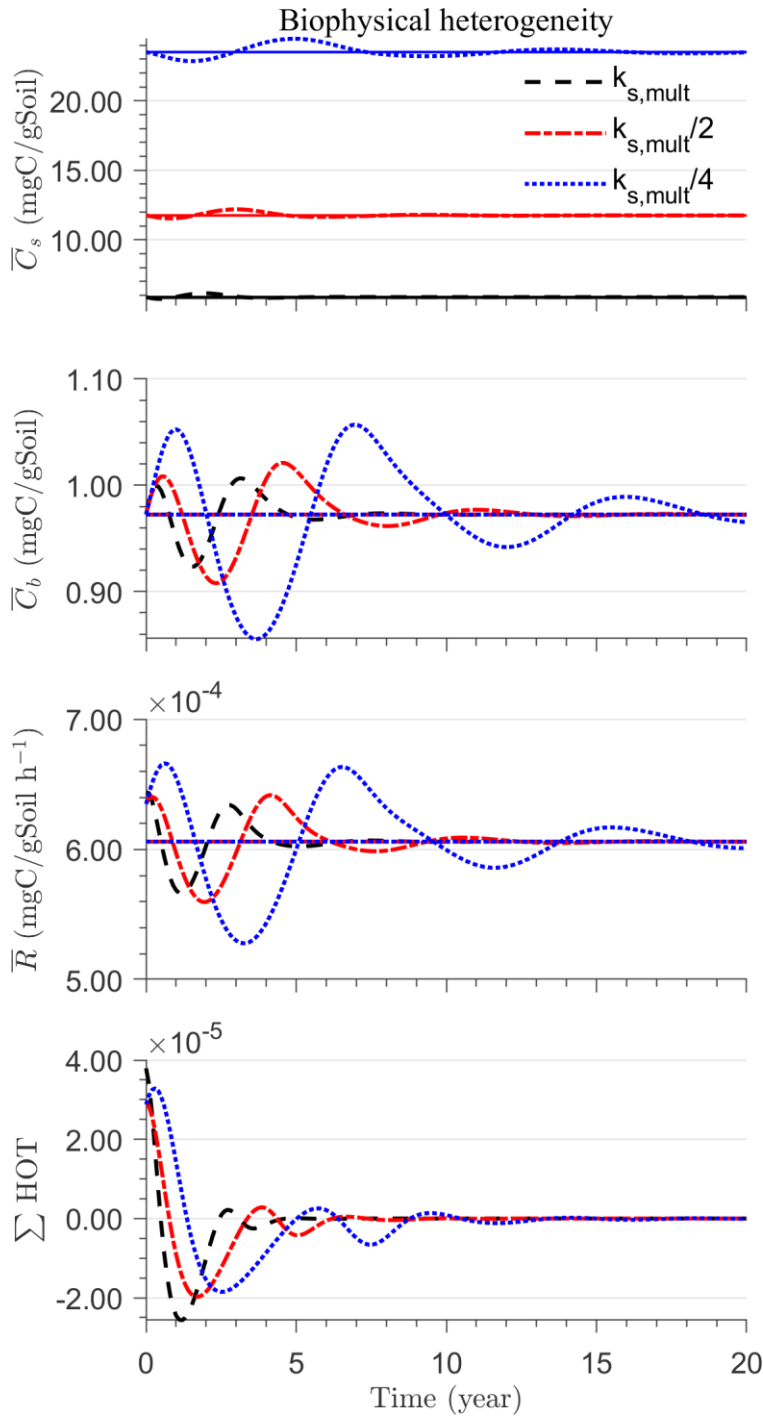


Figure R2 This figure is similar to Figure 4 left column in the manuscript. Different line colors represent varying levels of rate constant $k_{s,mult}$ with base case same as in Figure 4 of manuscript. Scenario 1 (initial condition at steady state): effect of biophysical on the macroscopic decomposition dynamics when the substrate is distributed randomly around the steady state: (a) mean substrate C (C_s), (b) mean microbial C (C_b), (c) mean respiration rate (R), and (d) sum of second and third order terms (ΣHOT).

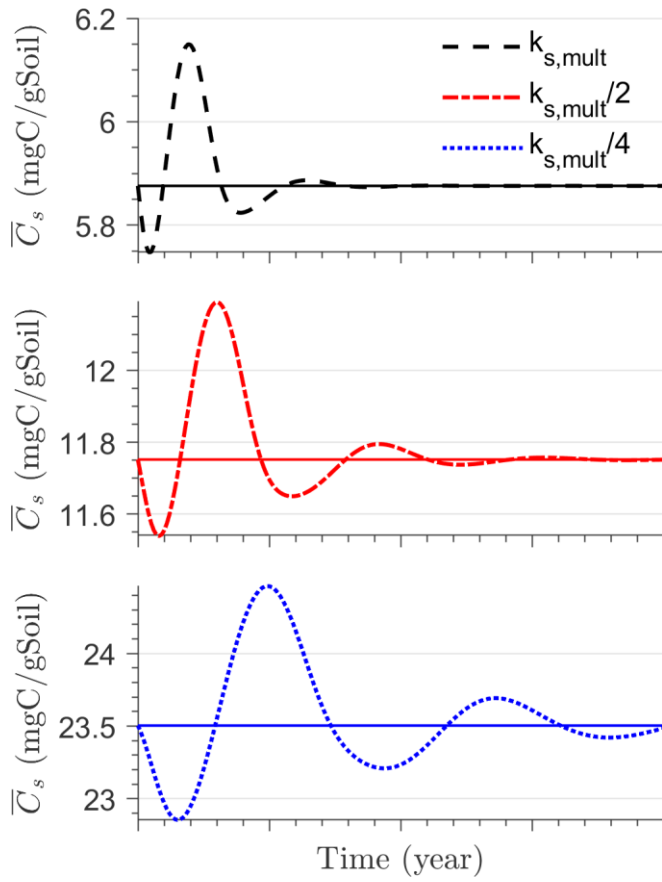


Figure R3 Enlarged view of the time trajectories of the mean substrate C concentration extracted from figure R2.

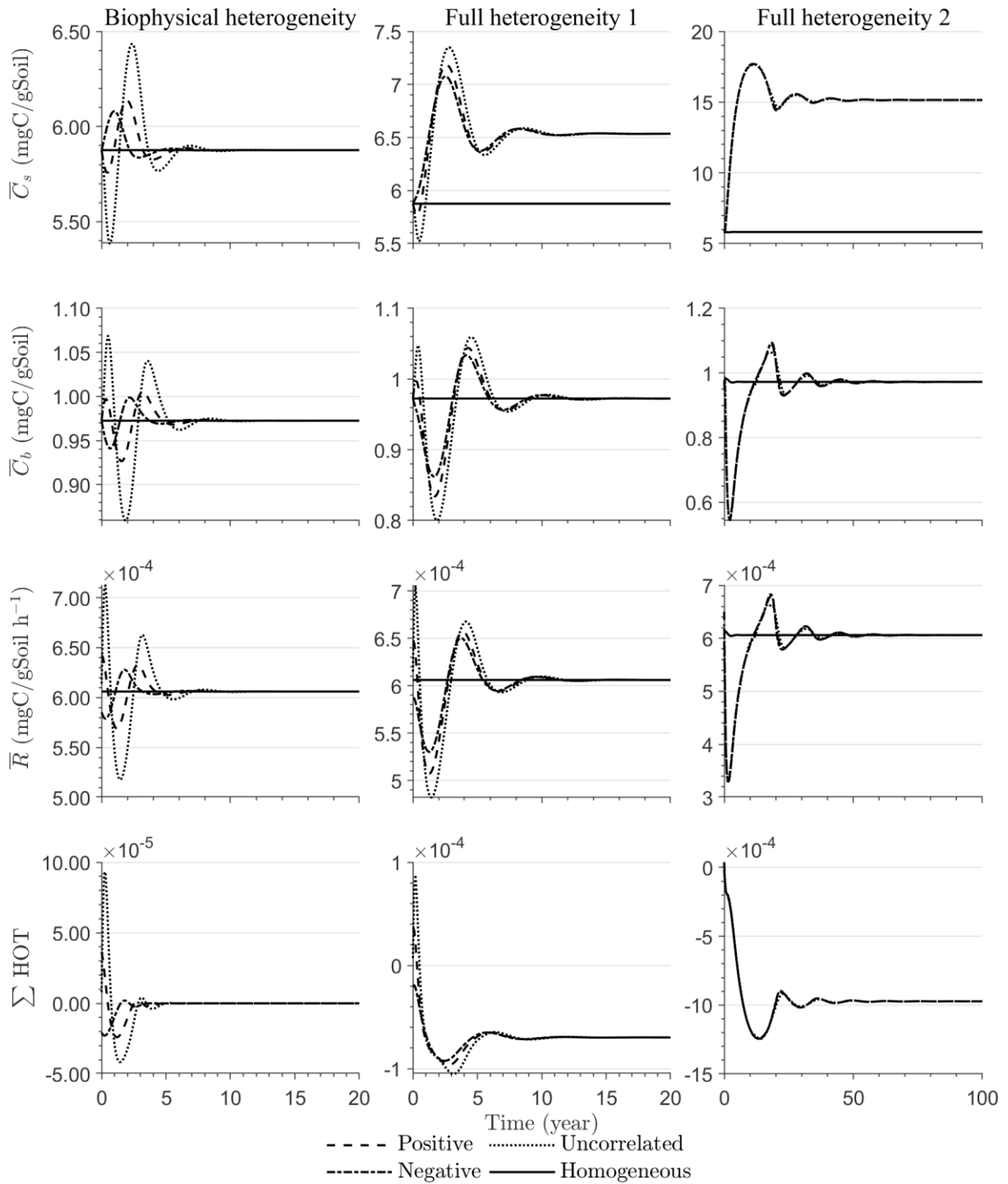


Figure R4: This figure is similar to Figure 4 in the manuscript, except for the right column, where we added trajectories for the full heterogeneity case, with increased heterogeneity of the rate constant ($k_{s,mult}$).

6. *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 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, $\bar{R} \neq (1 - Y)(\bar{k}_{s,mult} \bar{C}_s \bar{C}_b + \bar{C}_s \overline{k'_{s,mult} C'_b} + \bar{C}_b \overline{k'_{s,mult} C'_s} + \overline{k'_{s,mult} C'_s C'_b})$ because the third order moment $\overline{k'_{s,mult} C'_s C'_b}$ 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) contribute to smoothing spatial gradients.

In order to investigate if enough heterogeneities are included in the upscaled differential equation, a figure can be included in the revised manuscript exploring the effects of progressively adding higher order moments on the simulated dynamics of mean respiration rate. Such a figure would illustrate how errors are reduced when adding spatial moments to the mean field approximation.

- 7. 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. 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.

The linkages between these predictions with global change are not clear at this stage. We do not know if climatic changes alter the 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. In a revised manuscript, we could elaborate on this possibility.

As explained above, these preliminary replies are meant to continue the discussion and offer readers a glimpse at how we could address Dr. Wutzler's comments. A complete rebuttal will be provided in due time and if deemed useful by the editor.

References

Manzoni, S., and Porporato, A.: Theoretical analysis of nonlinearities and feedbacks in soil carbon and nitrogen cycles, *Soil Biology & Biochemistry*, 39, 1542-1556, 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.