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 2 (Ali Ebrahimi):

We would like to thank Ali Ebrahimi for the review of our manuscript. Our responses are highlighted in blue font. Some of the comments point to the approach limitations – indeed, this is a theoretical study the findings of which are hard to validate because there is no data at a fine-enough resolution. We would like to emphasize that the value of the proposed approach is to provide a framework for studying heterogeneity effects on measurable C fluxes and stimulate discussion in this area.

Major concerns:

1. *It is unclear to what extend the parameterization proposed in the analytical kinetic model could be experimentally validated. My major problem is that some of the quantities do not have real biogeochemical or physical meanings in which could be experimentally measured. For instance there is an emphasis on the second*

order moments as state variables used to close the model; however it is hard to think how such variable could be experimentally measured.

It is correctly stated by the reviewer that the second order moments (SOTs) do not represent 'real' biogeochemical fluxes, but they do have a clear physical meaning – SOTs represent spatial variability and co-variation of the state variables. SOTs should be considered as corrections to the mean-field approximation of the micro-scale model. State transition theory states that if the macro-scale system is heterogeneous, then rates calculated using the mean state variables are not accurate, i.e. the mean-field approximation does not offer a good representation of the dynamics. These SOT can be estimated from the spatial moments of the state variables, as done in applications of state transition theory in population ecology (e.g., Englund and Leonardsson, 2008). The problem is that these measurements in soil environments are difficult, so we hope that this theoretical study (as others being proposed lately) will stimulate advances in empirical approaches to fill this gap.

Experimental validation should be thought in the following sense: observations obtained from SOC decomposition represent the averaged response of the system, and this averaged response is expected to differ between a truly homogeneous system and a heterogeneous one. Therefore, experimental validation should stem from designing a truly homogeneous soil system and comparing it with regular soil based experiments, which are expected to be influenced by spatial heterogeneities in the sample. If any difference is observed between the homogeneous and heterogeneous systems, then our framework suggests that this difference should be attributed to spatial variability at the micro-scale (second order terms).

Furthermore, in this contribution we do not propose a parametrization of the upscaled equations – the so-called 'closure problem'. We simply compare the effect of micro-scale heterogeneities on the averaged C dynamics. While the current formulations based upon scale transition theory provide a way for conceptually including the effect of micro-scale heterogeneities in upscaled equations, finding a parametrization for SOTs remains a challenge. This challenge was presented in the original manuscript (P29L27, P30L22-26, P31L19), but we will expand on this in a revised version.

2. *The type of model and scenarios proposed in this study are relevant and could potentially address some of the inconsistency in our field measurements but it could only be possible if the model could establish a systematic link to relevant abiotic and biotic factors observed in the field. While in the discussion authors have tried to relate some of the scenarios in the study to soil aggregation or pore connectivity and an entire subsection is dedicated for that, I still find that the* ***modeling framework is too abstract that makes the explanations quite speculative*** *and hard to think to what extend the decomposition rate may vary under realistic settings.*

The modeling framework described in the manuscript is motivated by its simplicity to describe C dynamics at the micro-scale and a tractable number of SOTs that results from scale transition theory. This simplicity (and high level 'abstraction' to quote the reviewer) allow for theoretical insights on how spatial heterogeneities affect the macro-scale fluxes. Several experiments are now exploring how substrate placement affect respiration (e.g., Don et al., 2013; Schnecker et al., 2019) – these results point to spatial placement as a key driver of C fluxes. While the theory presented here can be used as a framework for interpreting those results, as explained in the Discussion a direct theory validation is not possible at this stage. Other approaches to soil heterogeneities have focused on spatial gradients in aggregates (as in recent papers by the reviewer); here we propose a more general – albeit harder to validate – approach based on a statistical description of substrate and microbial placement in the soil.

While we already acknowledge the theoretical nature of this study and its limitation in the original manuscript (which the reviewer correctly points out in his comment), it should be noted that statistical approaches as the one proposed have not been applied to soil systems and thus might offer novel solutions to the limitations of current microbial-explicit models. Here we do not claim that we fully address these limitations, but we hope that this work can contribute to the discussion in this area.

3. *The model could potentially describe some of the underlying abiotic and physio-logical mechanisms that shape the decomposition dynamics but in the current form of the manuscript this has not been explored. For instance, I was wondering to what extend half saturation to substrate and decomposition rate constant (KM and Ks) are shaping the dynamics observed in the model. I would guess if lower KM or high Ks would have been chosen the heterogeneous scenarios would have converged faster to the homogenous one.*

Indeed the values of the kinetic parameters affect the speed of convergence to the steady state, the actual value of the steady state (this is a novel result as well), and the nature of the fluctuations towards the steady state. We explored how varying the decomposition rate constant and its variability on the macro-scale respiration rate in a set of figures prepared in response to a related comment by reviewer 1 (Figures R2, R3, and R4).

Minor concerns:

4. *I was wondering to what extend the fluctuating environmental condition (for instance fluctuating in carbon distributions) could play a role in shaping the carbon decomposition dynamics. Do you expect to see faster convergence to homogenous scenario in high intensity fluctuations?*

We hope to interpret correctly the meaning of the term 'high-intensity fluctuations' in this comment, as conditions of higher contrast between substrate and microbial biomass concentrations. If our interpretation is correct, this question is best answered by comparing the convergence to homogeneous conditions of systems with different degrees of correlation between substrates and microbial biomass. With negative correlation (highest contrast), the system converges more or less at the same speed as in the case of positive correlation. Convergence is slower when there is no correlation between substrate and microbes (Figure 4).

5. *The system size that is modeled in grid based network is rather small. The number of grids, or pores equal to 10000, is basically enough to model an aggregate with the size of 0.5mm. I was wondering if this size is sufficiently large to capture heterogeneities in the soil?* ***For instance inter aggregate pores or macro-pores****?*

For system with no spatial interaction, 10000 grid points are enough for statistically meaningful mean dynamics and dynamics of second order term do not change by increasing the number of grid points. We have not explored the role of variability among aggregates or of a pore structure – these are all good suggestions for future work, but are beyond our scope here.

6. *Following up on the results for negative correlations**, I was wondering how much physical inaccessibility of the carbon to microbes could be relevant for the soil systems?** For instance most of the carbon protections in soil are often driven by soil aggregation and creation of anoxic microsites. In a broader term, the counter gradients created by carbon and other necessary substrates for carbon degradation could lead to inaccessibility of the carbon for microbes and not necessary physical inaccessibility. This is a phenomenon that has been previously shown in soil aggregates that due to creation of anoxic zones, the carbon configuration does not play a role in carbon consumption (Ebrahimi and Or, 2018 GCB) and in other studies showing carbon protection by aggregation (e.g., Keiluweitet al., 2017 Nat. comm.).*

   This is also an interesting point. Indeed, inaccessibility of substrate to microorganism can be caused by several bio-physio-chemical processes. Inaccessibility caused by any biophysical factor should decrease the mean respiration rate because inaccessible C is not contributing to the CO2 emission. In the spatially explicit mass transfer based model (described in the response to reviewer 3), we explored the effect of different degrees of spatial redistribution of the decomposition products. This analysis shows that increasing the level of spatial redistribution would result in decomposition of all the substrate in the domain even if substrate and microorganism are initially isolated i.e. negative initial correlation. Therefore, it is the combined effect of initial inaccessibility and spatial redistribution mechanisms that is responsible for making substrates available to microbes.

   Returning to the question of the reviewer: with the current model we cannot provide a clear answer as in some systems time-varying anoxic conditions will drive the spatial distribution of microbial activity (which we did not account for here), while in other systems physical protection or heterogeneous substrate 'quality' may matter more (which we did consider).

References

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