Interactive comment on “Dynamic upscaling of decomposition kinetics for carbon cycling models” by Arjun Chakrawal et al.

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Received and published: 6 July 2019

The authors study one very basic assumption of soil organic matter (SOM) modelling at theoretical level. They falsify the assumption that dynamic equations that work for the pore-scale can be used at the soil core-scale. This is because soil is heterogeneous and properties vary much at a scale longer than diffusion mixing length. Moreover, they present a framework that is able to derive equations at the soil core scale, albeit currently only for simple models and without the required information about the dynamics of the heterogeneity. This work is very interesting to the SOM modelling community, because it shows basic shortcomings in current model development and interpretation of simulation results. It could be a start for the development of a new class of SOM models. I enjoyed reading the manuscript and looking at the differences in results between homogeneous and heterogeneous simulation. The length is quite long and it was difficult to keep the storyline in mind. With the detailed explanations, the point was made clear, I understood and trust the claims, and got curious with even more questions to be discussed.

General comments
The methods and result sections are rather long. It would be nice to shorten it by deciding on the important points and moving less important points to the appendix. I give some suggestions in the detailed comments.

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.

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.

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

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

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, …).
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.

Development of the heterogeneity / damping of oscillations (Fig 4): The system 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.

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?

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?

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.

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?

Time scale: I am especially interested in modelling decadel 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.

Specific comments:

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.

P11L11: The sentence does not make sense to me. The variance itself is not always negative. Probably you ment: “This term is always negative because the variance of the spatial substrate distribution is a positive quantity and…”

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.

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

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

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.

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).
P17L11: It did not
P18L14: The equation is not understandable here (what is a and b). I suggest just referring to the appendix equation.
P19L1: I suggest to shortly inline write the definition of SGR or refer to Eq. 20.
P22L4ff: The details are hard to follow. I suggest moving this paragraph to the appendix near the referenced figures. However, I suggest keeping the conclusion that additional higher order terms cannot be ignored.

Fig5 is nice but actually does not add insight in addition to the dynamics already shown in the other figure 4. Another possibility to shorten the manuscript and moving the Figure to the appendix.
P22L15: I suggest to remove the first sentence – its essentially a figure caption. Better start with the subject of the paragraph: the relation between SGR and Cs. Why its important to look at SGR?

Fig8: I assume this refers to the transient simulations. Please indicate this in the figure caption. Further, I suggest adding a third column and move SOT lines out of the second panel and add color redundant to linetype, because it’s really hard to distinguish the lines. First, I was confused by R_hom in plots of correlations. I assume it was added for comparison and should be the same across all rows (it looks shifted, but that may be an optical illusion). Please, clarify in the figure caption. I initially thought from your description in 2.6 that in the transient scenario decomposed a large initial SOM field but did not receive any further inputs. However, this contradicts the behaviour in Fig. 8. Please clarify in 2.6. The respiration seems to run into a steady state, that is independent of the heterogeneity. Initially I was puzzled by the same respiration despite very different substrate and biomass values, but if this in steady state with an input rate this is the expected behaviour. Would be nice to read a little discussion on this.

C5

Fig9: May add an arrow to one line to indicate the development in time.
P27L12: “Early state of decomposition process”: In my interpretation of your results its more a “Period after disturbance” - but this relates to the missing presentation of development of spatial heterogeneity.
P28L14: Cited literature. There is another group who did much work on pore-scale modelling with H.J. Vogel in Leipzig although in the hydrological domain. He also suggested a “scaleway” (e.g. 2003 Moving through scales). Would be nice to reference some of their work for following links in literature.
P28L23: typo: differences “are” (instead of “is”)
P28L21: Here you discuss high frequency measurements of respiration in the range of minutes for moving forward to measure effects of heterogeneity. However, your simulated dynamics of heterogeneity works at multi-annual time scale. How does this relate to each other?

eq. A7: When checking the derivatives, I a get a different dF/dCSdCS with a different denominator of the second term: (kM+CS)³. I assume its a typo in the manuscript, but please, check your code, or show that your derivation is indeed correct.

Fig A1: How does this figure differ from Fig 2 in the main text?

eq. A13: Where does the log_e10 in the logUniform distribution come from? Do you expect your results to change, if you use the log to base e instead of the log to base 10?