Comment on bg-2021-72
Anonymous Referee #2

Referee comment on "Predicting the impact of spatial heterogeneity on microbial redox dynamics and nutrient cycling in the subsurface" by Swamini Khurana et al., Biogeosciences Discuss., https://doi.org/10.5194/bg-2021-72-RC2, 2021

General comments:

Khurana et al. used a numerical modelling approach to assess the impact of spatial heterogeneity in the subsurface on microbial activity and nutrient dynamics. The authors combined a biogeochemical process network to describe the turnover of carbon and nitrogen with reactive transport modeling and simulated scenarios that reflect different types of spatial heterogeneities in the subsurface. They propose that impacts of spatial heterogeneity on nutrient cycling can be estimated and scaled based on the residence time of solutes and the Damköhler number of reactions in the domain.

The research question that this manuscript addresses (what are the impacts of spatial heterogeneity on subsurface biogeochemistry?) is relevant to the readership of Biogeochemistry. I believe that the authors' numerical modeling approach provides valuable insights into the relevance of spatial heterogeneity for subsurface carbon and nitrogen cycling. In my opinion, the manuscript would benefit from a more in-depth discussion of how the results of the study could be applied at larger scales or to other subsurface systems and potential caveats that would come with this. Furthermore, I think some statements in the manuscript need clarification—see specific comments and questions below. My specific comments also include some suggestions to improve the readability manuscript.

Specific comments:

L1: The term "redox dynamics" is not used in the manuscript (except once when referring to the literature) and I am not entirely sure what the authors want to convey with it.

L58: "in this microbial ecosystems...": what does "in this" refer to?

L78: "Sufficiently well" for what?

L81: Please add citations for the statement on biogeochemical reaction networks.

L81-82: It is not clear to me how the sentence starting with "Working with ..." fits into the
line of arguments here.

L84: "A straight-forward application of the soil-based biogeochemical model approaches to conditions in deeper subsurface compartments is problematic because the nature of carbon source changes as it travels into the deeper zones." I believe the authors did not specifically look into this- is there a reason for this?

L99: I think using the term "mechanisms" is not great here as I think the manuscript does not address this.

L196: "established": can you add references for this?

L196: What are variance and anisotropy values used for the base case? When I first looked at Figs. S1 and S2, I was confused because the homogeneous base case was shown in all variance:anisotropy ratios.

L250: Based on equation 2, the Da value should depend on the size of the domain relative to the size of the "heterogeneity". Have the authors looked into this?

L312: "while the removal of TOC was the lowest there...": is this trend related to microbial biomass?

L391-392: The bars in Fig. S6 are not linked to redox conditions- is it possible to do so?

L411-451: Given that the prediction of the impact of spatial heterogeneity on redox regimes is the major posit of this manuscript, I believe this section needs to be improved. A few suggestions for improvement are given in the following few comments.

L444: What is AIC and what do these values mean?

L449: Where in Fig. 5 can I see these under-/overestimations?

L452: Does this Fig. include data for different reactive species? Also, why are Da numbers given in log10 base (given that per definition Da is already the ln of the concentration ratio between outflow and inflow)? If solutes are consumed in the domain, then Cout/Cin is always < 1 and hence the Da per eq. 2 is negative- which will give a complex number when taking log10. Is there something I am missing here?

L461: I think it would be beneficial to explicitly state the range of the scenarios.

L463: "correlation length": this is not discussed in detail in the results section and I am not sure how it fits in here.

L507-508: "We establish that the persistence of microbial species in the domain is governed by the presence of the appropriate carbon source and electron acceptor, ..." I am wondering how microbial species are linked to carbon sources and electron acceptors in the model. Is species distribution independently modelled or could this finding in part be a result of the way the reaction network and model are set up?

L627: Can the authors elaborate on the significance of this results for environmental systems? For example, when and where do they expect these heterogeneities to be most significant?

L654: Or underestimate nutrient removal six-fold as stated in L443?
Technical corrections:

L18: "used" instead of "undertake"
L83: "group" instead of "groups"
L115: "attempted" instead of "attempt"
L123: "Disentangle" from what? I think describe/define would be better.
L271: I think the "removal" before "impact" should be deleted.
L424: Why are some words bold?
L446: Seems like a repetition of L 443f.
L553-555: A verb is missing in this sentence.
L609: Delete "towards".

Tables: Captions should be above tables, not below.

Figures: It would be helpful to have different symbols for the three flow regimes so that the figures are readable in black and white.