

## Final response to all reviewers

*We thank all the reviewers for the constructive feedback which helped us improve the discussion of the results and overall readability of the manuscript. While we have already responded to the specific comments from the reviewers in our individual responses, we provide locations of the major changes in the revised marked up manuscript below. Reviewer comments are preceded with "RC" and our response is the italicised text following the reviewer comment.*

*A revised description of the AIC criterion and the derivation of Damköhler estimates is now included in the revision P10:L272 to P11:L301.*

10 RC: P1-L18: 'undertook'  
*P1-L19: Replaced with 'used'.*

15 RC: P1-L21: In biology we have a clear nomenclature. Conditions are either 'oxic' or 'anoxic', Organisms and processes are 'aerobic' or 'anaerobic'. I suggest to use this nomenclature concisely throughout the MS.  
*Changes made at several locations throughout the manuscript including P1-22*

20 RC: P2-L37: Here and at many other spots  
RC: P2-L49: Papers of potential interest for the authors: Zhou et al. (2012) FEMS Microbiol. Ecol. 81: 230-242, Hofmann et al. (2020) Front. Microbiol. 11: 543567  
RC: P2-L50: Papers of potential interest for the authors: McGuire et al. (2000) Chem Geol 169: 471-485, McGuire et al. (2005) Ground Water 43: 518-530

*P2-L50 onwards: References added at several locations in the Introduction section.*

25 RC: L58: "in this microbial ecosystems...": what does "in this" refer to?  
Lines 58-60: awkward wording, suggest rephrasing  
*P2: L60*

30 RC: In the Introduction section important issues such as the discrimination between 'active' and 'inactive' as well as 'mobile' and 'immobile' cells are not picked out as central points.  
*P2: L68-75.*

35 RC: Lines 76-78: consider simplifying to "...representative of a system's chemical and biological species, and second...representative of a system's flow and transport pathways."  
*P3:L84-87*

RC: L78: "Sufficiently well" for what?  
*P3: L88*

40 RC: L81: Please add citations for the statement on biogeochemical reaction networks.  
*P3: L90*

45 RC: L81-82: It is not clear to me how the sentence starting with "Working with ..." fits into the line of arguments here.  
*P3: L91*

RC: L83: "group" instead of "groups"  
*P3:L94.*

- 50 RC: L115: "attempted" instead of "attempt"  
*P4: L126*
- RC: L123: "Disentangle" from what? I think describe/define would be better.  
*P5: L135*
- 55 RC: As highlighted in the first paragraph, the conceptual model is simplistic. While the focus is to test for spatial heterogeneity and flow velocity as steering factors with respect to carbon, nutrient and microbial dynamics, frame conditions for the model simulations are non-dynamic with steady-state flow and constant inflow concentrations of dissolved
- 60 species. In this respect, I would expect an in-depth discussion of the model output. Are the set frame conditions sensitive factors? How may the results change with respect to transient input concentrations of carbon and nutrients.  
*P5-L137,L142,L160*  
*P22-L553-572*
- 65 *P28-L760-763*
- RC: The authors mention the 'use of geochemical and geomicrobial observations from a common study site' as basis of the conceptual model. However, I could not find any sources (papers cited) with respect to 'values'. The concentrations of TOC, DOC, NH<sub>4</sub>, NO<sub>3</sub>, O<sub>2</sub>, prokaryotic cells (active and inactive) have been selected and based on which studies and sites.).
- 70 *P5-L160-162*
- RC: Line 163: complete the second half of the sentence by describing how microbes become immobilized (biofilms etc.)
- 75 *P6:L183 onwards*
- RC: In P6-L182 you say: 'The concentrations of the reactive species mimicked conditions observed in the subject site'. However, in the discussion it is mentioned that there were two orders of magnitude difference in prokaryotic cell numbers. I ask the authors to carefully consider input values. Is it true that a prokaryotic concentration of mobile prokaryotic cells in groundwater of 10<sup>9</sup> have been found in the field? Seems very high to me.
- 80 *P23: L582-598*
- 85 RC: Line 195: What is the correlation length used in the simulations? I couldn't find it in the tables.  
*P8:L218-220.*
- RC: L196: "established": can you add references for this?
- 90 *P8: L221-224*
- RC: 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.
- 95 *P9: L240*
- RC: Lines 196-198: The outcomes may be sensitive to the assumption of a second-order stationary random field with horizontal anisotropy. Other types of heterogeneity (e.g.,

100 multipoint statistical models, geometric models, or depositional process models) could lead to different (and probably even more striking) conclusions. I don't view this as a flaw of the study, since this assumption is conventional, but the assumption and its potential implications should perhaps be discussed.

*P22:L550-552.*

105 RC: I know that it is hard to collect reliable information from the literature with respect to microbial features in shallow aquifers. Having this in mind, one need to carefully select values for 'rate constants', 'yield coefficients', ... The values summarized in Table A.4.1 originate from field studies and lab studies very different in nature, i.e. values derived from lab experiments with pure bacterial cultures. Are the chosen values sufficiently  
110 representative for the Critical Zone in Hainich and shallow aquifers in general? This at least needs to be critically discussed.

*P22: L553-565*

115 RC: With respect to DOC, an constant input concentration of 800µM has been chosen. DOC degradation in soil and in groundwater is determined not only by its concentration but more likely by its quality (degradability). Has this been considered.

120 There is dynamics in many aspects, including flow velocity, water retention time, activity and biomass of microbes, DOM concentration and transformation, N transformation, ... Only a subset of parameters, i.e. spatial heterogeneity and flow velocity (related to residence time) has been tested. This needs to be clearly mentioned already in the Introduction section.

*P5: L137-139*

125 RC: Lines 245-246: Clarification is needed here to elucidate what is meant by "fit of the model" in defining the AIC criterion. It isn't clear whether this is fit to actual field observations (there are some discussed in the paper but they are not described in detail) or fit to analytical solutions (e.g. Figure S8), or something else.

*P10:L273-278*

130 RC: Line 280: switch scale and spatial in the sentence

*P12:L328-329*

135 RC: P12-L321: Is there any evidence that the portions of active and inactive cells/species are realistic? In particular when these ratios are calculated for individual physiological guilds (nitrate reducers, ammonium oxidizers, ...). See also table 4.

*P23:L594-596*

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

RC: P16-L411: Provide a citation that supports this statement.

*P18-L472*

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

*P10: L273-278*

RC: L446: Seems like a repetition of L 443f.

*P20: L503-515*

150 RC: P19-L459: The 'available' process knowledge, does it refer to the Hainich study site?  
*P21:L537-538*

155 RC: L461: I think it would be beneficial to explicitly state the range of the scenarios.  
*P21: L540-541*

RC: P19-L474: from carbon concentration and carbon content per cell one will not end up  
with gene copies per volume but cells per volume.  
*P22-L576*

160 RC: Lines 487-489: clunky sentence, suggest rewording  
*P23:L607-609*

165 RC: P20-L490 & L516: There is techniques and reports available on high-resolution  
sampling in aquifers. The reader should not get the impression one cannot get spatially more  
resolved in sampling. E.g. Ronen et al. 1987 J. Hydrol. 92, 173–178, Báez-Cazull et al. 2007  
Appl. Geochem. 22, 2664–2683, Smith et al. 1991 Contam. Hydrol. 7, 285–300, Anneser et  
al. 2008 Appl Geochem 23:1715–1730.  
*P24:L641-645*

170 RC: P20-Fig. 6: What do you mean with 'oxic cells'. Please change.  
*P17: Figure 3*

175 RC: P21-L528: Consider the review paper of Smith et al. 2018 FEMS Microb. Ecol. 94:  
fy191  
*P25: 651-654.*

RC: L553-555: A verb is missing in this sentence.  
*P25:L679*

180 RC: P22-L565: I fully agree with this statement. In many cases the contribution of the mobile  
fraction of microbes can be neglected in terms of 'transformation processes'. Findings from  
other studies (like the one already cited Grösbacher et al. 2018) are not discussed in  
comparison to the model outcome.

185 *P23: L582-594*  
*P26: L689-692*

190 RC: 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?  
*P28: L754-763*

195 RC: P24-L630: mention at which spatial scale.  
*P28: L766*