

Biogeosciences Discuss., referee comment RC3
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Comment on bg-2021-72

Anonymous Referee #3

Referee comment on "Predicting the impact of spatial heterogeneity on microbially mediated nutrient cycling in the subsurface" by Swamini Khurana et al., *Biogeosciences Discuss.*, <https://doi.org/10.5194/bg-2021-72-RC3>, 2021

Review of Khurana et al, "Predicting the impact of spatial heterogeneity on microbial redox dynamics and nutrient cycling in the subsurface," submitted to the journal *Biogeosciences*.

Summary: This manuscript presents results of numerical experiments exploring the fate of reactive compounds within spatially heterogeneous subsurface environments. The conceptual model is based on in-situ observations of dissolved organic matter and microbial functional groups, and models of variably heterogeneity (ranging from homogeneous to highly heterogeneous). The numerical models use a sophisticated representation of reaction networks including biomass growth and transport as well as multi-species reactions. Overall, this manuscript is well-written and organized with only a couple points that require clarification and a few grammatical and formatting mistakes to address. The authors make a clear case for the inclusion of a scaling factor based on the Damköhler number which considers the reactivity of chemical species. The authors provided detailed explanations of the limitations of their model and dataset such as spatial variability of chemical and microbial species within the well screen, which might bias observations from the subsurface.

Specific Comments: There are a few matters that require clarification for the reader and provision of supporting information that is not in the current manuscript:

Line 170: "average hydraulic conductivity" – what average is used (arithmetic, geometric, harmonic)? I would assume arithmetic since not stated otherwise, but often the geometric mean is considered more representative of the average behavior of a heterogeneous permeability field.

Table 1: The "length scale" is given here as 0.1 meters, apparently as used to compute the Peclet number (ref. line 230). What is that value based on?

Line 195: What is the correlation length used in the simulations? I couldn't find it in the tables.

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., 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.

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.

Line 253 (Equation 2): Is this a standard definition of Da ? If so, please provide a citation. If not, please provide clarification as to how this equation represents the ratio of advective and reactive time scales.

Lines 265-270: These lines highlight a broader issue: What times were used for analysis and metrics of reactive processes? The flow field is clearly stated as being steady, but the concentration fields will be transient, and various times are mentioned in the manuscript. The breakthrough time is defined as the time at which $C_{out}/C_{in} = 0.5$ (for tracer), but what other times are considered for reactive species (they may not reach this value at the outlet)? This was confusing to me as a reader and should be clarified.

Technical Corrections:

Lines 58-60: awkward wording, suggest rephrasing

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."

Lines 102-103: suggest grouping citations at the end of the sentence

Line 153: e.g. seems out of place, consider deleting

Line 155: aerobic should be all lowercase

Line 162: necromass is one word, not two

Line 163: complete the second half of the sentence by describing how microbes become immobilized (biofilms etc.)

Table 1: "longitudinal" is misspelled

Line 270: this is "the" same (add "the" to the sentence)

Line 280: switch scale and spatial in the sentence

Figure 2: Is a title necessary? The figure caption should cover the topic of the figure.

Line 424: unbold sentence

Figure 4: Why is there a border around this figure?

Line 447: change to, "Since nutrient dynamics are..."

Line 482: Is there a difference between dormant and inactive? The term "dormant" is used sparingly within the manuscript, so I'd suggest sticking to inactive and defining that this pool includes dormant microbes to avoid confusion.

Lines 487-489: clunky sentence, suggest rewording

Figure 6: It's a bit unorthodox to present figures within the discussion section. Why didn't you introduce it within the results section and then reference it in the discussion?

Line 618: Change to "The regression model links the..."

Line 631: Change to "... was considered when evaluating..." (delete "for")