Comment on bg-2021-265
Julie Zilles (Referee)

Referee comment on "To what extent can soil moisture and soil Cu contamination stresses affect nitrous species emissions? Estimation through calibration of a nitrification/denitrification model" by Laura Sereni et al., Biogeosciences Discuss., https://doi.org/10.5194/bg-2021-265-RC1, 2021

Does the paper address relevant scientific questions within the scope of BG?

Yes, the topic is highly relevant to BG, encompassing physical, chemical, and biological processes as they impact nitrogen transformations in soil and subsequent emissions.

Does the paper present novel concepts, ideas, tools, or data?

Yes, to my knowledge, the combined focus on impacts of copper on nitrogen transformations and integration of those impacts into an existing biogeochemical model is novel.

Are substantial conclusions reached?

Unsure. I am not entirely clear on what the authors’ conclusions are, so I would request clarification of the conclusion section.

Are the scientific methods and assumptions valid and clearly outlined?

The overall approach is valid. It is difficult to integrate experimental and modeling work,
and this work does that well.

My most serious concern with the approach is that the bioassays investigating the effect of copper on nitrification were only conducted on soil that was not previously contaminated with copper. As microbial communities are quite adaptive, one could reasonably expect that there would be different results if the experiments were conducted on soil with a history of copper contamination. Indeed, there may already be studies on that topic; if so they would be relevant to incorporate. The question then becomes which situation is most relevant globally – short-term effects upon introduction of copper (such as the 3 days of exposure tested here), or longer-term consequences of contamination. Given the authors’ focus on improving predictive capability of continental models under climate change, I’d expect longer-term effects would be more relevant.

It would also be helpful to provide more justification for the selected soil type and the copper concentrations used here. Consideration of bioavailable copper would also seem appropriate and might allow for conclusions that are more generalizable to other soils.

*Are the results sufficient to support the interpretations and conclusions?*

(See comment on conclusions above)

The experimental results seem not to be considered as leading to any conclusions.

For the sentences in the conclusion about N2O, and the last sentence of the abstract, I do not find sufficient support in this paper. N2O was not measured here, and DNDC has difficulty predicting the proportion of N2O from denitrification (e.g. https://doi.org/10.1016/j.scitotenv.2018.07.364), so it seems quite speculative to make these conclusions based only on results from a model that was only calibrated and validated with respect to nitrate.

I have similar concerns about conclusions about the abundance of denitrifying bacteria, particularly since they are typically facultative and thus may not directly correspond to the concentration of nitrate.

Modeling is not my core expertise, as is probably evident from my comments. However, to conclude that a new model performs better, I would typically want to see it compared to calibrated versions of existing models.
Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?

I have several questions about how the experiments were conducted.

- No replication is mentioned in 2.2, but data from replicates is given in Table 1. In addition to having these be consistent, I’m wondering if the samples were from replicate microcosms or from replicate samples taken from the same microcosm.
- How was sampling conducted? In particular, were microcosm soils mixed before sampling for measurements and bioassays?
- I’m not clear about how the drying was done, or how long it took for microcosms to reach the drought/dry state.
- What temperature was used for the microcosm incubation?
- How long was the microcosm incubation? Section 2.2 says 45 days, but other places refer to one month and five weeks. This also relates to another question – were the drought and dry-rewetting treatments at a dry or wet state for their final week of incubation before the bioassays?
- When was NH4+ added to the bioassays, and at what concentration?
- I’m not clear on how much liquid was in the bioassays, not sure how to interpret soil solution 1:12. Does this mean that the approximately 5 g of soil was mixed with 60 mL of liquid? Did you account for the moisture differences, or simply take 5 g wet weight from the relevant microcosm?
- Line 124 and 130 contradict. Line 285 gives yet a third description.

On the modeling side, I have an even greater level of confusion. In the abstract it states that DNDC was used, with modifications to account for soil copper effects. Yet in the methods it states both DNDC and a model by Zaehle and Friend … which are two different models … and later it states that the model was written in R, which suggests that DNDC was not used at all. Given this fundamental confusion, I have not done a detailed review of section 2.3. It would be helpful to have more clarity on which equations are taken directly from previous models and which have been modified in this work.

Do the authors give proper credit to related work and clearly indicate their own new/original contribution?

There is a wide body of literature on the effects of copper on soil microbial communities, which is not really incorporated here. Also many studies looking at the effect of moisture on N cycling in soil. These omissions make it difficult to make a clear argument for the novel contribution here.

Does the title clearly reflect the contents of the paper?
In my opinion, the title is not representative of the paper, promising much more than is delivered. It examines copper, not a wide range of soil contaminants. Similarly the focus is on N2O, not the full array of greenhouse gases. There may be similar issues with the modeling description, but that is harder to evaluate given my confusion with the methods.

*Does the abstract provide a concise and complete summary?*

The abstract is well-organized and covers the expected content. Clarity could be improved, in particular around where the double stress came into the experiments. (see also language comments below)

*Is the overall presentation well structured and clear?*

Organization of the intro and methods was straightforward. I found the results very difficult to follow. It would be helpful to me if the experimental measurements were presented before the explanation of how they were incorporated into the model. Or, if those are not considered part of your results, then frame the whole paper as a modeling paper rather than an experimental and modeling paper. Similarly with the discussion – there is currently very little, if any, discussion of the experimental results.

*Is the language fluent and precise?*

The language is at times not fluent or precise, but the intent is generally clear.

Highlighting some early examples:

- Title Extend should be extent
- Abstract: prospect I think should be predict
- Abstract: nitrate production modulation
- Intro lines 70, 75

Another area of confusion for me is the word preincubation. From the figure I understand that this is referring to the initial incubation at different moisture levels, but in the abstract this period was referred to as an incubation, and in section 2.2 as an incubation and as microcosms. It would be helpful to be consistent about how you name this part of the experiment.
Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

No major concerns here. In my experience, the “N” would follow the compound name, e.g. N2O-N.

Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?

I found the discussion difficult to follow. You might consider organizing it around your conclusions.

Please use different symbols/line types as well as different colors in the figures. This is a fairly easy change that will make them more accessible for color blind readers and for those who still print in black and white.

Are the number and quality of references appropriate?

The paper is generally well-supported by references.

Some specific comments on references: I would have liked to see more recent references included in the first paragraph (lines 44 and 50). Although it is an excellent work I don’t find Jones et al 2014 a good support for the sentence in lines 46-47. The reference list is inconsistent in format and several references are lacking information such as page number or doi. See also comment on related work above.

Is the amount and quality of supplementary material appropriate?

Yes. I appreciate that the authors have posted so much data.