

Biogeosciences Discuss., author comment AC1  
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## Reply on RC1

Jie Zhang et al.

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Author comment on "Modeling nitrous oxide emissions from agricultural soil incubation experiments using CoupModel" by Jie Zhang et al., Biogeosciences Discuss.,  
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We would like to thank Reviewer 1 for the time and effort that they took to provide useful feedback for our manuscript. The comments and suggestions provide valuable input for revising and improving the paper, and our responses are outlined below.

Reviewer 1 (RC1):

Manuscript "Modeling nitrous oxide emissions from agricultural soil incubation experiments using CoupModel" by Jie Zhang et al.

**RC comment:** The manuscript is well written and provides an interesting review of challenges to biogeochemical modeling of N<sub>2</sub>O fluxes. It presents an incubation experiment paired with modeling to better resolve drivers of error in N<sub>2</sub>O modeling. However, the most interesting discovery from that effort, which is the contribution of biases in NO<sub>3</sub><sup>-</sup> and NH<sub>4</sub><sup>+</sup> towards N<sub>2</sub>O flux biases, is touched on fairly superficially and should be delved into in much more detail.

**Response:** We agree with the reviewer that regarding contributions of biases in mineral N and associated N<sub>2</sub>O fluxes, we should investigate it in much more detail. In the residual analysis in Figs. S1-S2, we found that the residual errors in NO<sub>3</sub><sup>-</sup> and NH<sub>4</sub><sup>+</sup> were only weakly correlated with the residual errors in N<sub>2</sub>O. In line 482-483 it was stated: "however, the weak and insignificant relationship between N<sub>2</sub>O flux residuals and the residuals for mineral N indicates that N<sub>2</sub>O underestimation at high flux ranges may be due to other factors". We are also aware that even though the calibrated model failed to capture magnitude of pulse fluxes in specific treatments but the variability in posterior model ensembles (Figure 5a and 5b) indicates large uncertainties in parametrization may exist in simulating peak flux. We will describe this result in the revised manuscript.

**RC comment:** Subsequently, the paper discusses many potential drivers of model error and challenges in experimentation to better identify and address contributions to this error. However, the study conducted does not help address these shortcomings much at all. Hence, in my opinion this article is of limited value as an original research paper and is in fact a mix of limited original research and interesting review. I urge the researchers to push towards work to unravel these meaningful issues they coherently discuss here.

**Response:** We agree with the reviewer that we need to put more efforts in addressing these shortcomings of the model and discuss with details of potential attributors, besides, we want to emphasize values of our article as an original research paper for the following reasons:

Process models are primarily used for field-scale simulations where the discussion of model deviations with respect to N<sub>2</sub>O estimation often refers to inaccurate pedo-climate subroutines (Brilli et al., 2017). The present study focused on the role of reactive C and N for N<sub>2</sub>O emissions, and used simulation of targeted experiments to identify key drivers. Simulating C and N dynamics in a short-term laboratory study may be considered to zoom in on a single field operation, in this case the incorporation of crop residues by standard tillage operations. Grosz et al. (2021) in a recent paper in Biogeosciences applied three process models, including CoupModel, to results from an incubation study, but without model calibrations. In contrast, the present study examined model parameters with respect to soil physical properties, but also decomposition, nitrification and denitrification, to learn about sensitivities and limitations.

The unamended soil treatments (controls) were well described by the model, indicating that the repacked and preincubated soil was a suitable representation of normal soil conditions. In contrast, C and N dynamics in residue-amended soil, especially at the high moisture level (Fig. 4a), were difficult to describe with the model, possibly because of the mixing of residues and soil accelerating C and N turnover.

The simulation of predominantly aerobic conditions on the basis of soil respiration and oxygen diffusion, despite significant N<sub>2</sub>O emissions, has not been reported before. Also, parameters related to denitrification and other processes ranked high in the sensitivity analyses, while there was a weak response of estimated N<sub>2</sub>O fluxes to soil moisture. This could be related to heterogeneous moisture distribution in the soil-residue mixture in the experiment, indicating the presence and importance of organic hotspots.

**We will revise the Introduction to better explain the motivation and focus of the study, and we also plan to add a new section to the Discussion on these modeling outcomes and need for better experimental design.**

Other comments:

**RC comment:** How were the parameter ranges derived? It's insufficient to just describe them as "with realistic ranges" or according to model defaults. The ranges are important to model sensitivity and calibration equifinality issues.

**Response:** The ranges of input parameters were derived around the mean values of measurements and estimations, and details will be added in Table S4, and justified in the text. For parameters supported by measurements, i.e. soil porosity and pH, the ranges

were within 25% of the mean values to represent realistic micro-scale variations in the laboratory setup. The residue porosity was estimated with a bulk density of  $0.18 \text{ g/cm}^3$  and a dry density of  $1.3 \text{ g/cm}^3$  (similar to a loose peat soil with high organic content) with a wider range of uncertainty due to compressibility. Soil porosity and residue porosity were used to calculate the soil-residue mixture bulk density and porosity which was beyond the CoupModel framework, and this description will be added in the revised version to section 2.3.1. The range of organic pool fractions were considered from the literature values for cultivated soil (references will be added in the revised Table S4), and for crop residues the range was bound by the estimated fractions of two crop residues.

Regarding process parameters, we looked through most relevant calibration studies using CoupModel and other process models, and adopted ranges defined in the model on the basis of previous applications as shown at the bottom of Table S4. The ranges of remaining model-specific parameters have not been reported in the existing literature, including those involved in nitrification and denitrification, we adopted the default ranges set by the model without better prior information.

**RC comment:** Too much is shown in the figure 5 subplots for interpretation. This data needs to be represented in a better manner.

**Response:** Agree. We will split Fig. 5 into two separate Figures by WFPS level. One Figure with treatments at 60% WFPS (with the most interesting gas emission dynamics) is kept in the manuscript, while a Figure with treatments at 40% WFPS will be included in the supplement.

**RC comment:** In table 1, why is the rRMSE so much different between the single treatment and multi-treatment for  $\text{NH}_4^+$ ?

**Response:** For  $\text{NH}_4^+$  in the multi-treatment calibration, high rRMSE was almost exclusively caused by larger biases between measured data and modeled data for red clover treatments compared to those in the single-treatment calibrations. This has been depicted in Fig. 6c and Fig. 7c, please note that a log-scale is used. The statistics rRMSE and RMSE are more sensitive to outliers compared to mean error (ME) and they would be reduced to 78% and 0.01, respectively, after removing the four treatments (green points in Fig. 7C). **In the revised paper, we will add relevant sentences in section 3.2.2.**

**RC comment:** You describe a pattern of better model fit as the simulations progress with time. This sounds like a model initialization issue. Did you make any attempts to spin-up the model?

**Response:** We did not spin-up the model but took the initial carbon pool sizes from literature values. Spin-up is intended to make the soil pools reach an equilibrium between carbon input and decomposition, which is often the assumed state in long-term studies of ecosystems (Hashimoto et al., 2011). In our study, we assumed that the pre-incubated

bulk soil was already close to a steady state at the start of incubations, in accordance with the C and N dynamics in control treatments, and that the changes observed during incubation were mainly caused by decomposition of residues introduced at time zero. **A statement will be included to clarify the initialization step.**

**RC comment:** Do you have ideas of what caused the second flux peak? Was it the residue decomposition? Something else?

**Response:** The observed secondary increase in CO<sub>2</sub> fluxes from treatments with wheat straw was most pronounced in treatments with elevated soil NO<sub>3</sub><sup>-</sup> (see Taghizadeh-Toosi et al., 2020; Fig. 1), and presumably it reflected growth of heterotrophic microorganisms, which could be enhanced by assimilatory NO<sub>3</sub><sup>-</sup> reduction. Without specific evidence, however, we prefer not to speculate on this.

**RC comment:** Isn't seeing ranges of calibrated parameters oscillating heavily across treatments a sign that the calibration is largely fitting noise?

**Response:** We understand the “noise” as measurement error. We used mean error (ME) as the main measure of calibration, aiming to have a ME close to zero by fitting daily measurements. Considering measurement errors often are normally distributed around zero, and thus their influence on parameter fitting may have been limited if we rule out serious experimental systematic errors. The limitation of the measurement dataset is that we only had mean values of recalculated measurements to compare with model simulations, and therefore any measurement error was included in parameter ranges. Future experiments should have explicit measurements in separate layers with error bars for model use. **We will add further relevant statements about measurement dataset limitations to the Discussion.**

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