Comment on bg-2021-77
Anonymous Referee #1

Referee comment on "Evaluation of denitrification from three biogeochemical models using laboratory measurements of N\textsubscript{2}, N\textsubscript{2}O and CO\textsubscript{2}" by Balázs Grosz et al., Biogeosciences Discuss., https://doi.org/10.5194/bg-2021-77-RC1, 2021

Manuscript “Evaluation of denitrification from three biogeochemical models using laboratory measurements of N\textsubscript{2}, N\textsubscript{2}O and CO\textsubscript{2}” by Grosz et al.

In the present study, gas fluxes (N\textsubscript{2}O+N\textsubscript{2}, CO\textsubscript{2}) modelled by three biogeochemical models (Coup, DeNi, DNDC) were compared to measured ones. For this, data from two laboratory experiments were used in which two different soils (one sand, one silt-loam) were incubated under various conditions (different temperatures, water contents, N addition, ryegrass incorporation, etc.). The models were run without calibration.

The topic is within the scope of the journal.

Due to enormous difficulties in quantifying N\textsubscript{2} fluxes from soils against its high natural atmospheric background, N\textsubscript{2} losses are the largest uncertainty of the N cycle at present. Therefore, there are very few studies that provide reliable information on N\textsubscript{2} losses and (N\textsubscript{2}+N\textsubscript{2}O)/N\textsubscript{2}O emission ratios, although such information is urgently needed for model validation. The manuscript, therefore, deals with an interesting and important topic, since it includes measured N\textsubscript{2}+N\textsubscript{2}O data and a comparison of three widely used biogeochemical models.

The manuscript is a quite long and partly difficult to read. This is amongst other reasons due to the fact that there are several inconsistencies in the manuscript (see general comment on "Inconsistencies" below) and also due to the large number of tables and figures (in total 14 figures and 17 tables in the text and the supplementary material, see general comment on "Tables and Figures" below). Some parts are redundant (see specific comments below). All sections including the title have to be revised to different degrees, especially the description of the results and parts of the Discussion. In my opinion, the manuscript cannot be published in Biogeosciences in the present form, revision is needed.

General comments
Language: Some proof-reading is needed, since there are some linguistic errors.

Abbreviations are not consistently used throughout the text (especially carbon/C). The abbreviation “SOC” is not defined (cf. l. 258, first appearance), "DOC” must be defined in l. 161 (not in l. 185).

Treatment numbers (silt-loam soil): In the Results and Discussion sections (including Table 7) treatment numbers are provided with subscripted information including water-filled pore space, bulk density and N addition. Theses superscripts should be left out, since they worsen the readability of the text. All important information about the treatments can be found in Table 2.

Inconsistencies: (i) Test criteria: According to l. 171/172, “comparing the magnitude of measured and modeled fluxes was not a criterion” for model evaluation. However, in l. 235/236 it is written, that this comparison “was considered a secondary criterion.” This should be clarified. (ii) Tables 1 and 3: For the silt-loam soil, the sum of NO3-N and NH4-N in Table 1 corresponds to the respective sum in Table 3 (14 mg N kg-1). This is not the case for the sand soil (19.2 vs 16 mg N kg-1). Do the numbers in Table 3 refer to pre-incubated soil material? If so, it is strange that the N concentrations of the silt-loam do not differ. This should also be clarified. (iii) Figures 3 and 7: In Figure 3d the measured CO2 fluxes of the four individual control cores of the sand soil are shown. Around day 10, a maximum respiration rate of about 0.4 g C m-2 d-1 is depicted for three of the cores, the fourth one had a lower respiration rate. However, in Figure 7 an average CO2 emission rate of almost 0.8 g C m-2 d-1 is shown. The peak around day 5 (Figure 7) seems not to be correct either. This is an important point (comparison of measured and modelled data) and should be carefully checked. (iv) Discussion: The summary of the results does partly not agree with the data shown in the respective figures and tables or is misleadingly formulated (l. 578-582; see detailed comment below).

Tables and figures: As outlined above, the huge number of tables and figures makes it sometimes difficult to follow the text. I strongly recommend to reduce the number of figures and tables and only keep those which are really necessary for the aims of the study (not all data generated must be shown). (i) It is obvious that not all tables provided as supplementary material are necessary, since there is no reference to some of these tables. All tables to which is not referred to in the text must be omitted (Tables S.3, S.4, S.5). (ii) The Tables 2 and 3 could be merged, since the only additional information in Table 3 is “Calculated 15N enrichment”. The initial mineral N concentrations are already shown in Table 1 and “Added N” in Table 2. (iii) Since one focus of the manuscript is on the comparison of measured and modelled data, the measured data need not to be presented in that detail as in the present manuscript. Therefore, I recommend omitting Figures 2 and 3, because all information needed for the comparison of measured and modelled data are included in Figure 7 (average N2O+N2 and CO2 emission rates). (iv) Figures 4, 6, and 7: The sub-figures (d) to (f) should be (a) to (c), since respiration rates are described first in the text, i.e. before the N2+N2O data. The order of the figures/tables should correspond to the order in which they are cited in the text. (v) There is no reasonable order of the figures and tables in the supplementary material, each
table/figure should be on a separate page; (vi) there are too many unnecessary references to figures or tables in the text (see specific comments below). (vii) If results for all three models are shown, they should always be presented in the same order, i.e. Coup, DeNi and DNDC. In some figures (Figures 4, 5, 6, S.7) and in Table S.5, the order is changed.

Specific comments

Title: The title must be revised. The title focuses on denitrification, but CO2 which is not an end-product of denitrification is also mentioned; “decomposition” should be included. “Denitrification” alone is too unspecific. It should be clearly mentioned what was evaluated (e.g. denitrification products, temporal variations).

Abstract:

The structure could be improved. The motivation of the study does not really become clear. The aim/objective provided is too vague or appears too late in the Abstract (l. 29/30).

l. 14/15: What is exactly the research gap that should be highlighted here? (Bad agreement between measured and modelled data, missing processes, …..?)

l. 16: “to test the denitrification sub-modules of existing biogeochemical models” is too unspecific. It has to be mentioned with regard to what the sub-modules were tested. The information provided in l. 22 should be included.

l. 20/21 “Three common…” and first part of l. 21/22 “No systematic….“: This information should be included in l. 16.

l. 28/29: uncertainties: More specific information is needed here, for instance, one or two examples or a short explanation.

l. 29: This information must be provided earlier.

Introduction:

Some additional background information is needed (see comment on l. 68-72).

l. 37: “nitrogen” must be replaced by “N”

l. 42: The colon should be left out.

l. 44 and l. 47: The information in brackets should be provided as subclauses (“which is a function…”, “i.e. high background….“)

l. 55: “input data may result” instead of “input data result”

l. 57/58: The references cited here are the descriptions of the models used in the present
study. Do they really demonstrate that “measurements of both N2O and N2 fluxes are necessary to develop and test algorithms”? Del Grosso et al. (2000) is missing in the reference list.

l. 61: Delete the colon before “Coup”

l. 59: Delete “these”

l. 65: Delete “(Coup, DNDC, DeNi)”, it is redundant

l. 68-72: This passage needs to be revised. It must be clearly shown that the models are not able to properly predict denitrification processes and the dynamics/fluxes of the end-products (research gap must be comprehensibly identified). Appropriate references must be cited. At the moment, it is only mentioned that the models were used with “success”. The fact that the use of the acetylene inhibition technique may lead to incorrect results does not prove that the denitrification sub-modules of biogeochemical models provide incorrect predictions.

l. 76-86: The first sentence (l- 76/77) should be left out. Instead, “specifically” in l. 83 should be deleted and the aims presented in l. 83-86 should be moved to the beginning of the paragraph (laboratory incubations are considered in the aims).

Materials and methods:

Some important information is missing.

l. 95: The soil classification system used (World Reference Base for Soil Resources) should be added and “organic matter” should be replaced by “organic carbon”

l. 97 and l. 110: More information is needed about how the soil samples were obtained. Using an auger, steel rings, a spade?

l. 97 and 111: Why were the soil samples sieved to 10 mm and not 2 mm? Soil chemical analysis are usually conducted on the fine-earth fraction (< 2 mm). No additional sieving for soil chemical analysis is mentioned.

Table 1: The number of decimal places should be consistent within the table, C/N ratios should be provided without decimal place. The unit of bulk density should be written as “g cm⁻³”; “CaCl₂” should be placed immediately after “pH” and not in the same line as the units of the other soil properties.

l. 111: Were the NO₃ and NH₄ concentrations also determined using air-dried soil material? Nitrate and NH₄ should be extracted as soon as possible after sampling, air-drying of the soil samples is not recommended. This may lead to erroneous results.

l. 117: How many replicates per treatment were used?

l. 118: Delete “then” before “added”

l. 120 reference to Fig. S.3: The order of the figures and tables in the supplementary material should be changed (Fig. S.3 should be Figure S.1, etc.)

l. 121: How was “water content kept constant”? 
I. 123-126 and l. 161/162: All information needed to understand and also interpret the results of the present study needs to be provided (even if they are already published), since some readers may not have the possibility to access the relevant article(s). Therefore, for all technical devices used, information about the model, the manufacturer and the location of the manufacturer’s headquarter should be added. The basic principle of the methods to determine NO3, NH4, etc. used should also be included; pH: Which solvent was used?

I. 125: “at the beginning”: Were the analyses conducted using pre-incubated soil material or the “original” soil material?

Table 2: The number of decimal places should be consistent within the table (bulk density, WFPS). The units of bulk density and water content are missing. All units must be written with squared brackets. The abbreviation “WFPS” has to be defined. What does the asterisks in the last columns mean?

Table 3: Tables 2 and 3 should be combined (see general comment on “Tables and Figures” above) and Table 3 left out.

I. 140: “C-to-N” should be replaced by “C/N” (cf. Table 1) and “nitrogen” by “N”

I. 149: At which days/time steps were gas samples collected manually?

Table 4: All units must be written with squared brackets.

I. 174-176: This is discussion material.

I. 189: I guess, NH4 would be correct (instead of NH3).

I. 207: Delete the colon

I. 215-217: This information would better fit in the Introduction.

I. 219: Table S.6 should be Table S.1, etc.

I. 259 “treatments”: There is only one treatment (ryegrass addition) and one control. “Treatments” should be replaced by “soil cores”.

I. 264: Which model parameters and settings were modified and how? More specific information must be provided.

I. 272-279: A clearer separation between silt-loam and sand soil is needed here.

I. 301: How was normality checked?

Results:

See general comment above on “Tables and figures”. There are several incorrect references to tables and figures.

I. 306/306: Delete reference to the Figures S. 3 and S. 4, since they do not show any results. Moreover, Fig. S. 4 depicts information about the WFPS of the sand soil, not of the silt-loam soil.
I. 309/310: The reference must be to Figure 1a (not S.1)

I. 311-313: The sentences should be combined (treatments III to V which were characterized by.....showed highest N2+N2O fluxes)

Table 5: The meaning of the letters needs to be explained.

Figure 1: How many replicates were measured? Standard deviations or errors should be included, if possible.

I. 339: Wrong and/or unnecessary references.

I. 340 "fluctuations in the CO2 fluxes": Is this information really needed here?

I. 344: The reference to Table S.2 should be replaced by information about relevant dates/time intervals.

I. 344/345 "Initially,...": This information is redundant and therefore not needed here.

I. 34/348: Is this information really needed here? What does “(09/02 and 14/02)” mean? The description do not agree with Figure 2a (N2+N2O: core 1 and 2 and limited core 3).

I. 375: “d-f” should be added after “Fig. 4”

I. 376-379: Where is this shown? Table 8?

I. 380: “and DNDC” should be added after “Coup”. The reference to Figure S.6 should be moved to the end of the sentence.

I. 391: “smaller” must be corrected to “higher”

I. 396-406: This paragraph needs to be revised. It is absolutely inconsistent. According to l. 396, it deals with “cumulative N2+N2O fluxes”. For Coup and DeNi, cumulative fluxes are described. However, for DNDC, there is a reference to Table 8 in which average fluxes are shown and l. 404-406 deal with Table 7 instead of describing the results shown in Figure 5 (cumulative fluxes). The explanation for the numbers in Table 7 is in the next paragraph (l. 407-413).

I. 431-434: See general comment on "Inconsistencies" above. The measured data shown may be partly incorrect.

I. 443: “are” should be corrected to “were”

Discussion:

References to figures and tables should be kept to an absolute minimum in the Discussion section (too many references are, for example, in l. 499, l. 501-503, l. 504-526, l. 545, l. 575-582). An informative summary of the results that are discussed in the following is sufficient., since the results were already described in detail in the Results section. Section 4.1.2 should be shortened. Not every change in gas fluxes must be explained in great detail. A more general description of the assumed processes and possible causes would be more useful.

I. 494/495: This section is confusing. According to the Materials and methods section, the
whole soil material was pre-incubated (not only the control soil).

I. 500-503: Shorter; the information provided here can be combined.

I. 505: delete “without organic...”; information not needed here (already known)

I. 505, I. 578: Delete “treatment” (the control is not a treatment)

I. 523/524: Delete the references to the Tables 6 and 1

I. 546/547: delete “because...fluxes. However,” (redundant)

I. 574: Change to “the results of DNDC did not reflect” (leave Coup out)

I. 578-582: The description of the results seems to be incorrect. In I. 578 it is mentioned that “40 % higher CO fluxes” were determined in the control of the sand soil compared to the ryegrass treatment. However, in the Figures 6f and 7f, the modelled and measured curves look quite similar and – according to Table 9 – the cumulative CO2 fluxes were around 10 % lower in the control. According to I. 581/582 “similar soil respiration and N2+N2O fluxes” were calculated by DeNi for the control and the ryegrass treatment of the sand soil. The description must be more specific. The course of the modelled fluxes look largely similar, but the modelled amounts of N2+N2O emitted which are addressed in the preceding text are not similar. With respect to the cumulative N2+N2O fluxes, DeNi calculated 32 % lower fluxes for the control (Table 9). In this respect, DeNi was comparable to DNDC (33 % lower cumulative N2+N2O fluxes for the control), not to Coup (10 % lower cumulative N2+N2O fluxes for the control).

I. 601-604: This paragraph should either be included in sub-section 4.2.4 or the sub-sections 4.2.3 and 4.2.4 should be merged.

I. 625-627: A reference should be added.

I. 644: Delete “(as was done in this study)”, since no data obtained using the Helium gas flow soil core method were used.

I. 648: “These models” should be replaced by “The models tested in the present study”

Conclusions:

I. 657/658: The focus of the present manuscript is not only on denitrification end-products, but also on CO2. It should, therefore, be mentioned here, too.

I. 657: “these....” should be replaced by “the biogeochemical models Coup, DeNi and DNDC”

References:

Del Grosso et al. (2000) is missing in the reference list.

Other references were not checked.
Supplementary Material

Figure S.4: The red line (mean values) and the blue areas (SD or SE?) must be explained.