Response to reviewers' and editor's comments

Associate Editor decision: Reconsider after major revisions
by Ben Bond-Lamberty
Comments to the author:
Thanks for your submission to Biogeosciences. This manuscript was read by two referees, who both provide thoughtful and in-depth comments. Referee 1 is positive overall but notes many aspects of the text, methods, and results presentation aren't clear, and asks about availability of the model used. Referee 2 is also positive but similarly notes problems with clarity in many areas; suggests doing a parameter sensitivity exercise (even a basic one would be valuable, I agree); and has good suggestions to improve the structure, and reduce repetition, of the discussion and conclusions. Both referees have many useful minor questions and comments.

I have read the manuscript and broadly agree with the reviewers. This is an interesting analysis in many respects, but it does need substantial revisions in many areas to address the issues raised by R1 and R2; I have reviewed your responses and think there's a reasonable path forward in this respect. Please note that it is crucially important to clearly describe the model calibration procedure. Also, in your response you provide a link to the model code on figshare. Thanks—this is useful! However, please improve it by (i) adding comments describing what each function does, (iii) making sure that all the manuscript equations are noted in comments in the code (e.g. "// This is Equation X in Li et al. 2022") and (iii) providing a full example of running the code for a site.

The revised ms will then be re-assessed by the referees if they are available.

*(Note: although I see you already provide a revised ms, I have not looked at this yet, as it's supposed to be uploaded *after* considering this decision.)*

>>Thanks for your time.
First of all, the reviewers' comments were fully incorporated into the revised MS accordingly.
Moreover, according to your comments, we added the description about each function into the model code on figshare and matched each function in the code with the equation in the revise MS.
Furthermore, we provided and revised the documentation (Readme.txt) to illustrate how to run the executable file at the example site (Changshu).

A brief introduction to the revision of the manuscript (MS) as follows:

In the revised MS, the reviewers' comments were fully incorporated into the text accordingly. The text of the MS was revised by us: i) providing more details of the original model and the modifications; ii) reorganizing and rewriting the Abstract, Results and Discussion sections; iii) the sensitivity analysis for the parameters of the improved model was added. Furthermore, we recompiled the Supplementary materials by adding Table S1 and S2 to present the equations and symbols of the regulatory factors affecting NH_3 volatilization from uplands in the original and modified CNMM-DNDC.

Referee #1:

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

The paper present results of a modified version of DNDC-CMMM to better represent the NH_3 volatilization of paddy rice field and upland crop. Considering the importance of N cycles in soil biogeochemistry and of NH_3 emissions in global change the paper seems within the scope of BG.

>> Thanks.

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

The paper improve existing model of N emissions for two types of cultivation and performed sensitivity analysis to several environmental factors. In this way, tools and findings are novel.

>> Thanks.

3. Are substantial conclusions reached?

Yes, however it is a bit difficult to follow which simulations are considered as valid and which one are considered as non relevant. Maybe a table or few clear sentences to sum up might be helpful.

>> Fully agreed. In the revised MS, we summed up the performance of the original and modified models in a newly-added separate subsection. Please see changes in the 3.4 subsection.

4. Are the scientific methods and assumptions valid and clearly outlined?

The methods are well detailed, however the authors combined 3 different models (DNDC, CNMM and Jayaweera-Mikkelsen) while only Jayaweera-Mikkelsen model is accompanied by a schema. In my opinion, taking into account the numerous processes involved in each model and the successive optimizations performed by the authors, a complete scheme of the full model including the parameters used by default or optimized could be helpful.

>> Fully agreed. Our MS was based on the application of CNMM-DNDC model regarding the prediction of NH_3 emission from soils. The original model has a NH_3 algorithm. The attempt in this MS was to incorporate the J-M algorithm into the CNMM-DNDC to improve its performance for the NH_3 prediction. As

the result, we revised the statements regarding the descriptions of the original model and the modifications. Please see changes in Lines 143-146.

5. Are the results sufficient to support the interpretations and conclusions?
The results are well detailed but the difference in the Fig 3 to 5 is not very clear for me. Also, a comparison of the NH_3 volatilization sensitivity to environmental factor between rice paddy field and upland crops might be interesting. I found that the 4.1 title does not precisely correspond to the paragraph and that the 4.3 is a bit long and difficult to follow.

>> Fully agreed and revised the MS accordingly.

- **i) we added the detailed description regarding the difference of Figs. 3-5. And the cases with the same observed variables were associated in a figure for unified formatting. Please see changes in Lines 444-446.**
- **ii) we rewrote the title of the 4.1 subsection and reorganized the Discussion section. Please see changes in the Discussion section.**
- **iii) we are sorry for missing out the title of 4.3 and jumping the titles from 4.2 to 4.4. We renumbered the titles and reorganized the Discussion section to make it more readable in the revised MS. Please see changes in the Discussion section.**

6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?
I think all the data and results are provided, however, as noticed above the numerous processes and step involved in modification make it difficult to evaluate without a complete scheme (especially because several parameters were took from other model).
Also, it is not very clear if the data of re-calibration was the same than used in the last version of DNDC of Li et al., 2019 (l.117). Several parameters have been recalibrated (l. 168 to l.176) without mentioning how they were recalibrated (algorithms and data).
Also, I don't understand why the time conversion factor is 0.75 (so not a ratio of the two initial models time step) while one model is based on 3 hours and the other on 24 hours.

>> Agreed and revised the MS accordingly.

The two new Table S1 and S2 were added to present the equations and symbols of the regulatory factors affecting NH_3 volatilization from uplands in the original and modified CNMM-DNDC. Please see changes in the Supplementary materials.

The sensitivity analysis of the improved parameters was added. Please see changes in Fig. 8 and the 2.4 subsection.

The calibration and parameterization of the regulating factors except f_{depth} and f_{Tstep} were adopted from Dubache et al. (2019) and Li et al. (2019). Please see changes in Lines 189-190.

In this revised MS, the zero-intercept linear regression was applied for the calibration of f_{depth} and f_{Tstep}. Please see changes in Lines 200-210. In Fig. S2, we

provided the calibration process of f_{Tstep} as an instance.

The ratio of time steps of the two models (T_{layer}, with the value of 8) was involved in the modified model. But T_{layer} was missed out in Eq. (1) in the original MS due to our negligence. We are sorry for that. In the revised MS, we added the ratio of time steps (T_{layer}) of the two models into Eq. (1). Nevertheless, the deviation derived from the different time steps existed, as shown in Table S3. To solve the above deviation, a time-step parameter (f_{Tstep}) was introduced into Eq. (1) and the calibration process of f_{Tstep} was provided. Please see the new added Fig. S2.

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

For the major parts of the manuscript their is enough references, however the 4.4 lack of some references

>> Fully agreed. We added several references and sentences to support the subsection 4.3. Please see changes in the subsection 4.3.

8. Does the title clearly reflect the contents of the paper?

Yes

>> Thanks.

9. Does the abstract provide a concise and complete summary?

Yes but maybe the description of the sensitivity analysis could have been a bit more longer. Also, the validation part is presented after the sensitivity analysis in the abstract while in the results it came afterwards.

>> Agreed and revised the abstract accordingly. Please see changes in Lines 27-42.

10. Is the overall presentation well structured and clear?

The results are relatively clear except that in my opinion the fig 6 should be cited earlier in the text while comparing the model performance. Also, large part of the results focused on ABC treatment which is only 2 sites, in my opinion the results for others amendment are more robusts. The material and methods part is long and, as mentioned above the model and model parameter fitting is complicated to follow. The material and methods sections on data analysis are much clearer.

>> Fully agreed and revised accordingly. As a result, we summed up the performance of the modified model in a newly-added separate subsection 3.4 and especially focused on the performance of the model in simulating NH_3 volatilization from urea application. Please see changes in the 3.4 subsection.

In addition, Table S1 and S2 were provided to present the equations and symbols for the simulation of NH_3 volatilization from uplands in the original and modified CNMM-DNDC. Please see changes in the Supplementary materials.

Is the language fluent and precise?

Yes

>> Thanks.

11. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

Yes

>> Thanks.

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

As mentioned above the fig 3 and 5 are similar and a conjugated presentation of these two figures would be easier. Also, I there is several subplot in each of them but the whole figures seems somehow similar. Also, the text police is not the same in the whole manuscript, please adjust.

>> Fully agreed and revised accordingly. Please see changes in Lines 444-446.

We also double-checked the whole MS carefully and adjusted the inconsistent expressions throughout the revised MS.

13. Are the number and quality of references appropriate?

Yes

>> Thanks.

14. Is the amount and quality of supplementary material appropriate?

I would have appreciated if the model the authors build was available for re-use.

>> Agreed. The code and executive program of the modified model can be obtained from http://doi.org/10.6084/m9.figshare.19388756. Please see the additional descriptions in Lines 757-758.

Referee #2:

The authors describe an update to the CNMM-DNDC model to improve ammonia emission simulations. First, they performed a calibration and parameterization across upland agriculture sites. Second, they added a new algorithm to simulate ammonia emissions from rice paddy fields with flood irrigation. Finally, the authors conduct a sensitivity study to analyze the contributions to ammonia emissions over a variety of environmental factors (including atmospheric conditions, soil properties, and management of irrigation and fertilizer).

The manuscript is novel in that it brings a new management practice, flood irrigation, into a biogeochemistry model for calculation of ammonia emissions. This is a valuable addition to the field and should be considered in future models because of the differences in volatilization from management practices. I think the paper is well written and interesting and fits in the Biogeosciences scope. However, the paper could benefit from some additional clarification before it is ready for publication.

>> Thanks. We revised the MS strictly according to reviewers' comments as follows.

General comments:

Line 47-50: Might also want to mention efforts in ESMs such as Riddick et al., 2016 and Vira et al., 2020.

>> Revised. Please see changes in Lines 56-57.

Line 63: "dose and application methods…" The type of fertilizer used (e.g., manure vs. synthetic fertilizer) will also have an effect on volatilization of NH_3.

>> Revised. Please see the change in Line 71.

Line 102-104: The algorithms were already in the model, my understanding from reading the manuscript is they calibrated and parameterized the model further. However, this is never fully explained in the text under the materials and methods section.

>> Revised. The calibration and parameterization of the regulating factors except f_{depth} and f_{Tstep} were adopted from Dubache et al. (2019) and Li et al. (2019). Please see changes in Lines 189-190.

In the revised MS, the zero-intercept linear regression was applied for the calibration of f_{depth} and f_{Tstep}. Please see changes in Lines 200-210. In Fig. S2, we provided the calibration of f_{Tstep} as an instance.

Materials and methods section, I suggest organizing this differently. The authors start with a description of the sites, but I think it would be better after the model description, but this is optional

>> Fully agreed and revised. Please see changes in the subsections 2.1 and 2.2.

Line 155: What regional scale simulations were performed?

>> Revised. The objective of this study was aimed at modifying the CNMM-DNDC and evaluating the performance of the modified model at the site scale. The regional scale simulation was not tested and will be continued in the future. Therefore, we only conducted the site scale simulations in the MS and we rephrased the sentences to clarify. Please see changes in Lines 170-171.

Section 2.2.2:

The authors indicate recalibration and parameterization, but don't indicate how this was done or which components were included in the process.

Line 267-272: As noted previously, can the authors provide a description of the method used to calibrate the model? More explanation is needed for the process used to calibrate parameters.

>> Revised. The calibration and parameterization of the regulating factors except f_{depth} and f_{Tstep} were adopted from Dubache et al. (2019) and Li et al. (2019). Please see changes in Lines 189-190. In the revised MS, the zero-intercept linear regression was applied for the calibration of f_{depth} and f_{Tstep}. Please see changes in Lines 199-210. In Fig. S2, we provided the calibration of f_{Tstep} as an instance.

Were NH_3 emissions calculated differently from different fertilizer applications (e.g.., manure vs. synthetic fertilizer or urea vs. ABC) or was only synthetic fertilizer applied at the sites?

>> Revised. Different fertilizers (e.g., urea, ABC and other synthetic fertilizers) were simulated separately in CNMM-DNDC model. Please see changes in Lines 174-180.

In fact, since the authors don't introduce the original model, it is difficult to understand the significance of the modifications to upland volatilization. Perhaps the authors can expand this section or include a supplement that provides more detail on the original and modified algorithms. Also, how the f values are calculated is also missing in the documentation.

For eq 1, how does the depth of the fertilizer application play a role in the NH_3 flux?

>> Revised accordingly. We introduced the original CNMM-DNDC model in simulating NH_3 volatilization from uplands, described in Lines 174-180. Meanwhile, Table S1 and S2 were added to present the equations and symbols for the simulation of NH_3 volatilization from uplands in the original and modified CNMM-DNDC. Please see changes in the Supplementary materials.

Because there isn't a good introduction to the initial model, I am left to wonder about the role the parameters play in the emissions process and how sensitive the model is to parameter modification. This would be another good opportunity for a sensitivity analysis. Also, are the final parameter values used for all the sites or are they site/environment specific. Perhaps include a table of the parameters changed and

their initial and final values would help.

>> Revised. The sensitivity analysis for the parameters of the improved model was added. Please see changes in Fig. 8 and subsection 2.4.

Section 2.4: I think it would also be interesting to look at a sensitivity of the model parameters as well. This would provide an indication of which parameters have the largest influence in the model simulations of emissions and which parameters are

>> Revised. The sensitivity analysis for the parameters of the improved model was added. Please see changes in Fig. 8 and subsection 2.4.

Section 4:

The section begins with discussion of the factors affecting emissions and moves into why the model performs poorly for certain conditions. Perhaps split into two sections or separate in different paragraphs.

Section 4.2 begins by unnecessarily repeating methods (line 473-483), and again discusses model limitations rather than influences on emissions as the section heading suggests.

I suggest a separate section for model limitations or changing the header of 4.1 and 4.2.

>> Fully agreed and revised. We reorganized the Discussion section and rephrased the titles and the contents as well to make them more readable. Please see changes in the Discussion section.

Section 4.4 reads more like a conclusion than the actual conclusion in the paper.

>> Fully agreed and revised. We rewrote this section, which currently it is Section 4.3 in the revised MS. Please see changes in Lines 673-720.

The conclusion feels like more of an abstract and repeats methodology.

>> Agreed and revised. We rewrote the Conclusion section. Please see changes in the Conclusion section.

Data availability: Providing model output is useful but does not allow duplication of this effort. A suggestion would be to provide the actual model used by the authors.

>> Revised. The code and executive program of the modified model can be obtained from http://doi.org/10.6084/m9.figshare.19388756. Please see the additional description in Lines 757-758.

Technical comments:

Line 16-18 (and elsewhere): "...evaluated and modified using NH_3 volatilization observations from 44 and 19 fertilizer application events in cultivated upland areas and paddy rice fields in China, respectively." The wording is slightly confusing. I suggest "evaluated and modified using NH_3 volatilization observations from fertilizer application events in 44 cultivated upland areas and 19 paddy rice fields in China."

>> Response. The NH_3 volatilization observations from 44 and 19 fertilizer application events used in the MS were collected from 6 upland sites, 4 paddy rice sites and 1 site with upland and paddy rice area. Placing the numbers of 44 and 19 in front of fertilizer application events were more accurate. Therefore, we retained the expression of '44 and 19 fertilizer application events' instead of 44 cultivated upland areas and 19 paddy rice fields.

Section 2.1: The authors should reference Table S6 when discussing the upland sites.
>> Corrected. The citation was added in Line 308.

Line 451: is missing a space between placement and 5.
>> Corrected. Please see the change in Line 556.

Text is awkward, particularly Line 452-454.
>> Agreed. We rewrote the mentioned sentences and shortened other long sentences throughout the MS. Please see changes in Lines 557-559 and Lines 143-146.

Section 4.3 is missing; the titles jump from 4.2 to 4.4
>> Corrected. Please see changes in Line 673.

References:
Riddick, S., Ward, D., Hess, P., Mahowald, N., Massad, R., and Holland, E.: Estimate of changes in agricultural terrestrial nitrogen pathways and ammonia emissions from 1850 to present in the Community Earth System Model, Biogeosciences, 13, 3397–3426, https://doi.org/10.5194/bg-13-3397-2016, 2016.
Vira, J., Hess, P., Melkonian, J., and Wieder, W. R.: An improved mechanistic model for ammonia volatilization in Earth system models: Flow of Agricultural Nitrogen version 2 (FANv2), Geosci. Model Dev., 13, 4459–4490, https://doi.org/10.5194/gmd-13-4459-2020, 2020.
>> Revised. The above two references on CESM were added in the reference section and cited in the text. Please see changes in Lines 56-57, Lines 909-911 and Lines 930-932.