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Interactive comment on “The effect of aggregates on N₂O emission from denitrification in an agricultural peat soil” by P. C. Stolk et al.

J. Léonard (Referee)

leonard@laon.inra.fr

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This is a very interesting paper which focuses on the modelling of N₂O emissions, and especially on modelling the complex behaviour associated to the coexistence of very different environmental conditions and processes in the same volume of soil at a given time. Daily variations in N₂O emissions are often very difficult to simulate, and difficulties due to the influence of many control variables are accentuated by the fact that emissions both depend on the production in the soil and on the transfer between different zones in the soil and to the atmosphere. The strong dependence of emissions on transfers mainly results in the frequent occurrence of a variable lag time between production and emission as well as through the spreading, smoothing and even attenuation of peak emissions.

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The authors propose here a conceptual way to deal with this complexity through the distinction between a mobile and an immobile compartment in the soil, the distribution of the different processes between these compartments and the description of exchanges between them. This is not completely new as there is for example a similar conceptualization in the DNDC model where the soil is dynamically partitioned into an aerobic and an anaerobic component. However the author argue that their proposed approach has the additional advantage that the parameterization controlling the partition between the mobile and immobile component can be based on soil structure observations. An approach also focusing on the role of soil structure, where the size distribution of clods is used as a model input, had been tested by P. Renault and colleagues from INRA a few years ago and integrated into the PASTIS model (http://w3.avignon.inra.fr/pastis/description.php?module=den&trad=en_GB).

The title of the paper is a little bit misleading: it may suggest for example an experimental analysis of the effect of aggregates on N₂O emissions from denitrification, which is clearly not the case. “effect of aggregates” is also a bit exaggerated in my opinion as aggregates are here considered in a very conceptual manner and from a modelling approach only. I would suggest a title more like : “Modelling the effect of soil structure on N₂O emission of a peat soil with a mobile-immobile approach”, which would insist on the fact that this is a modelling work, and on the specificity of the model.

I think that the paper could be significantly improved through two main axis: i) a better description of the model and the concepts used (I will make suggestions below); ii) giving more room in results for the analysis and interpretation of the changes induced by the incorporation of the mobile-immobile concept in the original SWAP-ANIMO model.

For what concerns the first point, I would suggest:

- to include a scheme of the mobile-immobile model, showing the compartments, how the processes are distributed into these compartments, the fluxes which are considered (of course with a focus on what is related to N₂O production, consumption and

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emissions). That would be of great help as a complement to the description in the text; - to focus right from the start on the mobile-immobile model, the hypothesis, description of where processes occur and why, what fluxes and exchanges between compartments are considered (using the scheme to hep), so that we could have quickly a general view of that original part of the modelling work. In addition, the equations will be easier to understand for the reader if he already has a complete conceptual scheme in mind and if the variables used already have a meaning. I think the integration of the mobile-immobile sub-model into the general SWAP-ANIMO model should be presented only after; - to better separate what concerns the description of the model itself and what concerns its numerical resolution.

I would also appreciate to have figures illustrating some of the proposed relationships such as eq. 10 and 11 for example, or at least tables with parameter values or range so that the reader could visualize the functions if needed.

Finally, reference to the work of Hendriks et al. for further information on some aspects of the model (especially the section on N₂O production and reduction) is somewhat problematic as it is not easily available to the reader (unpublished report).

As regard to the second point, I think that figure 1 is not sufficient to really analyse the improvements brought by the incorporation of the mobile-immobile approach and reasons for eventual better performances (this is accentuated by the fact that the y scale in figure 1 does not allow for an accurate comparison between the different plots). Careful observation of figure 1 shows that despite gas transfer between the immobile and mobile compartment is now taken into account, that does not always result in better simulation of the lag between observed and simulated fluxes. There are also long periods with rather bad performances (for example between day 250 and 270), which should be commented. The statement that the improvement is 'spectacular' is thus a little bit exaggerated. The main interest of this work is in my opinion how the introduced modifications which allow to take into account the effects of soil structure can result in better simulation of emissions. I would thus like very much to see a

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more in depth comparison between the original and new model, showing also how nitrification and denitrification rates are modified, comparing production/consumption of N₂O between models and showing the effect of gas transfer on the transformation of N₂O production into N₂O emissions.

I list below some additional questions or comments which arose during the reading of the manuscript, and I hope that my questions, comments and suggestions will help improve the manuscript so that it could be published, which I would like very much, considering its interest to help us going a step forward in understanding and simulating N₂O emissions.

- Some parameters were calibrated in the case of the new model, but was it the case also for the simulation with the original model ? This is important to know exactly what is compared, and if possible to compare both models with a very close set of parameters.
- Does the introduction of new input parameters associated to the incorporation of the mobile-immobile approach induced some changes in the original parameter set (other than the new ones) ?
- The quantitative evaluation of both differences between simulations and between a given simulation and observations (through R₂, RMSE...) is not so obvious because any lag time between signals will have an influence on the estimation of the error. For example, it may be possible to have quite similar results between two situations with respect to the general tendencies and amounts of emissions, but a significant time lag can result in low R₂ and RMSE. How do you manage this difficulty ? (note that this is a potential interest of your improved model to have more phased signals between simulations and observations).
- 3255 l. 8-10 : because they often last for long time, background emissions can also contribute significantly to total emissions, this is why they are important to consider.

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- 3256 l. 11-19 : this is an interesting discussion about the interest and need for models that consider explicitly the effect of soil structure. I agree with the general idea, but we generally end with a more sophisticated model, with more parameters, that often are not really measurable and thus are also to be calibrated. I think the real interest of such models is rather on testing our understanding of the processes than on being used as such for prediction. They may be also useful for deriving better simplified models.

- 3256 : the description of the different models of soil structure is a little bit superficial, which makes it not so useful. What are the main differences between these approaches ? the potential consequences ? Maybe you should focus more directly on the mobile-immobile approach, and explain more in depth its interest.

- 3257 l. 4 : you mention three zones; what is the third one when there is one ? l. 12-13 : there exists at least one example (http://w3.avignon.inra.fr/pastis/description.php?module=den&trad=en_GB). but I did not find a corresponding publication.

- 3258 l. 16-17 : details on how aeration status is estimated would be useful.

- 3260 l. 2-3 : all vertical *gas* transport ?

l. 7-8 : 'Therefore all air filled pore space is assigned to the mobile zone and the immobile zone is always water saturated'. What happens when the water content change ? For example, when the immobile compartment volume decreases, does the N₂O present immediately become available for diffusion through the mobile compartment to the atmosphere ?

l. 8-9 : what exactly do you mean by "stagnant" ?

- 3262, eq. 10 and 11 : an illustration or a table with parameters values would be useful to help visualize the functions.

- 3262 l. 12 : 'The implicit assumption is that all reduction of NO₃ is located in the immobile zone and that the aggregates do not hamper NO₃ diffusion'. This assump-

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tion appears a little bit late. It would be preferable that all assumption be stated at the beginning of the model description, with the accompanying scheme.

- 3262 l. 19-24 : how do we know which of NO₃ or OM is limiting denitrification ?

- 3265 l. 26-28 : what is the method used to estimate the size of aggregates ?

-3266, Values for input parameters : it is not clear if calibrated parameters are the same for both the original and new model. Also, was the calibration done over the entire dataset ?

- figure 1 : the y range is very large, and it's difficult to really compare observations and simulations. Maybe crop the y range to the max of observed emissions ?

Discussion :

- 'Another advantage of this concept is that the parameterization is based on soil characteristics and that input values can be derived from observations'. This is not so obvious, aggregate size is not very easy to determinate, and the method used for that was not explained.

- The sensitivity to the aggregate size parameter seems very high (that was also a result obtained with the PASTIS model). That raises again the question of the necessity of a calibration (like in simpler more empirical models). I am thus not sure that we will gain predictive power through the incorporation of a more complex model taking into account soil structure. However, we will certainly gain a deeper understanding of the processes at work and potential consequences, and that is probably the main interest of the incorporation of the mobile-immobile approach.

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