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## ***Interactive comment on “The effect of aggregates on N<sub>2</sub>O emission from denitrification in an agricultural peat soil” by P. C. Stolk et al.***

**R. Grant (Referee)**

robert.grant@ales.ualberta.ca

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This work is a potentially useful contribution to the field of N<sub>2</sub>O modelling in that it addresses a key transfer mechanism that affects N<sub>2</sub>O emissions but which is overlooked in most (but certainly not all) earlier modelling studies. I think that this contribution could be enhanced if the following key points could be addressed in the paper before publication:

1. How temporally variable are N<sub>2</sub>O emissions and therefore what is the most appropriate time scale at which they should be modelled? There is good experimental evidence that diurnal variation can be large, because the environmental conditions by which emissions are driven (SWC, temperature) can vary greatly within a day. Perhaps such evidence is apparent in the EC measurements used in this study (1/2-hourly,

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hourly?), only daily-aggregated values of which were presented in the paper with no description of aggregation methodology. What is the basis and justification for selecting a daily time step in this model?

2. The effects of O<sub>2</sub> uptake on electron transfer rates that drive denitrification need to be further described. Is the immobile zone assumed to be completely anaerobic? How do varying SWC and temperature affect anaerobicity in the mobile and immobile zones? This may have been described earlier papers, but given its importance to the results, should be given here.
3. Include precipitation and fertilization events and SWC in Figs. showing N<sub>2</sub>O emissions to help readers understand model behaviour.
4. Parameterizing transfer functions as done in Eq. 13 for Eq. 12 is always problematic. Clearly the model results are extremely sensitive to the value for alf in Eq. 13. How well constrained is this value from independent observations? Was this value fitted to the model to give the results in Fig. 1? If so, then the model with this value of alf must be further tested against independent measurements to establish its robustness before the model can be applied.
5. Distinguish more clearly between model and experimental findings.

These points are made with more specific reference to the paper in the comments below:

#### Abstract

3254 l. 2: 'as couple of days'

3254 l. 12: 'The results of this study showed that aggregates strongly affect N<sub>2</sub>O emissions ...' Do you mean aggregates in the model?

3254 l. 15-16: Give more quantitative description of measured vs. modelled N<sub>2</sub>O flux ranges, and evidence of improved agreement such as greater R<sup>2</sup>, smaller RMSD.

**BGD**

8, C1408–C1412, 2011

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3254 I. 19-21: 'The effects of changing conditions on reduction of N<sub>2</sub>O relative to N<sub>2</sub>O production is dependent on the NO<sub>3</sub> content of the soil' This is rather vague. Specify these effects.

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Introduction

Method

3258 I. 11-14: Given the large diurnal variation in N<sub>2</sub>O emissions, and of the their highly non-linear relationships with drivers such as temperature, water content and gas exchange, a daily time step seems too long. An hourly or sub-hourly time step would be more appropriate.

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3259 Eq. 1: The earlier modelling approach assumed instantaneous equilibrium between aqueous and gaseous phases, represented by the Bunsen solubility coefficient. Note that this coefficient is very temperature sensitive, and that temperature varies diurnally.

3260 Eq. 4: There are 2 key parameters with unconstrained values: FIM,max and 0.95. Sensitivity to these parameters will need to be examined. I see that this is done later.

3262 Eqs. 10, 11: Shouldn't the coefficient for NO<sub>3</sub> be 2/14? The rationale for these eqns needs more explanation, particularly the calculation of Rpr,el and its sensitivity to O<sub>2</sub>. I had expected to see an actual affinity parameter (e.g. Km) for both NO<sub>3</sub> and N<sub>2</sub>O, rather than a relative one for N<sub>2</sub>O.

3262 I. 11-12: Why should cNO<sub>3</sub> be the same in both aqueous zones while cN<sub>2</sub>O is not? I see that this is explained later in the Discussion, although it could be mentioned here. I found this assumption to be somewhat arbitrary.

3262 I. 16-19: The lack of an O<sub>2</sub> effect on N<sub>2</sub>O:N<sub>2</sub> under these conditions is a big assumption, and not consistent with experimental evidence.

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3262 l. 22-24: Actually there is a delay between  $\text{NO}_3$  reduction and  $\text{N}_2\text{O}$  production during the generation and reduction of intermediate e- acceptors  $\text{NO}_2$  and  $\text{NO}$ . Perhaps the absence of these steps in the original model caused the rapid onset of emissions.

3263 Eq. 12: This sort of eqn is best solved by considering both water volumes to ensure that gradient reversals do not occur.

3263 Eq. 13: Values of beta and alf will give  $k_{tr} > 1 \text{ d}^{-1}$  in some cases. Are these value constrained in any way? These are clearly key parameters that will determine model behaviour.

3263 l. 20: Do you mean eqs (12) and (14)?

3264 l. 7: conform?

3265 l. 17-20: What was the frequency of measurement?

## Results

3267 Fig. 1: How were the short-term EC measurements aggregated into daily values? This absolutely needs to be described before the paper can be published. Also show dates of rainfall, fertilizer or manure application, SWC if available. These are needed to understand ecological controls on the emissions. In this Fig., would total  $\text{N}_2\text{O} + \text{N}_2$  production be similar in both model formulations? What  $\text{N}_2\text{O}:\text{N}_2$  ratios were generated, and how realistic were they with changing SWC? Can these ratios be inferred from Figs 3, 4 and 5?

3268 Fig. 2: It would be helpful if the direction of the relationship between model inputs and outputs were indicated (+ve or -ve).

3269 Figs. 3, 4: Model results are clearly very sensitive to alf, likely because it is squared when calculating  $k_{tr}$ . Were the results in Fig. 1 achieved by fitting the value of alf? How well constrained is this value by experimental evidence? Is there an

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independent test of the value used in this study?

3269 l. 7-14: Clarify that these are findings from model results. What experimental evidence exists to corroborate these findings?

#### Discussion

3269 l. 25-27. The effects of compaction on BD will affect simulated denitrification through the parameter p2 in Eq. 9, even without considering aggregate size.

3271 Fig. 5. Again, data for precipitation and fertilization events, and SWC would help readers understand the model response to Ksat.

3272 l. 9-10: Check wording.

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