Comment to the paper „Evaluation of a new inference method for estimating ammonia volatilisation from multiple agronomic plots"by Benjamin Loubet et al.

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This paper presents an appealing and low-cost approach to determine NH_3 losses from adjacent multiple agronomical plots by a combination of concentration measurements using passive sampler devices and a dispersion model that is driven by turbulent parameters inferred from standard 30 minutes meteorological data.

The aim of the paper is described as: *"Can inverse dispersion modelling approaches be used for inferring NH_3 emissions from multiple small plots (agronomic trials) using passive samplers, and to which degree of accuracy?"*

The overall answer is encouraging with the statement in the conclusions *"In this study we have demonstrated that it is possible to infer with reasonable biases ammonia emissions from multiple small fields located near each other using a combination of a dispersion model and a set of passive diffusion sensors which integrate over a few hours to weekly periods".*

According to our judgement the accuracy will be mainly determined by two aspects addressed below.

a) Bias related to the applied dispersion modelling

Dispersion models are a simplified mathematical representation of the turbulent motion in the surface layer and will always deviate from reality. Systematic biases can be expected when modelling the lower heights of the measurements that are discussed in this paper. For concentration sensors place close to the ground (e.g. 25cm above ground) transfer functions are likely to be biased due to e.g. the needed simplifications that must be made to describe the exchange process at the ground, the natural heterogeneity on a small scale at the surface or the violation of model assumptions such as the failure of K-theory close to the canopy (Raupach and Legg, 1984). Furthermore, the translation of the sensor height in a model framework is challenging for very low heights since the sensor height value (and with that the resulting value of D at that location) becomes very sensitive to sensor height measurement errors as well as to the absolute values of z0 and d. To us, a sensor height of 25 cm seems too close to the surfaces.

The authors are using their FIDES-3D model that is based on an analytical solution of the advection-diffusion equation. This model is compared with the backward Lagrangian Stochastic dispersion (bLS) model described in Flesch et al. (2004) (the "WindTrax" software, Thunder Beach Scientific, Nanaimo, Canada). For the presented analysis the FIDES model K_z was adopted to match the far field approximation of K_z of the bLS model. We are missing an explanation, why this was done.

In the supplement, a detailed investigation is presented how the two models differ in their formulation of the vertical diffusivity K_z. The assumed far field vertical diffusivity in the bLS model is approximated by parametrizations provided in Flesch et al. (1995). We would like to remark that WindTrax uses slightly different default parametrizations of σ_w than provided in Flesch et al. (1995) (see e.g. the manual on the WindTrax homepage1). This is resulting in vertical diffusivities given as:

$$K_z(Z) = 0.5 * 1.25 * u_* Z/(1 + 5Z/L) \qquad \text{for z/L} \geq 0$$

$$K_z(Z) = 0.5 * 1.25 * u_* Z \times (1 - 6Z/L)^{0.25}(1 - 3Z/L)^{(1/3)} \qquad \text{for z/L} < 0$$

with a Schmidt number value of $Sc \cong 0.64$ for near-neutral stabilities with a smooth transition from L = ∞ to L = -∞. These equations differ from the equations S7 and S8, and imply a different interpretation of the differences between FIDES and WindTrax, though without changing the numeric results of the comparison.

In the supplement Figure S3 presents a comparison between evaluated concentrations with FIDES and WindTrax respectively using the prescribed emission sources with the SVAT model. This figure is hiding the apparent differences as a double logarithmic representation is used and the concentrations are shown using an emission source that shows a positive correlation between the meteo input parameters of the models and the source strength. E.g. for neutral conditions the regression of ratio of the concentrations calculated with FIDES and WindTrax at a height of 0.25m is indicated as $c_{FIDES} = 0.97 \cdot c_{Windtrax}{}^{0.87}$. For a concentration of 1 the ratio is 0.97 and for a concentration of 100 the ratio becomes 0.53. As the transfer function D in FIDES and WindTrax are only depending on the prevailing turbulent parameters it would be more instructive to use a constant unit emission of 1 and show the ratio on a linear scale as function of u* and L in a similar way as the authors have done in a previous paper (Carozzi et al., 2013).

b) Bias related to the concentration measurements

The use of passive diffusive samplers is a challenging business. Within different networks the reliability of PS such as ALPHA samplers or Radiellos have been proven, but the use of them close to emitting source showed major deviations compared to other measurements. E.g. Misselbrook et al. (2005) found severe overestimations of passive diffusive samplers. The latest investigation stems from the Dronten experiment and is discussed in a paper by Michael Bell et al. (submitted to AFM). In this experiment the ALPHA samplers were affected by a positive bias in the order of 50% relative to the other devices. We speculated that the exposure of the PS with the protection hat above them cached eddies from below loaded with higher NH_3 concentrations but shielded eddies with lower concentrations from above.

Figure 1 illustrates the NH_3 dynamic that occur over an emitting surface. The concentration was measured with a fast device described in Sintermann et al. (2011). Immediately after application of slurry with a splash plate the NH_3 concentration was measured at a height of 1m above ground with an ionization technique and a strongly heated inlet line to avoid as much as possible damping effects.

[1] http://www.thunderbeachscientific.com/downloads/atmosphericdata.pdf

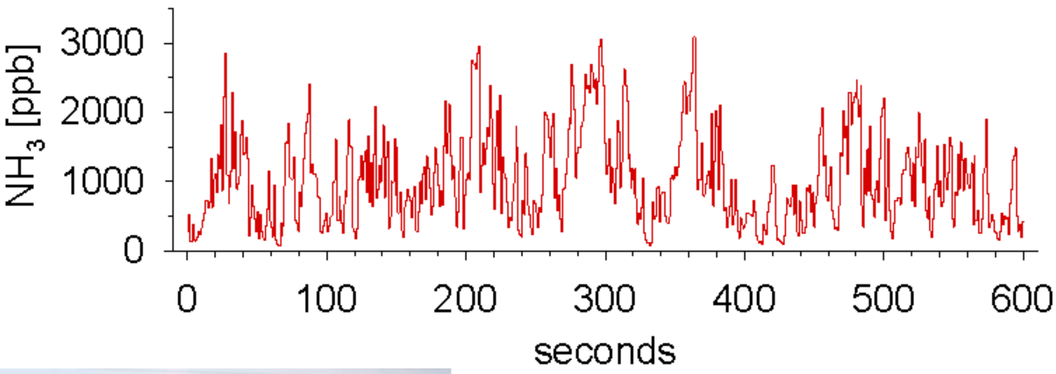

Figure 1: NH_3 concentration timeseries measured 1m above ground over a manured surface with splash plate.

Concluding comments:

We judge that the most important potential biases of the proposed multiplot approach are related to biases of the concentration measurements and the used dispersion coefficient. It would be instructive to calculate probability density functions of the estimated emissions with a dataset that reflect the distributions of the measurements and the turbulence parameters that drive the dispersion model.

The authors have tested their setup in field trial in April 2011 applying slurry with a DM content of 6% and an application rate of 41 kg N-NH_3/ha. According to the details given in the text, we assume that broadband application was used and was compared to fast incorporation and no application. The cumulated loss amounted to 8 to 10% of the applied NH_3. For broadband application, this is a loss on the low side (see e.g. Häni et al.,2016). We would not be astonished if the real emissions would be double as high.

The presented approach to perform NH_3 emission measurements in a multiplot arrangement is encouraging and goes in a good direction. To make the approach more robust, the employed ALPHA NH_3 sampling systems should be validated under real conditions, i.e. over an emitting source in comparison with e.g. MiniDOAS systems (Sintermann et al., 2016).

Finally, we would like to invite the authors to collaborate with us to compare the FIDES and WindTrax approach. We have an extensive dataset from field trials where we released CH_4 or a mixture of NH_3 and CH_4 from a circular artificial source with a diameter of 20 meters (Häni et al., 2017).

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