# Can we estimate ammonia emissions by inverse modelling with time averaged concentrations?

Loubet B.[1], Génermont S.[1], Personne E.[1], Massad R.S.[1]
(1) UMR EGC, 1091 INRA-AgroParisTech, 78850 Thiverval-Grignon, FR.

## Context

• Atmospheric ammonia ($NH_3$) is a major threat to the environment. It is mainly emitted by agricultural activities, especially following organic and mineral fertilization.

• There is still a need for a method easy to deploy under real conditions, to better characterize the variability of $NH_3$ emissions with respect to agronomic practices. This implies many repetitions. The use of micrometeorological methods is therefore difficult as it requires large fields, although the development of COTAG methods is promising (Famulari et al. 2004).

• One option is the use of the inverse modelling approach such as Windtrax (Flesch et al. 2004) or the FIDES model of Loubet et al. (2010). However such an approach requires to measure $NH_3$ concentrations at a hourly time step. Unfortunately there are no low cost $NH_3$ analysers to deploy over several fields.

• The use of passive diffusion sensors (alpha badges, Sutton et al. 2001) is a very easy method to deploy over a large number of locations. However these sensors need a longer time integration to allow sufficient quantities of $NH_3$ to be captured on the acid coated filters.

## Objectives

The objective of this study is to evaluate *in silico* the feasibility of using diffusion samplers to estimate ammonia emissions from individual bare soils fields. This method is thereafter called "integrated inverse modelling method".

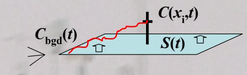
Four main parameters are tested :
(1) The size of the emitting field (from 10 to 100 m squared fields)
(2) The height of the sampler (from 0.5 m to 2 m height)
(3) The sampling periods (2 hours to 4 weeks)
(4) The application date (6 dates throughout the year)

## Methods

▪ For that purpose, we simulate the volatilization of $NH_3$ following fertilization with the Surfatm-NH3 SVAT model (Personne et al. 2009)
▪ To explore the variability of the $NH_3$ source, four patterns of surface emission potentials ($\Gamma$) are generated over a period of 28 days ($\tau_0$):
(1) a constant $\Gamma = \Gamma_0$,
(2) a linearly decreasing $\Gamma = \Gamma_0 \times (1 - t/\tau_0)$,
(3) an exponentially decreasing $\Gamma = \Gamma_0 \exp(-4.6\, t/\tau_0)$,
(4) a Gaussian $\Gamma = N(\Gamma_0, \sigma_\Gamma)$.

▪ The meteorological dataset is from the Grignon L3 Site in 2008.
▪ Six application periods are considered: 1st of Mar, Apr, May, Sep, Oct and Nov.
▪ The FIDES and the Windtrax models are used to generate the transfer time between the source and the receptor $D(x_i,t)$. The concentration at each receptor $C(x_i,t)$ is then estimated given the source strength $S(t)$ and the background $C_{bgd}(t)$ (eq. 1).

$$C(x_i,t) = D(x_i,t) \times S(t) + C_{bgd}(t) \qquad (1)$$




▪ These concentrations are then averaged (overbars) over a sampling period $\tau$ ranging from 2 hours to 4 weeks (eq. 2).

$$\overline{C(x_i)}^{\tau} = \overline{D(x_i)}^{\tau} \times \overline{S}^{\tau} + \overline{D'(x_i)S'}^{\tau} + \overline{C_{bgd}}^{\tau} \qquad (2)$$

▪ The average $NH_3$ emission over the whole period is estimated from these averaged concentrations (eq. 3).

$$\overline{S}^{\tau} = \frac{\overline{C(x_i)}^{\tau} - \overline{C_{bgd}}^{\tau}}{\overline{D(x_i)}^{\tau}} - \underbrace{\frac{\overline{D'(x_i)S'}^{\tau}}{\overline{D(x_i)}^{\tau}}}_{\text{Relative error}} \qquad (3)$$

▪ The second term in the right hand side of eq. (3) is the error introduced by the time integration. It is equal to the correlation between $S(t)$ and $D(x_i,t)$ divided by the averaged $D(x_i,t)$.

## Results

• The modelled $NH_3$ emission patterns were variable according to the $\Gamma$ pattern (Fig. 1a) and the application period (Fig. 1b-c).

• In particular the daily variability of the $NH_3$ source is completely different between May and November with sharp daily variations in May and more chaotic variations in November.

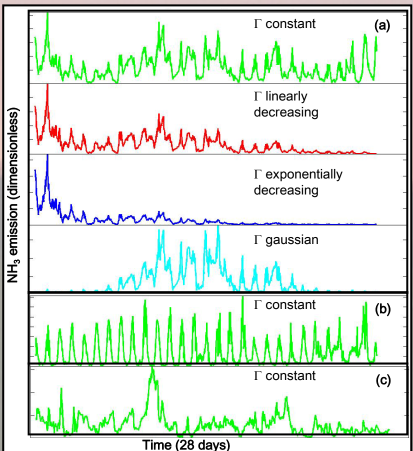



**Fig. 1.** $NH_3$ emission pattern modelled with Surfatm-$NH_3$ over a 28 days period starting **(a)** 1st March, **(b)** 1st May and **(c)** 1st November.

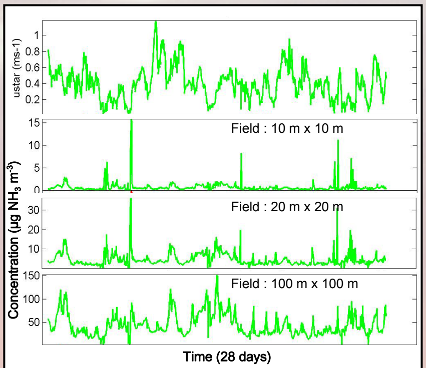



**Fig. 2.** $u_*$ and $NH_3$ concentration at 1.5 m height in the centre of the square field for fields of varying sizes. March application, constant $\Gamma$.

• The concentration modelled with the forward dispersion models using Eq. (1) vary with the height of the receptor relative to the source dimensions (Fig. 2).

• One of the difficulty of the method is linked to the fact that the source is sometimes out of the footprint of the receptor. In such case the source is undetermined.

• Another issue is linked to the fact that the concentration can peak during rare events (of especially low wind speeds). These spikes can dominate the signal.

• This is shown in Fig. 2 where, in the case of the 10x10 $m^2$ field, the concentration pattern is similar to that of the 100x100 $m^2$ field but with some spikes that correspond to low wind $u_*$ (and high $D(x_i,t)$).

• The error of the inversion method:
- ranges from 0 to -40% for 100 m square field (Fig. 3).
- is mostly negative: the fluxes are underestimated.
- increases in magnitude with increasing integration period.
- decreases with receptor height.
- does not depend much on the potential emission pattern $\Gamma$.
- depends on the application date.

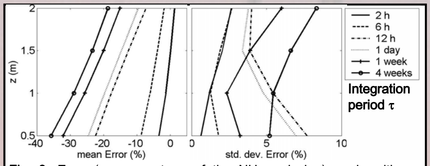



**Fig. 3.** Error (as percentage of the $NH_3$ emission) made with an inverse modeling method for several heights of receptors located in the middle of a 100x100 $m^2$ field.

• For a given field size, the main factor influencing the error in the "integrated inverse modelling method" is the daily $NH_3$ emission pattern which is mainly governed by the wind speed and the surface temperature pattern (Fig. 1).

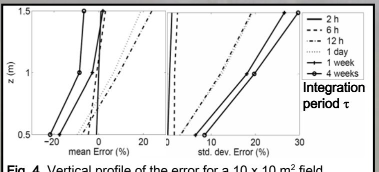



**Fig. 4.** Vertical profile of the error for a 10 x 10 $m^2$ field

• The size of the field is also essential and it must be related to the measurement height. For small fields (10 m), the error can become positive due to undetermination of the source as $D$ tends to zero (Fig. 4). The uncertainty is accordingly also much larger.

## Conclusions - perspectives

• The variability of the error is limited to within less than 10% (Fig. 1, right panel).
• Despite this variability, we can already draw some conclusions for a 100x100 $m^2$ field:
(1) for integration periods below 12h, the underestimation of the $NH_3$ emissions is not expected to be larger than 5 to 10% (± ~5%),
(2) for longer integration periods, the underestimation may be up to 30% (± ~5%).
• For smaller fields (10x10 $m^2$), or equivalently for larger receptor heights, the main concern is that since $D(x_i,t)$ can reach 0, the source is then undetermined for some periods. As a consequence the error is much more variable (systematically larger than 10%) and it changes sign for higher levels.
• This study will be continued to analyse further the differences between FIDES and Windtrax, although preliminary comparison shows a general tendency of FIDES to give larger transfer time.

## References

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http://www-egc.grignon.inra.fr/ Loubet@grignon.inra.fr

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