Modeling bi-directional fluxes of NH3 in a forest ecosystem using SURFATM-NH3 model: A study with a dataset from a deciduous montane forest in the southeastern

Nebila Lichiheb, Erwan Personne, John T. Walker, Rick Saylor, Zhiyong Wu, Xi Chen, Donna B. Schwede, A. Christopher Oishi

Modeling bi-directional fluxes of NH_3 in a forest ecosystem using SURFATM-NH_3 model: A study with a dataset from a deciduous montane forest in the southeastern

Nebila Lichiheb[a], Erwan Personne[b], John T. Walker[c], Rick Saylor[a], Zhiyong Wu[c], Xi Chen[d], Donna B. Schwede[c], and A. Christopher Oishi[e]

[a]National Oceanic and Atmospheric Administration, Air Resources Laboratory, Atmospheric Turbulence and Diffusion Division, Oak Ridge, TN 37831-2456, USA.
[b]AgroParisTech, UMR ECOSYS INRA-AgroParisTech, Université Paris-Saclay, 78850 Thiverval-Grignon, France.
[c]U. S. EPA, Office of Research and Development, Research Triangle Park, NC 27711
[d]U. S. EPA, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711
[e]U. S. Forest Service, Southern Research Station, Otto, NC 28763

***Nebila.Lichiheb@noaa.gov**

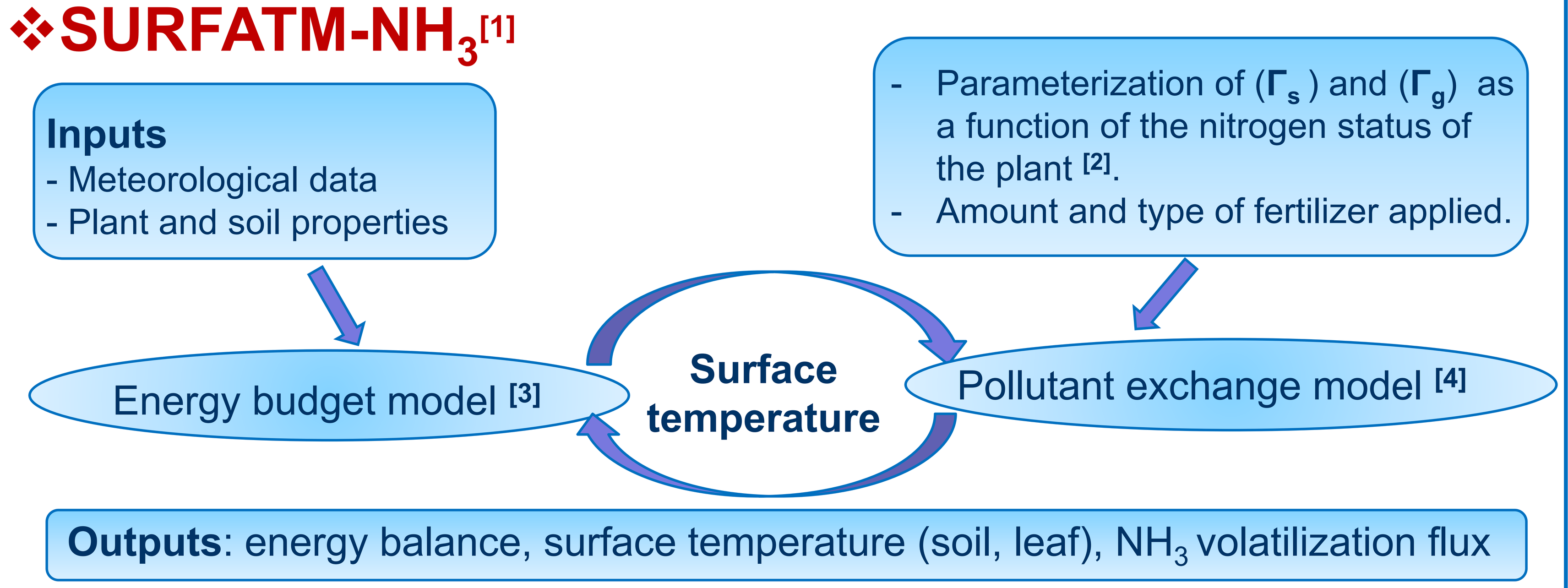
Context & Objective

Ammonia (NH_3) is the most abundant alkaline component in the atmosphere, and is therefore of great importance in the neutralization of atmospheric acids and formation of aerosol particles. Numerous studies have been published investigating the effects of NH_3 fluxes on agricultural ecosystems since emissions of atmospheric NH_3 are mainly related to agriculture. However, NH_3 emissions also occur from natural sources and deposition may affect sensitive ecosystems such as forests. Understanding and predicting the biosphere-atmosphere interactions of NH_3 in a forest canopy is challenging due to the complex nature of this ecosystem.

The aim of this study is to investigate the NH_3 flux partitioning between the ground layer, cuticle and stomata compartments for a deciduous forest using a two-layer NH_3 compensation point model SURFATM-NH_3 as a comparison and interpretation tool. Modeling results are evaluated with data collected during the Southern Appalachian Nitrogen Deposition (SANDS) study in southwestern North Carolina.

Materials and Methods

❖ SURFATM-NH_3[1]



- The emission potential for the vegetation (Γ_s) and ground layer (Γ_g) are given by the NH_3 gas concentrations at equilibrium with the ammonium (NH_4^+) concentration in the apoplastic fluid or soil solution.

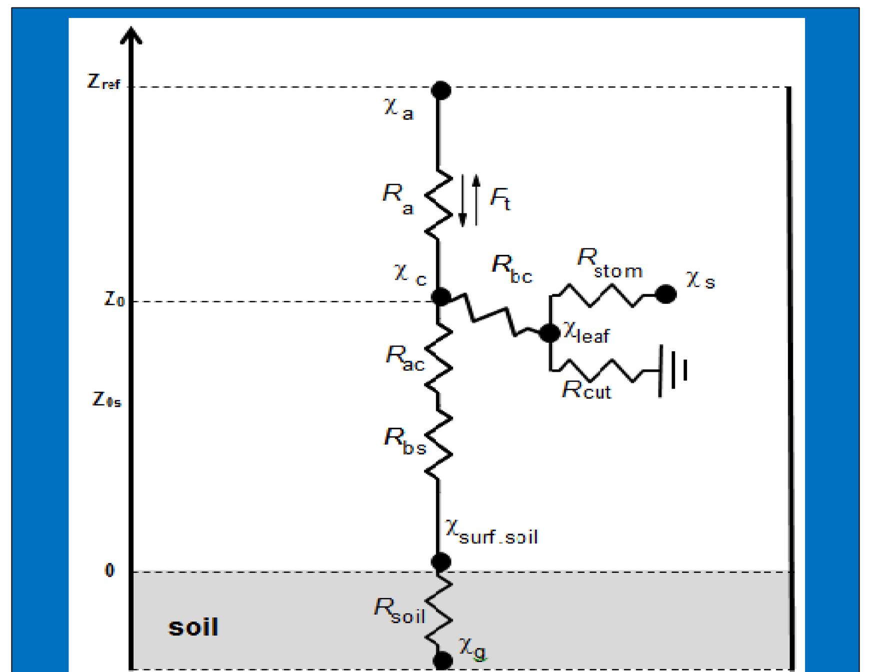


Fig.1: Resistive Scheme for NH_3 exchange model.

R_a, R_{ac}, R_{bc}, R_{stom}, R_{cut}, R_{bs} and **R_{soil}** are respectively aerodynamic resistance above the canopy, aerodynamic resistance inside the canopy, canopy boundary layer resistance, stomatal resistance, cuticular resistance, soil boundary layer resistance and soil resistance; **χ_a , χ_c, χ_s $\chi_{surf.soil}$** and **χ_g** refer to atmospheric NH_3 concentration, canopy NH_3 compensation point, stomatal compensation point, NH_3 concentration on the soil surface and the ground layer compensation point.

- **Volatilization flux of NH_3 (F_t)**

$$F_t = -\frac{1}{R_a}(\chi_a - \chi_c)$$

with $\chi_c = f(\chi_a, \chi_s, \chi_g, R_a, R_{ac}, R_{bs}, R_{bc}, R_{stom}, R_{cut}, R_{soil})$

- **Stomatal compensation point (χ_s)**

$$\chi_s = K_d \times K_H \times \exp\left(\frac{\Delta H_d^0 + \Delta H_H^0}{R} \times \left(\frac{1}{298.15} - \frac{1}{T_s}\right)\right) \times \Gamma_s$$

- **Ground layer compensation point (χ_g)**

$$\chi_g = K_d \times K_H \times \exp\left(\frac{\Delta H_d^0 + \Delta H_H^0}{R} \times \left(\frac{1}{298.15} - \frac{1}{T_g}\right)\right) \times \Gamma_g$$

T_s and **T_g** refer to leaf temperature and soil temperature, **K_d** the dissociation constant for acid-base dissociation NH_4^+/NH_3, **K_H** the Henry constant, **ΔH_d^0** and **ΔH_H^0** are the free enthalpies of acid-base dissociation and volatilization, **R** is the perfect gas constant.

❖ Parameterization of R_{stom}

Improvement of R_{stom} description by coupling the stomatal conductance (g_{stom}) model formulated by Medlyn et al. (2011) [5] and the mechanistic simulation of photosynthesis (A_n) proposed by Collatz et al. (1991) [6] .

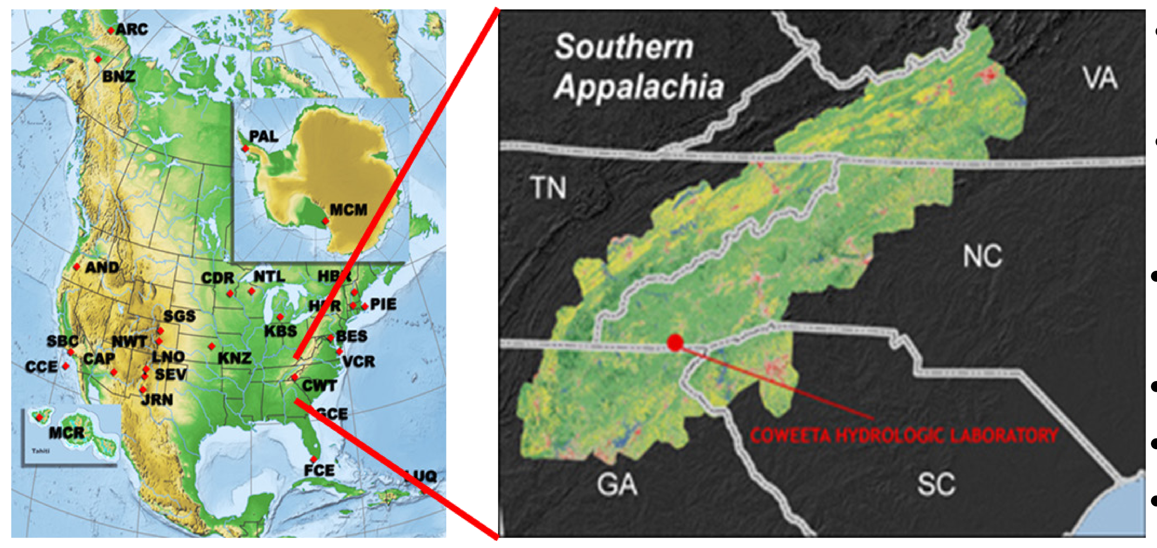
$$g_{stom} = g_0 + 1.6\left(1 + \frac{g_1}{\sqrt{D}}\right)\frac{A_n}{C_{CO_2}} \quad \text{with} \quad A_n = \min\{J_E, J_C, J_S\} - R_D$$

g_0 and **g_1** are fitted parameters, **D** the vapor pressure deficit, **C_{co2}** the atmospheric CO_2 concentration, **J_E** the light-limited assimilation rate, **J_c** the rubisco-limited assimilation rate, **J_s** the assimilation rate due to the limitation of the export of assimilates inside the leaf, **R_D** the leaf dark respiration.

❖ Dataset for model validation

- **Field site location**

Coweeta Hydrologic Laboratory, North Carolina



- Deciduous overstory (tulip poplar, red maple, oak, hickory)
- Evergreen understory (rhododendron, mountain laurel)
- Mature southern Appalachian forest (~85 years since harvesting)
- Mean annual temperature: 12.7 °C
- Average canopy height: 35 m
- Total canopy LAI: 4.6

- **Measurements**
  - Air : NH_3 concentration (denuder and MARGA data), wind speed, friction velocity, sensible and latent heat flux, chemical fluxes, solar radiation, rainfall, air temperature
  - Canopy: height, LAI, stomatal emission potential (Γ_s) and litter emission potentials
  - Soil: temperature, moisture, pH, heat flux, soil emission potential (Γ_g)

- **Initial model testing**

- **Initial focus:** July 20-30, 2016 • **Implemented emission potentials:** Γ_s = 40, Γ_g =200

Initial results

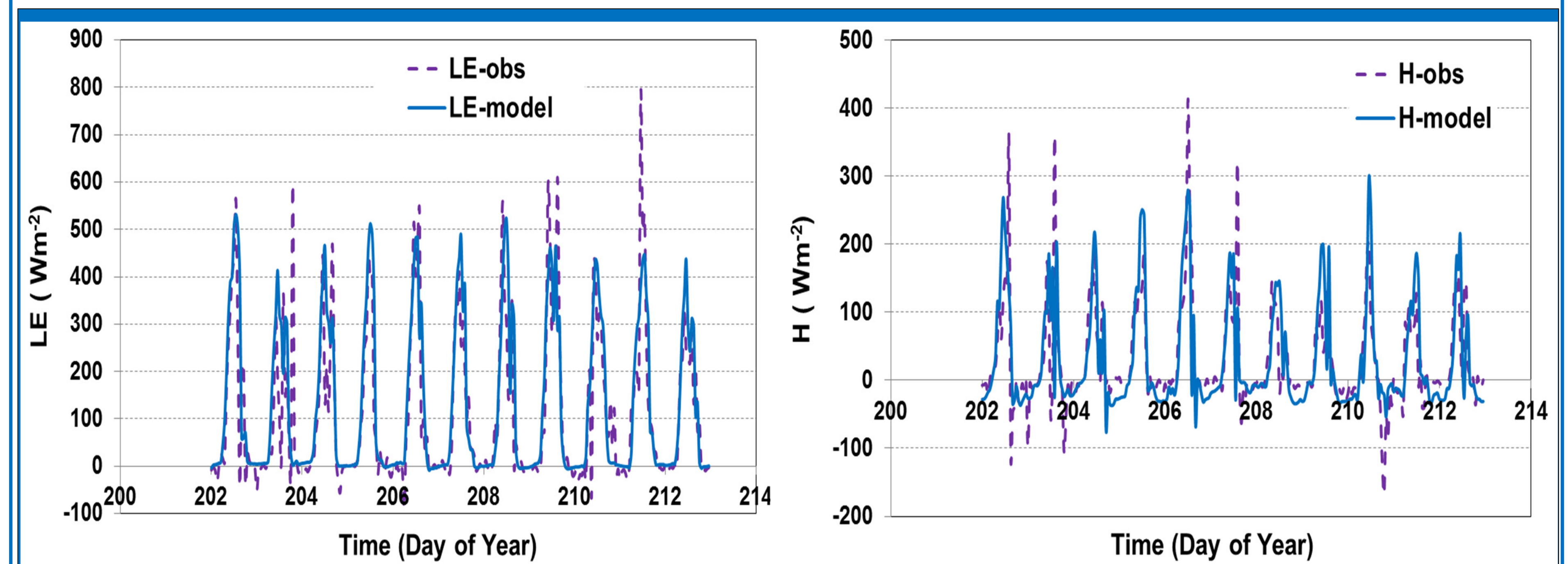


Fig.2: Comparison of modeled and measured latent heat flux (LE) and sensible heat flux (H)

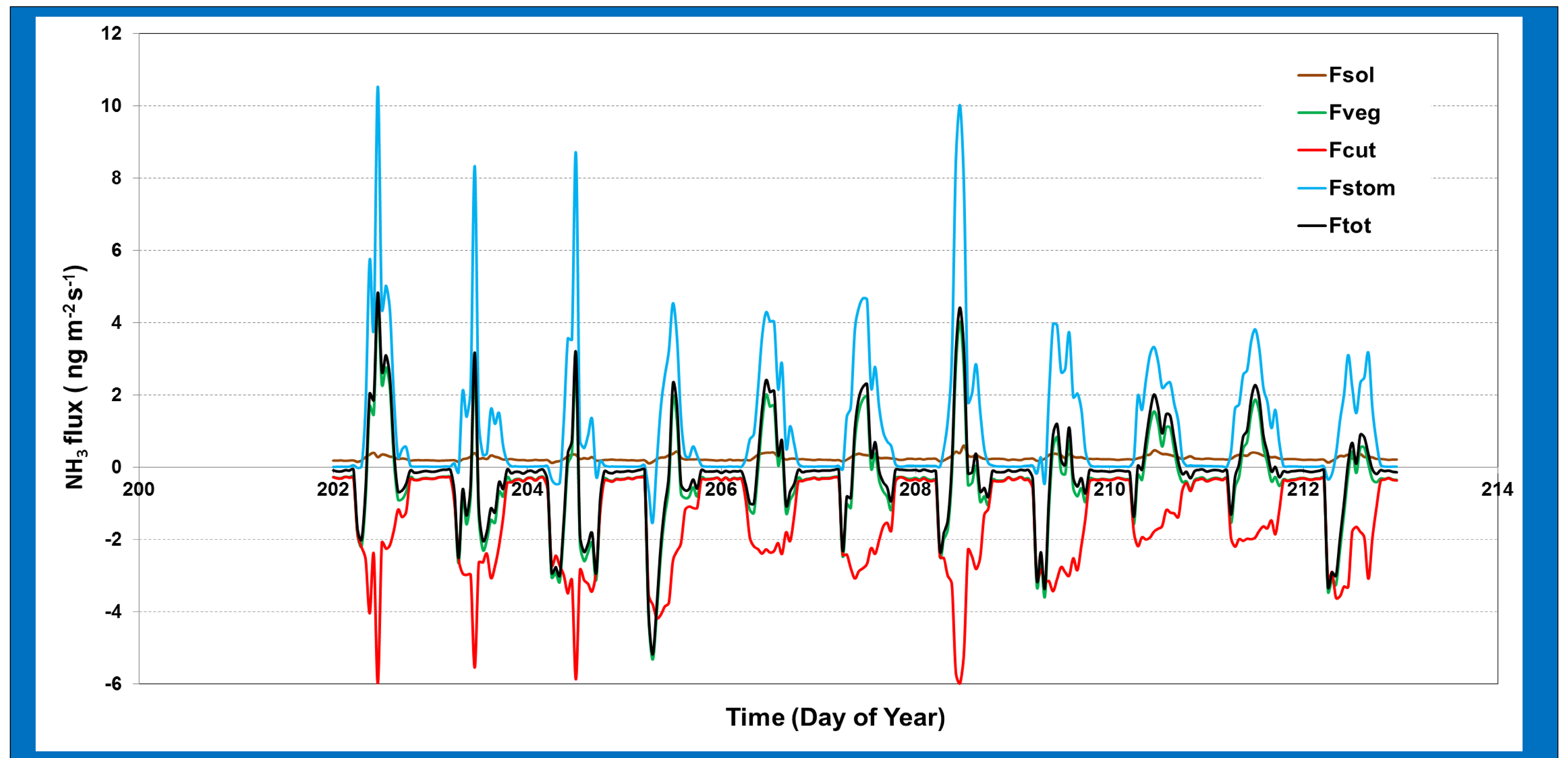


Fig.2: Simulation of the different sources of NH_3 fluxes with SURFATM-NH_3 model

- SURFATM-NH_3 simulates LE and H which are in good agreement with the experimental data.
- The stomatal exchange is the main contributor to the simulated forest NH_3 emissions.
- The total modeled NH_3 fluxes over this forest ecosystem are relatively small.

Future work

- Implement a litter emission potential (**Γ_{litter}**) in the model;
- Improve the description of **R_{cut}** by implementing: (i) the effect of temperature suggested by Flechard et al. (2010) [7], (ii) the effect of LAI suggested by Zhang et al. (2003) [8], and (iii) the molar ratio of total acid / NH_3 in the atmosphere (**AR**) proposed by Massad et al. (2010) [9];
- Study the sensitivity of the model to various parameters ;
- Simulate NH3 fluxes for the whole experimental study and compare the model outputs to the measurements;
- Compare SURFATM-NH3 results with other models.

References

[1]: Personne E. *et al.* (2009). SURFATM-NH3: a model combining the surface energy balance and bi-directional exchanges of ammonia applied at the leaf scale. Biogeosc. 6,1371-1388.
[2]: Massad, R.S. *et al.* (2010). Review and parameterisation of bi-directional ammonia exchange between vegetation and the atmosphere. Atmos. Chem. Phys.10, 359–386.
[3]: Choudhury B.J. and Monteith J.I. (1988). A four-layer for the heat budget of homogeneous land surfaces. Q.J.R.Meterol.Soc. 144, 373-398.
[4]: Nemitz, E. *et al.* (2000): Resistance modelling of ammonia exchange over oilseed rape, Agric. Forest Meteorol. 105, 405–425.
[5]: Medlyn, B.E. *et al.* (2011) Reconciling the optimal and empirical approaches to modelling stomatal conductance. Global Change Biology, 17, 2134–2144.
[6]: Collatz, G.J. *et al.* (1991). Physiological and environmental regulation of stomatal conductance, photosynthesis and transpiration: a model that includes a laminar boundary layer. Agric. Forest Meteorol .54, 107-136.
[7]: Flechard, C.R., *et al.*, 2010. The annual ammonia budget of fertilised cut grassland – Part 2: Seasonal variations and compensation point modeling. Biogeosciences 7, 537-556.
[8]: Zhang, L., *et al.*, 2003. A revised parameterization for gaseous dry deposition in air-quality models, Atmos. Chem. Phys., 3, 2067–2082,
[9]: Massad R.-S., *et al.*, 2010. Review and parameterisation of bi-directional ammonia exchange between vegetation and the atmosphere. Atmospheric Chemistry and Physics, 10:359–386.

99th AMS annual Meeting, 6-10 January 2019, Phoenix, AZ