Project Number 282910

ÉCLAIRE

Effects of Climate Change on Air Pollution Impacts and Response Strategies for European Ecosystems

Seventh Framework Programme

Theme: Environment

MS13: Summary report on site applications of improved NH_3 / NO and VOC models, including uncertainty assessment and comparison with original approaches

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1. Executive Summary

- Two ammonia exchange models were compared to measured NH_3 fluxes from the ECLAIRE sites and previously available datasets: The process-based volt'air model for situations following slurry applications and the Massad Nemitz Sutton (2010; MNS-2010) resistive model based on prescribed emission potentials.
- The MNS-2010 model was revised to incorporate a meta-model of the soil emission potential derived from Volt'air following slurry application and a crop model CERES-EGC for background conditions. The non-stomatal resistance was also revised.
- Comparison of the revised MNS-2010 with data showed considerable improvement and demonstrated that the concept of a simple resistance scheme with meta-modelled emission potential is a way forward for improving ammonia exchange in regional and global chemistry transport models.
- The Volt'air model was compared with measurements from three sites in Europe (FR-Gri, CH-Oen and CH-Poi), two of which were grasslands. The model tends to overestimate the emissions during the first peak following application. Likely causes are the parameterisation of the additional resistance due to turbulent transfer in the vegetation canopy as well as the timing of the
- The Bayesian uncertainty assessment of parameter induced uncertainty in simulated yearly NO emissions resulted in simulation uncertainties approximately in the range of the yearly NO emission strength.

Objectives:
The aim of WP3 was to provide improved parameterisations of biogenic and agricultural emissions to the modellers which include a robust response to climatic conditions that are predicted to change in the future. The individual objectives were to:

- To improve the climate response characteristics of NH_3 emission models for agricultural sources and vegetation,
- To improve the climate response characteristics of soil NO emission models,
- To improve European BVOC emission models and their response to meteorological drivers and stresses

The milestone MS12 objective was to give a summary report on site applications of improved NH_3 / NO and VOC models, including uncertainty assessment and comparison with original approaches.

However, due to delayed availability of VOC emissions datasets, the VOC is not reported here.

2. Activities:

2.1. Site applications of improved NH_3 exchange

Modelling strategy.
Ammonia exchange between the surface and the atmosphere is bi-directional: large emissions occur following fertilizer applications while deposition dominates when the surface is wet and cold (Flechard et al., 2013; Massad et al., 2010). Modelling NH_3 exchange may therefore require different types of modeling approaches: an approach based on emission potential from the soil and the canopy is adapted for background conditions (away from nitrogen application) (Massad et al., 2010), while following nitrogen application, physically and chemically explicit dynamical models like Volt'air or DNDC are required (Genermont and Cellier, 1997). Two models were therefore selected for testing against ECLAIRE datasets:

- The Massad, Nemtiz, Sutton (2010) model (hereafter named MNS-2010; (Massad et al., 2010) was used for simulating NH_3 fluxes under background conditions;
- The Volt'air model (Genermont and Cellier, 1997) was used for simulating NH_3 volatilisation following slurry application.

The two models were compared to measurements performed before and during the ECLAIRE project. This comparison led to revision of the models which are briefly presented here.

Ammonia fluxes datasets at the Eclaire sites.
The European field sites and associated NH_3 flux datasets available for evaluating the NH_3 exchange models spanned 20 years. These data included :

- Unfertilised (semi-natural) ecosystems:
  - UK-AMO, Auchencorth Moss, extensively grazed moorland, 1995-96-98 (LIFE project)
  - NL-Spe, Speulderbos, temperate mixed forest, 2009-10 (NitroEurope), 2013 (ECLAIRE)
  - IT-BFo, Bosco Fontana, medit. forest, 2012 (ECLAIRE)
- Fertilised agro-ecosystems:
  - UK-EBu, Easter Bush, grazed grassland, 2007-08 (NitroEurope)
  - CH-Oe1, Oensingen, cut grassland, 2006-07-08-09 (NitroEurope)
  - CH-Pos, Posieux, grazed grassland, 2013 (ECLAIRE)
  - FR-Gri, Grignon, crop rotation, 2008-09 (NitroEurope), 2012 (ECLAIRE)
  - FR-Mej, Méjusseaume, grazed grassland, 2014-2015 (FR-ADEME BTEP project)

Volt'air modelling of the NH_3 emissions following slurry applications.

The Volt'air ammonia volatilisation model was detailed at length in (Genermont and Cellier, 1997). It is a process-based model accounting for the water and solutes transfer and energy balance in the soil as well as the thermodynamical and chemical equilibrium between phases. The soil is discretized in shallow layers at the surface.

The Volt'air model was compared to measurements performed in Oensingen, Posieux and Grignon. Figure 1 shows an example comparison of measured and modelled NH_3 fluxes in Oensingen, and Figure 2 shows the same for Grignon. Overall the model tends to overestimate the first peak of emissions expect in some cases as in Grignon 2009. The overall evolution of the flux is however well reproduced over a large range of scale indicating that the soil processes are correctly simulated (Figure 1 and Figure 2).

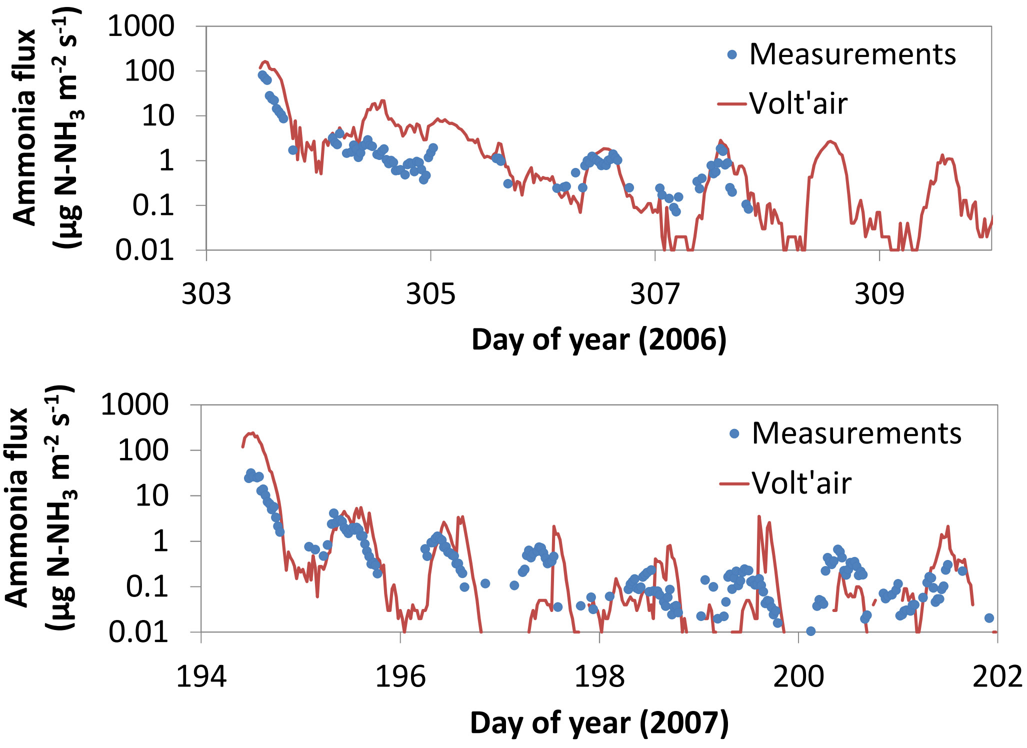

Figure 1 *Comparison of modelled (continous lines) and measured (points) NH_3 fluxes at CH-Oe (Oensigen, NitroEurope Data), following slurry application in a grassland field.*

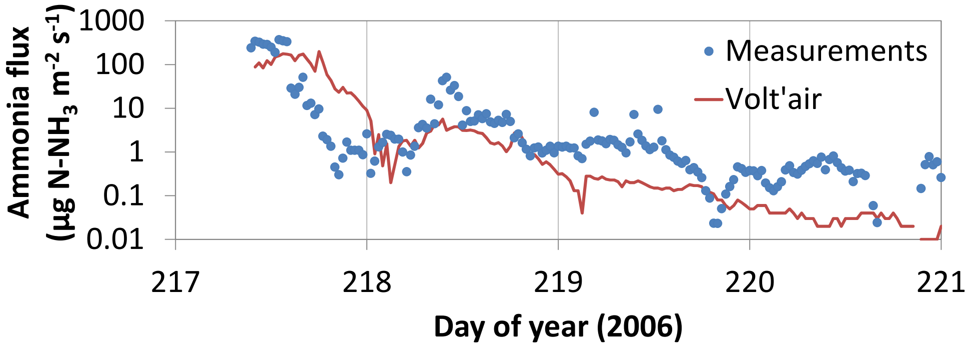

Figure 2 *Comparison of modelled (continous lines) and measured (points) NH_3 fluxes at FR-Gri (Grignon, NitroEurope Data), following slurry application in a grassland field.*

A borader analysis on the differences between Volt'air and measurements is hown for Oensigen in Table 1. It shows that the parameters controlling the slurry infiltration and incorporation in the first layer will modify substantially the percentage losses simulated only in some configurations (30/10/2006 and 24/10/2007), but that in some other cases these parameters cannot explain the overall overestimation of the Volt'air model in Oensigen. The addition of a vegetation layer in Voltair that will modify the turbulent transfer and the energy balance of the surface is a required improvement which will likely diminish the simulated emissions in grasslands.

Table 1 **Comparison of modelled cumulated losses of NH_3 at CH-Oen for several Volt'air model configurations following slurry application: Mono: the slurry is supposed to stay on the surface. Mixed: the slurry is mixed with the first soil layer. Infiltration is a parameter controlling the infiltration of slurry in the soil.**

	cumulated ammonia emissions (% of TAN)		
	modelled		
	Mono, infiltration = 0.02	Mono, infiltration = 1	Mixed
13/07/2006	94%	95%	95%
27/06/2006	48%	45%	49%
30/10/2006	54%	44%	28%
03/04/2007	67%	65%	66%
13/07/2007	86%	74%	78%
24/10/2007	80%	74%	70%

Improved MNS-2010 modelling of NH_3 fluxes.

The MNS-2010 parameterisation for bi-directional NH_3 exchange was based on an extensive literature review of NH_3 flux datasets, soil and vegetation emission potentials and resistance formulations for in-canopy transfer and deposition (Massad et al., 2010). The MNS-2010 scheme was developed to provide general parameter tables and functions for the Nemitz-Milford-Sutton 2-layer NH_3 canopy compensation point model with a view to implementing bi-directional NH_3 exchange schemes in CTMs. Briefly, the exchange of NH_3 between the atmosphere and the ecosystem is mediated by a network of physical resistances accounting for turbulent transfer above- and in-canopy, molecular diffusion through laminar sub-layers and through stomates, and uptake by wetness and by other non-stomatal surfaces. A revision of the MNS-2010 parameters was performed in ECLAIRE as detailed in delivrables 4.1 and 3.2:

- A first revision consisted in dividing by 3 the minimum non-stomatal resistance and its response to temperature.
- A second revision consisted in replacing the prescribed soil emission potential (Γ_g) by a meta-modelled Γ_g derived from Volt'air after slurry application and from CERES-EGC for background conditions.

The two revisions improved considerably the model performance: reduced non-stomatal resistance led to a better representation of the daily dynamics of NH_3 deposition (Figure 3); and revision of Γ_g following fertilization led to a decrease of duration of the emission peak which better fits the available observations (Figure 4).

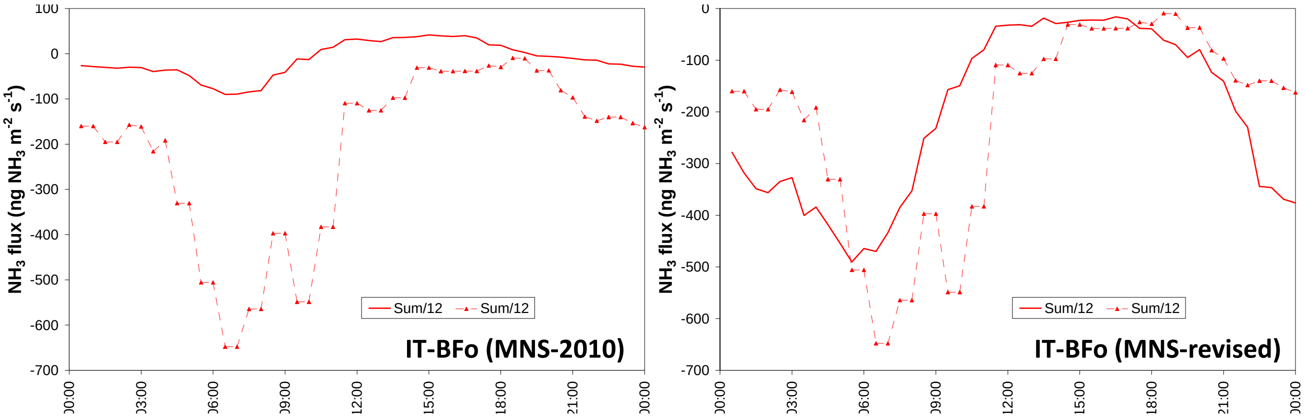

Figure 3 *Comparison of modelled (continous lines) and measured (dashed lines) NH_3 fluxes at the ECLAIRE IT-BFo (mediterranean forest). Modelled fluxes were simulated using either the default parameters as per MNS-2010 (left-hand side) or revised parameters for R_w (right-hand side) (see text for details).*

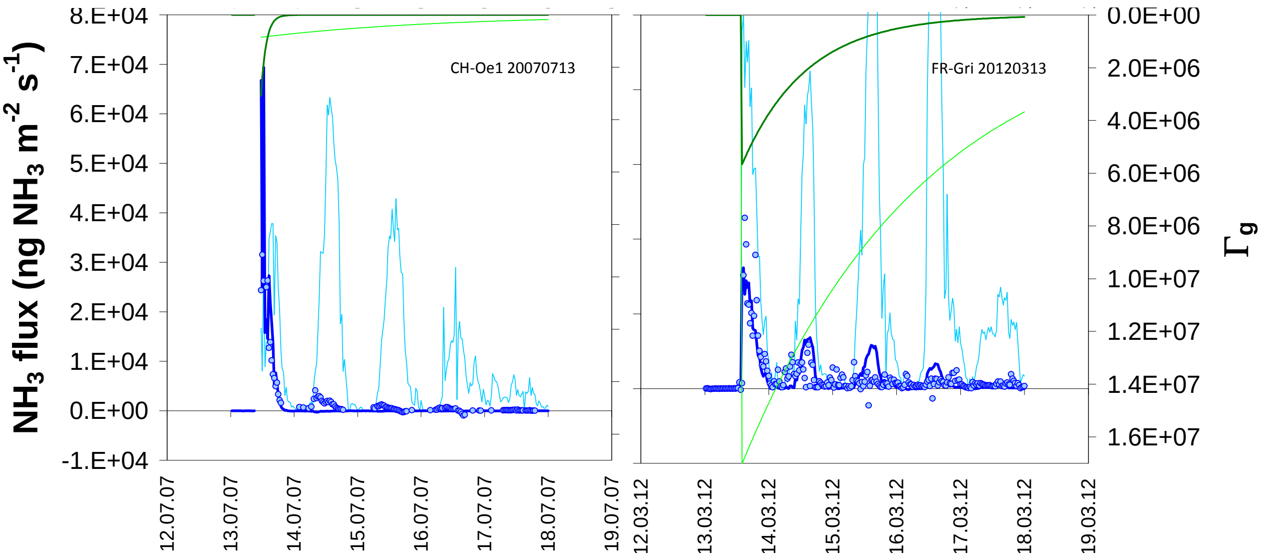

Figure 4 *Example runs of original (cyan) and improved (bold blue) MNS-2010 model against the NitrooEurope site CH-Oe1 (Oensingen, 2008-2009) and the ECLAIRE site FR-Gri (Grignon, arable, 2008-2012). The original Γ_g is shown in light green and the meta-modelled Γ_g is shown in dark green.*

2.2. Site applications of NO emission module

To improve the processes describing the soil carbon and nitrogen cycle a calibration of the process parameters was performed in order to optimize the prediction accuracy of the model. First a parameter sensitivity analysis for the new soil biogeochemistry module has been performed in order to identify the most sensitive parameters describing soil borne NO and N_2O emissions. In the next step parameter calibrations for different ecosystems including the available field observations of NO and N_2O emissions have been performed using a Bayesian Model Calibration method (BC). The parameters addressed within the calibration are summarized in Table 2. The BC method has been proved to be a powerful approach to obtain very good optimized parameters sets for process-based models. Figure 5 illustrates the Metropolis algorithm for the Bayesian model calibration of the LandscapeDNDC soil biogeochemistry.

Table 2 The 15 most sensitive process parameters with respect to soil NO and N_2O emissions used for the calibration and Bayesian parameter uncertainty quantification

Symbol	Description	Units
CO_2_PROD_DECOMP	Factor of CO_2 production during decomposition	
F_DENIT_N_2O	Factor that regulates how much of the denitrified N goes to N_2 (directly)	
MUEMAX_C_DENIT	Microbial use efficiency for C consumption during de-nitrification	kg C d^{-1}
KF_NIT_N_2O	Factor reaction rate for N_2O reductase	
KMM_N_DENIT	Michaelis-Menten constant for N during denitrification	Kg N m^{-3}
AMAX	Maximal specific microbial death/reutilization rate	kg C d^{-1}
KR_HU_AORG	Humufication rate for heterotrophic microbial biomass	kg C d^{-1}
F_DENIT_NO	Factor of NO production during denitrification	
KMM_C_DENIT	Michaelis-Menten constant for C use during de-nitrification	Kg C m^{-3}
MUEMAX_C_NIT	Microbial use efficiency for C consumption during nitrification	kg C d^{-1}
KR_HU_HUM_1	Rate of Humufication of humus pool one	kg C d^{-1}
KR_DC_HUM_1	Rate of decomposition of humus pool one	kg C d^{-1}
KF_REDUCTION_ANVF	Reduction factor of the anaerobic volume fraction	
BIOSYNTH_EFF	Biosyntheis efficiency factor	
KR_DC_HUM_0	Rate of decomposition of humus pool cero	kg C d^{-1}

Performing four different Bayesian calibrations in parallel (Markov chains) for these parameter sets and using the convergence criteria of Gelman and Rubin, 1992 a calibrated joint parameter distribution will be generated (Figure 6). This joint parameter distribution represents the posterior parameter distribution of the calibration, from where we sampled optimum sets for uncertainty quantification.

Results

The Bayesian calibration resulted in a joint parameter distribution for the 15 most sensitive parameters (Figure 6). Model calibration was carried out for different sites using daily NO and N_2O measurement. Table 2 summarizes and Figure 5 illustrates the distribution of each parameter after the calibration.

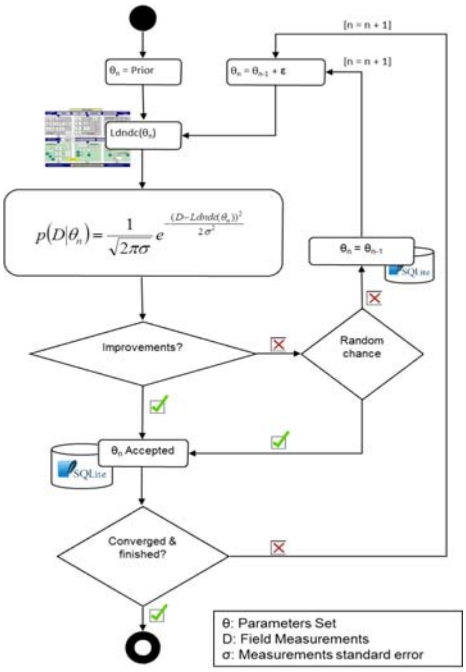

Figure 5 Metropolis algorithm for the Bayesian Calibration of the LandscapeDNDC soil biogeochemistry module following the approach of Van Oijen *et al.*, 2005, Rahn *et al.*, 2012.

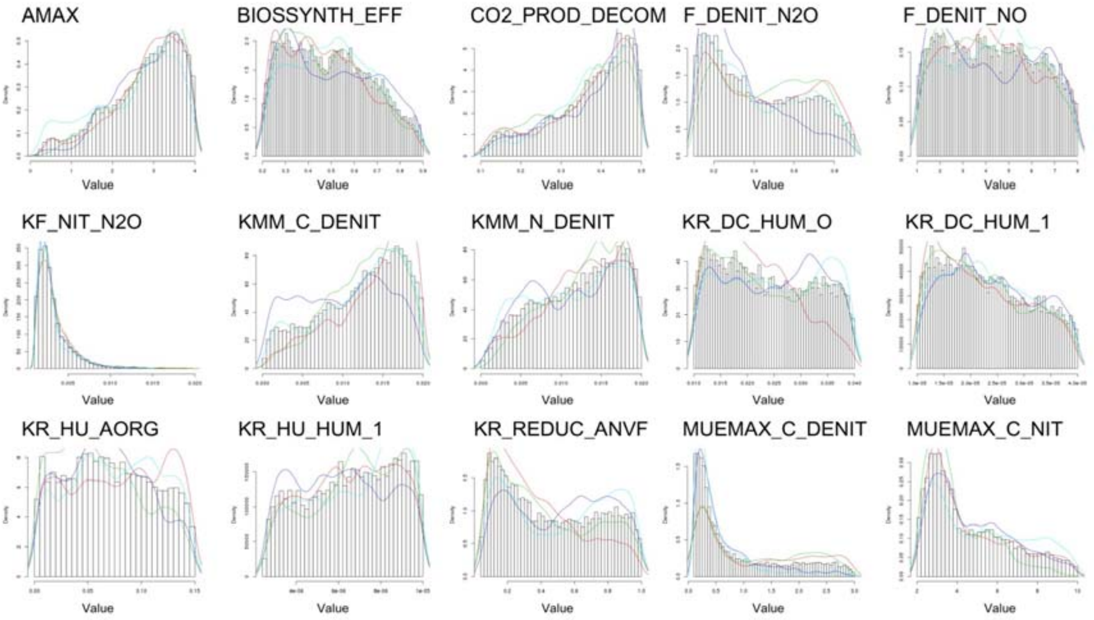

Figure 6 Joint parameter distributions resulting from the 4 parallel BC chains (indicated by the 4 coloured lines) after the conversion of the Markov-Chains was reached

The posterior parameter values were assigned uniform probability within their given ranges. The uncertainty of the prior parameter values (pre calibration model default values given with minimum and maximum values) were minimized considerably during the BC (e.g. see KF_NIT_N2O in Figure 6) while some parameters (like KR_HU_AORG, see Figure 6) did not reduce their uncertainty significantly. This parameter corresponds to the humufication constant from heterotrophic microbes and it suggests that all values ranging from 0.001 to 0.15 present a similar probability. For this kind of parameter, uncertainty is not reduced by the BC method. Values exceeding 0.14 are less likely than the others.

Performing an uncertainty quantification from the results of the BC by sampling parameters sets out of the joint parameter distribution and evaluating the model predictions for all sampled parameter sets (up to hundreds of site simulations) will result in uncertainty ranges of predicted NO and N_2O emissions when statistically analysing (see example Figure 7 and Figure 8). The uncertainty ranges for the predicted NO and N_2O emission strengths for all validation sites will be evaluated (publication in preparation)

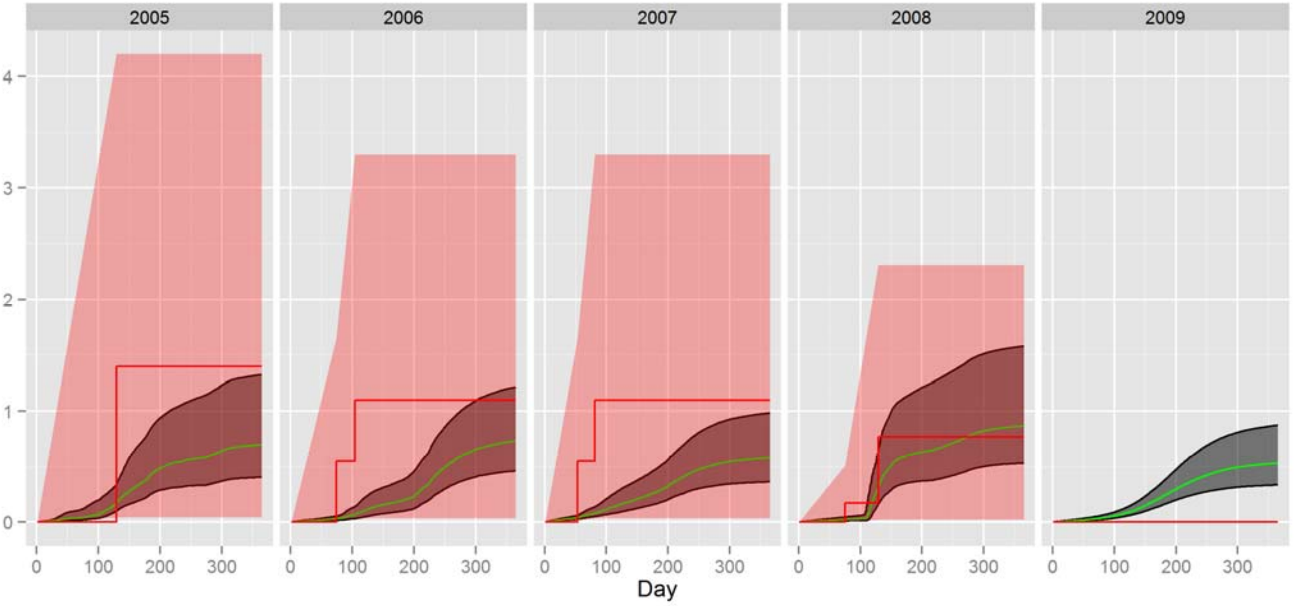

Figure 7 Uncertainty range in simulated soil N_2O emissions [kg N-N_2O / ha] for the Grignon-France site as resulting from the BC. Green line: median, black lines: 25 and 75 percentile, grey area: estimated uncertainty range, red line: N_2O emission estimated via IPCC direct N_2O EF (1.0 %), red area: IPCC uncertainty range for IPCC N_2O emission estimate. (For 2009, no N Fertilizer data was available)

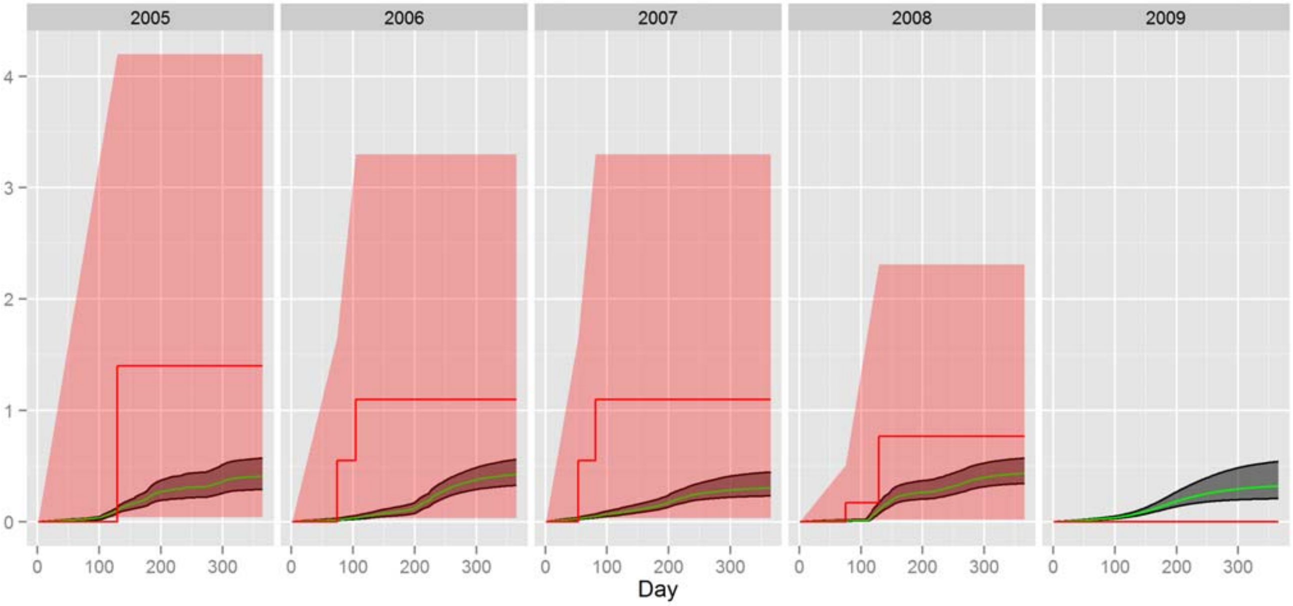

Figure 8 Uncertainty range in simulated soil NO emissions [kg N-NO / ha] for the Grignon-France site as resulting from the BC. Green line: median, black lines: 25 and 75 percentile, grey area: estimated uncertainty range, red line: NO emission estimated via IPCC direct NO EF (1.0 %), red area: IPCC uncertainty range for IPCC NO emission estimate. (For 2009, no N Fertilizer data was available)

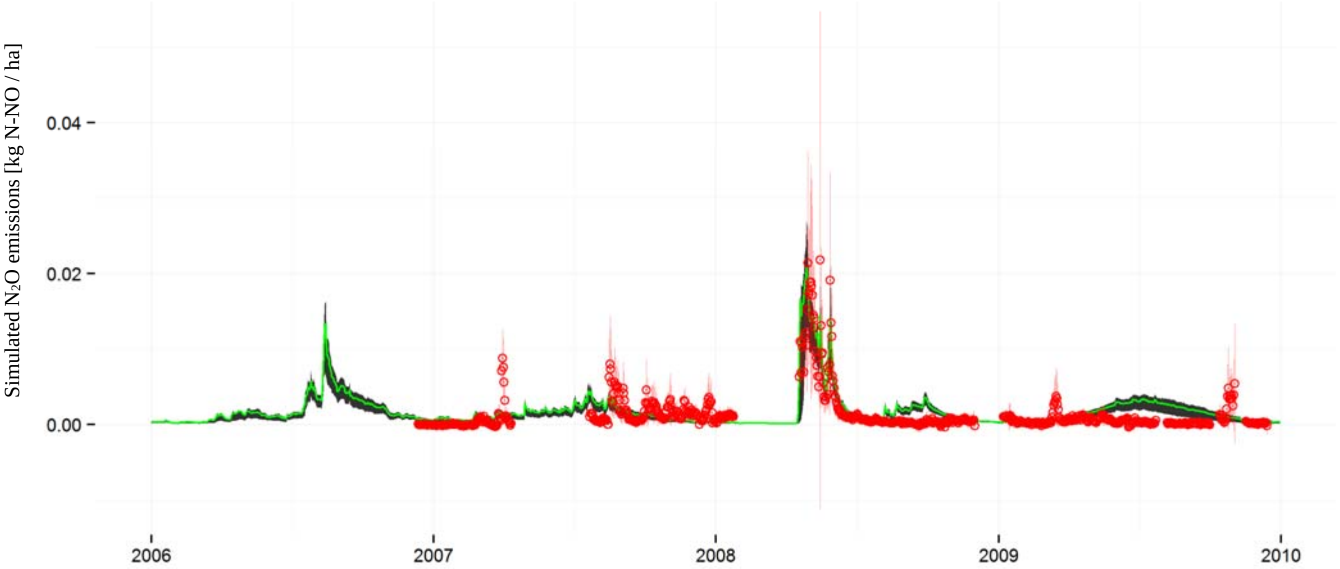

Figure 9 Simulated N_2O emissions [kg N-N_2O / ha] including the uncertainty bands resulting from the BC. Green line: median, black lines: 25 and 75 percentile, grey area: estimated uncertainty range, red circles: field measurements and measurement errors

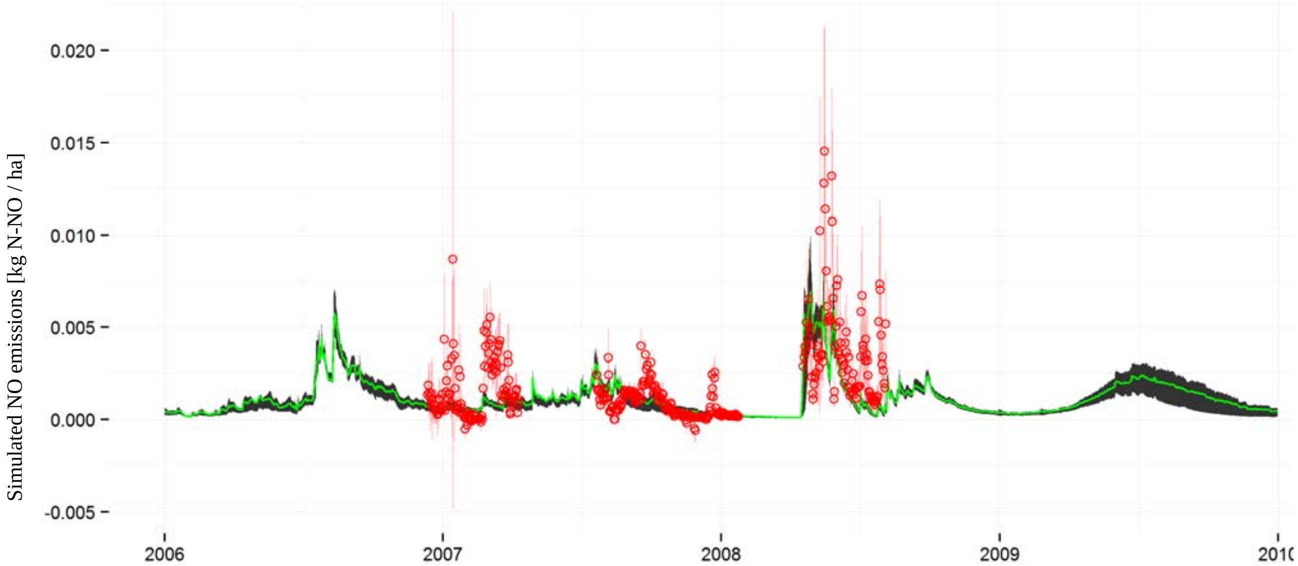

Figure 10 Simulated NO emissions [kg N-N_2O / ha] including the uncertainty bands resulting from the BC. Green line: median, black lines: 25 and 75 percentile, grey area: estimated uncertainty range, red circles: field measurements and measurement errors

3. Milestones achieved:

MS12: Summary report on site applications of improved NH3 / NO and VOC models, including uncertainty assessment and comparison with original approaches

4. Deviations and reasons:

This milestone was delayed because of the delayed development of the ESX model which was supposed to be used for such comparison. A different strategy was therefore developed in the last year of the project to revise parameterisation of the MNS-2010 model and develop meta-models out of existing CERES-EGC and Volt’air models.

No report on VOC models is included in this milestone due to delayed VOC emissions data from the ECLAIRE project.

5. Publications:

Ferrara R.M., Loubet B., Decuq C., Palumbo A.D., Di Tommasi P., Magliulo V., Masson S., Personne E., Cellier P., Rana G., 2014. Ammonia volatilisation following urea fertilisation in an irrigated sorghum crop in Italy. Agricultural and Forest Meteorology, 195-196, 179-191.

Flechard, C.R., Massad, R.-S., Loubet, B., Personne, E., Simpson, D., Bash, J.O., Cooter, E.J., Nemitz, E. and Sutton, M.A. 2013. Advances in understanding, models and parameterisations of biosphere-atmosphere ammonia exchange, Biogeosciences 10, 5183–5225.

Personne, E., Tardy, F., Génermont, S., Decuq, C., Gueudet, J.-C., Mascher, N., Durand, B., Masson, S., Lauransot, M., Fléchard, C., Burkhardt, J. and Loubet, B., 2015. Investigating sources and sinks for ammonia exchanges between the atmosphere and a wheat canopy following slurry application with trailing hose. Agric. For. Meteorol., 207: 11-23.

6. Meetings:

19-23 March 2012, CEH, Edinburgh. WP4 meeting, launch of ESX project

06-08 May 2013, Univ. Bonn. WP4-ESX meeting

7. List of Documents/Annexes:

None

8. References

Flechard, C.R. et al., 2013. Advances in understanding, models and parameterizations of biosphere-atmosphere ammonia exchange. Biogeosciences, 10(7): 5183-5225.

Genermont, S. and Cellier, P., 1997. A mechanistic model for estimating ammonia volatilization from slurry applied to bare soil. Agric. For. Meteorol., 88(1-4): 145-167.

Gelman, A., Rubin, D.B., 1992. Interference from iterative simulation using multiple sequences. Statitical Science 7, 55.

Massad, R.S., Nemitz, E. and Sutton, M.A., 2010. Review and parameterisation of bi-directional ammonia exchange between vegetation and the atmosphere. Atmospheric Chemistry and Physics, 10(21): 10359-10386.

Rahn, K.H., Werner, C., Kiese, R., Haas, E., Butterbach-Bahl, K., 2012. Parameter-induced uncertainty quantification of soil N2O, NO and CO2 emission from Höglwald spruce forest (Germany) using the LandscapeDNDC model. Biogeosciences 9, 3983-3998.

Van Oijen, M., Rougier, J., Smith, R., 2005. Bayesian calibration of process-based forest models: bridging the gap between models and data. Tree Physiology 25, 915-927.