

Project Number 282910

ÉCLAIRE

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

Seventh Framework Programme

Theme: Environment

MS35: Update of NitroScape to reflect ÉCLAIRE needs

Due date of milestone: **31/01/2013**

Actual submission date: **30/09/2015**

Start Date of Project: **01/10/2011**

Duration: **48 months**

Organisation name of lead contractor for this deliverable :
INSTITUT NATIONAL DE LA RECHERCHE AGRONOMIQUE (INRA)

Project co-funded by the European Commission within the Seventh Framework Programme		
Dissemination Level		
PU	Public	<input type="checkbox"/>
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1. Executive Summary

- Although the development of NitroScape has been delayed due to technical reasons and researchers leaving the project, significant improvements and modifications have been made to the model throughout the duration of the project up to the point that the model has now been updated to reflect ÉCLAIRE needs
- Problems with the incorporation of the FASSET farm model led to the development of a simpler substitute model (FARM-EF) to model NH₃ and N₂O emissions from animals in stables, grazing animals and manure storage areas
- A new version of the agro-ecosystem model CERES-EGC, was integrated into NitroScape that includes new modules of denitrification and nitrification simultaneously models all plots of the landscape using the PALM coupler
- The TNT hydrological model has been updated with the integration of new modules (NH₄⁺ transfer and transformation, especially in lowland areas...) or the improvement of existing modules
- An alternative atmospheric model was implemented into NitroScape. The FIDES-3D-Surfatm model results from the coupling between a soil-vegetation-atmosphere exchange model (Surfatm) and a model of Gaussian dispersion (FIDES)
- In addition, many model errors resulting from compiler changes, changes of operating system, and inconsistencies between component models have been corrected
- NitroScape was applied and tested on a French landscape, for which datasets were complete and ready to be used
- The model is now ready to be used on other landscapes, especially the Scottish and the Dutch landscapes of the ÉCLAIRE project
- A parallel study to evaluate the sub-grid variability of regional models by using a landscape scale approach (NitroScape) has also been carried out

2. Objectives:

To extend the NitroScape modelling framework to the needs of ÉCLAIRE to analyse sensitivity to climate change, especially in relation to atmospheric deposition to sensitive ecosystems

3. Activities:

3.1. Nitroscape status at the beginning of the ÉCLAIRE project

NitroScape overview

NitroScape is a coupled, spatial and dynamic model which integrates processes of transfer and transformation of reactive nitrogen (N_r : NH_3 , NO_x , NO_3^- , NH_4^+ , DON, N_2O) in four compartments of the landscape: farms, agro-ecosystems, atmosphere and hydrosphere (Duret et al, 2011; Drouet et al, 2012). It simulates fluxes, losses and budgets of N_r within landscapes of a few km^2 for periods of several years. The NitroScape model is coupled to a spatial database, which contains the parameters and the input and output data necessary to calibrate and evaluate the model on the six European landscapes of the NitroEurope project (2006-2011), including the two landscapes used in the ÉCLAIRE project.

NitroScape specifications

NitroScape specifications were defined for the NitroEurope project. They are the same for the ÉCLAIRE project:

- NitroScape must simulate the flows of N_r within landscapes of a few km^2 for periods of several years;
- NitroScape must account for landscape structure and spatial heterogeneity, especially the position and intensity of N_r sources and sinks, as well as spatial interactions between landscape elements;
- NitroScape must be dynamic (i.e. it is not a steady-state model);
- NitroScape must integrate, as far as possible, existing models (called elementary models) for each landscape compartment;
- NitroScape must be consistent between models describing the landscape compartments, in terms of process complexity, spatial resolution and time resolution;
- The elementary models of NitroScape must be freely available;
- The code of each elementary model must be fully available and use the more common programming languages (C, C ++, Fortran, Java, Python), it should preferentially be run on Linux systems but also should be compatible with Windows operating systems;
- Updates of each elementary model when needed must be made by the team developing the model;
- The NitroScape structure must be generic and modular to ease the integration of new elementary models or the exchange of an elementary model by another in each landscape compartment;
- NitroScape must be able to exchange data with a spatial database.

Elementary models

At the beginning of the ÉCLAIRE project, the NitroScape model integrated four models describing the N_r processes in four landscape compartments:

- The FASSET model (Bernsten et al., 2003) simulates nitrogen management of farms within the landscape and also exchanges with farms outside the landscape; NH_3 and N_2O emissions are modelled from emission factors (IPCC, 2006) for animals in stables, effluent stores and fields; FASSET operates on a daily time step integrated over a year;
- The CERES-EGC model (Gabrielle et al, 2006) simulates nitrogen transformations and transfers in agro-ecosystems: water, carbon and nitrogen cycles, crop growth and production, energy balance, evapotranspiration, heat and water flows in the soil above 180

cm; NH₃ emissions are modelled from the approach developed in the Volt'Air model (Génermont and Cellier, 1997); N₂O emissions from nitrification and denitrification processes are modelled by integrating the NOE model (Hénault et al., 2005); NO emissions are modelled from the nitrification model developed by Laville et al. (2005); CERES-EGC works at the plot level and at a daily time step integrated over a year;

- The TNT model (Beaujouan et al., 2002) simulates water and NO₃⁻ transfers in agro-ecosystems through the hydrological pathway; it integrates surface runoff, leaching and exfiltration, exchanges between the surface layers of soil and groundwater, and deep flows (below 180 cm); TNT works on a regular grid at a daily time step integrated over one year and for the whole catchment;
- The short-term version of the OPS model (OPS-st, van Jaarsveld et al., 2004) simulates the NH₃ fluxes between agro-ecosystems through the atmosphere by integrating processes of NH₃ dispersion, transfer and deposition; it can work on areas of different sizes by integrating short nitrogen transfers (OPS-st, Gaussian approach) and longer distance transport; the landscape is represented by a regular grid; OPS-st works at a hourly time step; it is a proprietary model (RIVM, the Netherlands) and can be used under agreed conditions.

An additional elementary model namely the linker (Duret et al., 2008) manages data exchange between the elementary models and calculates the nitrogen budget at the pixel or the landscape scale at every time step (one day) or at the end of one simulation (one to a few years). The linker manages the exchanges of variables between the elementary models on the one hand and between the elementary models and the spatial database on the other hand; the linker also verifies the consistency of the simulated values, especially in terms of nitrogen budget of the whole landscape or for specific parts of the landscape.

The PALM coupler (Buis et al., 2006) couples all elementary models. Pre-processing and post-processing routines were developed to prepare data extracted from the database and format NitroScape outputs for analysis and graphical representations.

NitroScape application to theoretical landscapes

At the beginning of the ÉCLAIRE project, NitroScape was able to simulate N_r fluxes within a theoretical idealized landscape of 304 ha (1.75 x 1.75 km²) described by a regular grid of 70 × 70 grid squares of 25 x 25 m² each (Duret et al., 2011). This theoretical landscape was designed to highlight the vertical and lateral N_r flows in rural areas of mixed farming with high animal densities resulting in high N_r flows (Drouet et al., 2012). This first version of NitroScape was not designed to work on real landscapes.

3.2. NitroScape updates to reflect ÉCLAIRE needs

New developments and many tests were made for the ÉCLAIRE project to produce a more reliable user-friendly version of NitroScape that could be applied to real landscapes. Obtaining a reliable model code was the priority before applying it to real landscapes, where interpretations of results may strongly influence choices related to nitrogen policy or landscape planning.

Overall NitroScape structure

Initial NitroScape simulations revealed inconsistencies in N_r fluxes. Checking data flows and data exchanges between the elementary models was a major task for the ÉCLAIRE project and was carried out at INRA. Many errors in the initial codes were detected when running NitroScape: errors resulting from changes in the compiler, changes of operating system, inconsistencies of units used by models for a given variable and inconsistent exchange of variables between models, especially between the CERES-EGC model and the TNT model, which both simulate N_r in the first soil layers. Solving these errors generated more errors in the model output (as is common in programming). Development and testing of a complex model such as NitroScape is a long iterative process that is very time-consuming. Time for development and testing was underestimated resulting in delays in progress (as highlighted in

the WP reports). The PALM coupler was updated with an open source code (Open-PALM) in collaboration between INRA and CERFACS, which has made the coupler easier to implement and has reduced simulation duration. Solving errors, improving communication between elementary models and using the new version of PALM made it possible to improve the computational performances of NitroScape. Code optimization and parallelisation are still in progress to facilitate the application of NitroScape to real landscapes, which are potentially represented by a very large number of pixels.

Farm model

The version of FASSET integrated in the first version of NitroScape could only be run on the theoretical landscape. Much time was used in the ÉCLAIRE project to update the FASSET model (in collaboration between INRA and Aarhus University) and to make it able to read data from the database. This work could not be completed and it was decided at the 4th General Assembly (2014) to abandon the integration of an updated version of FASSET into NitroScape. A simplified farm model namely FARM-EF was developed at INRA by the end of 2014 to model NH₃ and N₂O emissions by animals in stables, grazing animals and effluent storage areas. It uses the IPCC emission factors (2006) and the results from the collective expertise on "Nitrogen and livestock" carried out by INRA (2012).

Agro-ecosystem model

A new version of CERES-EGC, developed at INRA, was integrated into NitroScape. It includes modules of denitrification and nitrification updated from Lehuger (2009). It also includes an automatic transformation of the reference version (CERES-EGC 1D operating at the scale of individual plots) to a spatial 2D version (simulating simultaneously all plots of the landscape by using the PALM coupler). A system of code versioning (subversion) has made it easier to integrate the new developments in the CERES-EGC code into NitroScape. All crop modules were tested, checked and corrected when needed. A simplified grassland module based on existing formulations and information from the literature was implemented in 2015. Although this grassland module has produced consistent initial results, it still needs to be tested more thoroughly before being applied to real landscapes. The work on implementing a forest module has also been started.

Hydrological model

The TNT model was updated with the integration of new modules (NH₄⁺ transfer and transformation, especially in lowland areas...) or the improvement of existing modules (deep water transfer...) to better simulate N_r fluxes and concentrations in the hydrological network.

Atmospheric model

Since the OPS-st model is a proprietary model, an alternative atmospheric model was implemented into NitroScape. The FIDES-3D-Surfatm model (Blanchon, 2013) developed at INRA results from the coupling between a soil-vegetation-atmosphere exchange model (Surfatm, Personne et al., 2009) and a model of Gaussian dispersion (FIDES, Loubet et al, 2001). Surfatm calculates the density of NH₃ sources from vegetation parameters and atmospheric concentration, whereas FIDES calculates the matrix of NH₃ dispersion in the atmosphere and the contribution of each source cell to each sink cell of the domain. FIDES-3D-Surfatm models NH₃ concentrations and fluxes in the atmosphere at a given height. This work was carried out under French-funded projects. It clearly benefits ÉCLAIRE since the description of processes for NH₃ emission, dispersion, transport and deposition, especially bi-directional exchanges in the soil-vegetation-atmosphere module, are an improvement on those of the OPS-st model. The generic and modular structure of NitroScape makes it easy to compare different models for a given landscape compartment (e.g. the atmosphere).

NitroScape application to theoretical and real landscapes

The updated version of NitroScape integrates the linker and four models: FARM-EF, CERES-EGC, TNT and OPS-st or FIDES-3D-Surfatm. The code structure is now stabilised. Numerous tests carried out on the theoretical idealized landscape of 304 ha have produced consistent results in terms of nitrogen flows within each landscape compartment and consistency with the input data.

The calibration and evaluation of NitroScape was done on the landscape of Kervidy-Naizin (Brittany, France) for which the dataset was the most complete and ready to be use among the six NitroEurope landscapes. Initial simulations have produced satisfactory results, which were consistent with measurement data.

Conclusions and perspectives

The NitroScape model was updated to reflect ÉCLAIRE needs. The computational codes were improved, tested and checked to make NitroScape a reliable tool to simulate nitrogen transfer and transformation within landscapes. New modules were integrated and several existing models were improved to model all relevant processes related to the transfer and transformation of N_r within landscapes. NitroScape was made more user-friendly to be used on various landscapes and in relationship with a spatial database.

Development and testing of a complex model, such as NitroScape, is very time-consuming, a task that is very often underestimated. In addition, the computing engineer who was working part time on NitroScape by mid-2012 left the lab at the end of 2014. This led to delays in the progress of NitroScape. NitroScape was applied and tested on a French landscape, for which datasets were complete and ready to be used.

NitroScape is now ready to be used on other landscapes, especially the Scottish and the Dutch landscapes of the ÉCLAIRE project, subject to the availability of the input data required by NitroScape.

3.3. Use of NitroScape to evaluate the sub-grid variability of regional models

A PhD student, Niramson Azouz, was recruited to evaluate the sub-grid variability of regional models by using a local approach at the landscape scale. This works fits within the objectives of WP8. Models of nitrogen fluxes or air pollution operating at regional scales use large spatial resolutions (typically ranging from $5 \times 5 \text{ km}^2$ up to $50 \times 50 \text{ km}^2$). Simulations may lead to the under- or over-estimation of N_r concentrations and fluxes since those models do not take into account spatial interactions in N_r fluxes and their variability within grid cells. However, spatial interactions may be significant between nitrogen sources (animal housing, manure storage, manure spreading) and sinks (e.g. semi-natural agro-ecosystems) at the landscape scale (a few km^2 or tens of km^2). They depend on nitrogen management by farmers and landscape structure which play a role in atmospheric and hydrological transfer of nitrogen between landscape elements and subsequent environmental impacts.

The objectives of the thesis were to:

- Develop and test a methodology to quantify biases and uncertainties in predictions of nitrogen fluxes and air pollution by a regional model of atmospheric transfer (CHIMERE, Menut et al., 2013), by assessing the sub-grid variability using a process-based model at the landscape scale (NitroScape model);
- Implement this methodology to quantify the variability of nitrogen fluxes within large grid squares;
- Provide tools or recommendations (e.g. simplified landscape model, initialization of regional models, determination of thresholds or formulations for gridding regional models, quantification of uncertainties...) for the improvement and use of regional atmospheric models;
- Analyse the impact of agricultural activities, land use change within landscapes and climate change on issues related to nitrogen (e.g. nitrogen transfer and deposition, air quality, pollution of sensitive areas).

Initial results show large differences between NH_3 concentrations and NH_3 dry deposition predicted by the CHIMERE model and the NitroScape model, the effect of the position of NH_3 sources on the spatial distribution of NH_3 fluxes and the effect of model resolution of NH_3 fluxes. They also showed

statistical relationships between NH₃ dry deposition simulated by OPS-st and the distance from the source.

The beginning of the thesis was delayed due to the difficulty to obtain the other part of the funding and the correct candidate. The thesis started in September 2013 and will end in August 2016.

References

- Beaujouan V., Durand P., Ruiz L., Aurousseau P., Cotteret G., 2002. A hydrological model dedicated to topography-based simulation of nitrogen transfer and transformation: rationale and application to the geomorphology-denitrification relationship. *Hydrological Processes*, 16, 493-507.
- Berntsen J., Petersen B.M., Jacobsen B.H., Olesen J.E., Hutchings N.J., 2003. Evaluating nitrogen taxation scenarios using the dynamic whole farm simulation model FASSET. *Agricultural Systems*, 76, 817-839.
- Buis S., Piacentini A., Declat, D., 2006. PALM: a computational framework for assembling high-performance computing applications. *Concurrency and Computation-Practice and Experience*, 18, 231-245.
- Drouet J.L., Duret S., Durand P., Cellier P., 2012. Modelling the contribution of the short range atmospheric and hydrological transfers to nitrogen fluxes, budgets, and indirect emissions in rural landscapes. *Environmental pollution*, 159, 3162-3170.
- Duret S., Drouet J.L., Durand P., Hutchings N.J., Theobald M.R., Salmon-Monviola J., Dragosits U., Maury O., Cellier P., 2008. NitroScape specifications. NitroEurope-IP Internal report, 33 p.
- Duret S., Drouet J.L., Durand P., Hutchings N.J., Theobald M.R., Salmon-Monviola J., Dragosits U., Maury O., Sutton M.A., Cellier P., 2011. NitroScape: a model to integrate nitrogen transfers and transformations in rural landscapes. *Environmental Pollution*, 159, 3162-3170.
- Gabrielle B., Laville P., Duval O., Nicoullaud B., Germon J.C., Hénault, C., 2006. Process-based modeling of nitrous oxide emissions from wheat-cropped soils at the subregional scale, *Global Biogeochemical Cycles*, 20, GB4018.
- Génermont S., Cellier P., 1997. A mechanistic model for estimating ammoniacal volatilization from slurry applied to bare soil. *Agriculture and Forest Meteorology*, **88**, 145–167.
- Hénault C., Bizouard F., Laville P., Gabrielle B., Nicoullaud B., Germon J.C., Cellier P., 2005. Predicting in situ soil N₂O emission using NOE algorithm and soil database. *Global Change Biology*, 11, 115-127.
- Laville P., Hénault C., Gabrielle B., Serça, D., 2005. Measurement and modelling of NO fluxes on maize and wheat crops during their growing seasons: effect of crop management. *Nutrient Cycling in Agroecosystems*, 72, 159–171.
- Loubet B., Milford C. Sutton M.A., Cellier P., 2001. Investigation of the interaction between sources and sinks of atmospheric ammonia in an upland landscape using a simplified dispersion-exchange model. *Journal of Geophysical Research*, vol. 106, NO. D20, Pages 24,183-24,195.
- Personne E., Loubet B., Herrmann B., Mattsson M., Schjoerring J.K., Nemitz E., Sutton M.A., Cellier P., 2009. SURFATM-NH₃: a model combining the surface energy balance and bi-directional exchanges of ammonia applied at the field scale. *Biogeosciences*, 6, 1371-1388.
- van Jaarsveld J.A., 2004. The Operational Priority Substances model. Description and validation of OPS-Pro 4.1, RIVM-report 500045001, RIVM, Bilthoven, The Netherlands.

4. Milestones achieved:

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5. Deviations and reasons:

Although NitroScape was improved substantially during the project, this work didn't result in a useable product within the timescale of ÉCLAIRE for the reasons highlighted above. Since model outputs were needed for WP17, a contingency plan of using concentration/deposition maps from existing models and previous projects was required.

6. Publications:

Niramson Azouz, Jean-Louis Drouet, Matthias Beekmann, Olivier Maury, Pierre Cellier. Evaluation of the sub-grid variability of models simulating atmospheric nitrogen fluxes at regional scale from models integrating processes at landscape scale. Poster presented at the ÉCLAIRE Open Science Conference: Integrating Impacts of Air Pollution and Climate Change on Ecosystems, Budapest, 1-2 October, 2014.

Niramson Azouz, Jean-Louis Drouet, Matthias Beekmann, Olivier Maury, Pierre Cellier. An Intercomparison of models used to simulate the agricultural nitrogen fluxes at regional and landscape scale. Poster presented at the ÉCLAIRE Annual Meeting, Edinburgh, 1-4 September, 2015.

7. Meetings:

Discussions of the work plan, delays to the work and the development of contingency plans have taken place at the annual project meetings and via teleconferences (25 June 2012 and 22 July 2013)

8. List of Documents/Annexes:

None