How to use a process-based model for generating simple ammonia volatilization functions after manure application to arable land

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Abstract
Robust calculations of atmospheric ammonia emission are critical for understanding and predicting impacts, identifying key sources and mitigation measures. The aim of the present study is to use process-based model of ammonia volatilization after manure application to arable land Volt'Air to assess the effects of the main environmental and management conditions on ammonia emissions and to generate simple ammonia volatilization response curves for large ranges of soil, climate and agricultural conditions. Scenarios representative of French conditions were chosen from realistic combinations of these factors.

Introduction
Crops are the source of many gaseous compounds that may have an impact on the atmospheric environment or neighbouring ecosystems: this is particularly the case of ammonia which is 97% from agricultural activities, and for more than one third is related to the application of manure and mineral fertilizer in the field. It is involved in the formation of dust having an impact on human health (PM2.5) and after deposition contributes to soil acidification, declining biodiversity of semi-natural ecosystems, and eutrophication of inland waters. Control of ammonia emissions is a major concern at the international level with the current revision of the Gothenburg Protocol (1999) of the Geneva Convention on Long Range Transboundary Air Pollution distance (1979). This control requires robust calculations of atmospheric ammonia emissions (i) for modelling nitrogen dynamics in agricultural Decision Support System (DSS) e.g. Syst'N [1], (ii) for assessing national ammonia emission inventories using either the tier 2 or the tier 3 approaches following e.g. the EMEP/EEA guide book [2], as well as (iii) for modelling atmospheric ammonia transport, transformation and deposition in air quality models e.g. CHIMERE [3].
Available models of ammonia emission are either empirical or process-based. On the one hand, empirical models are not robust beyond the range of conditions which they were derived from. On the other hand, process-based models are more robust, but they require many input data, which makes them difficult to use for the applications listed above. Ammonia volatilization is indeed a process whose intensity and duration greatly depend on soil and climate conditions, and effluent characteristics [4], that encounter a high variability in agricultural practices. The aim of the present study is to explore the feasibility of using the process-based model of ammonia volatilization after manure application to arable land Volt'Air [5, 6] together with available databases (i) to assess the effects of the main environmental and management conditions on ammonia emissions at the regional and/or national scale for France and (ii) to generate simple ammonia volatilization response curves representative of French agricultural conditions.
The analysis has to be carried out in three steps: 1) uncertainty and sensitivity analysis of the Volt'Air model : uncertainty analysis aims at evaluating the probability distribution on model output from the set of probability distributions on model inputs and sensitivity analysis aims at ranking inputs according to their influence on the output; 2) scenario analysis to assess the actual spatial and temporal variability of ammonia volatilization after application of organic matter for French conditions and 3) conception of the ammonia volatilization functions.

Material and Methods

The Volt'Air model [5, 6]

It has been developed for simulating ammonia volatilisation after liquid organic waste and synthetic fertilizer application on arable land. It consisted in several sub-models that simulate the application of organic and mineral fertilizers, the chemical and physical equilibria between the various species of ammoniacal N in the soil, the transfer of heat, water and ammoniacal N within the soil, and the transfers of ammonia, heat and evaporation between the topsoil and the lower atmosphere. Processes are simulated with short time intervals over several days, or several weeks following the application of ammoniacal nitrogen in the field. The model can operate at an hourly time-step and has the capability to simulate several emission abatement methods such as timing of application, changing fertilizer characteristics and incorporation of the fertilizer following application.

Types and sources of input data

The Volt'Air model requires 3 types of input data to simulate ammonia volatilization: (i) soil types, (ii) climates and (iii) agricultural practices including fertilizer types.

The French soil data come from the INRA, Infosol: the Geographic Database Soil of France (BDGSF) « *Le millionième* » which is currently the only database on spatial soil covering the whole French territory and the Database Analysis of Earth (BDAT) to complete the physico-chemical properties of soil [7].

The meteorological data come from 13 weather stations belonging to INRA and MeteoFrance selected in a way to represent a large range of climatic conditions encountered throughout the French territory. Meteorological data required are air temperature, precipitation, wind speed, air humidity and global radiation collected at an hourly time-step from January 2000 to December 2011.

The agricultural practices data come from the typology of regional cropping systems developed within the framework of the DSS Syst'N by regional experts, dealing with type of fertilizer, amounts applied, date of application... Six types of organic fertilizers applied to arable land are investigated: cattle slurry, cattle manure, pig manure, poultry manure, sewage sludge and compost. Emissions from urea, ammonitrate and nitrogen solution also will be studied in the case of mineral fertilizer.

Choice of the ranges of the input data and parameters for the sensitivity screening

A preliminary work is to define for each parameter and variable of Volt'Air their actual distribution for values encountered in field conditions. In this feasibility study, we focus on the soil properties, that is to say texture and pH and on agricultural practices: for example, the day of nitrogen application vary from 2 days before and 2 days after the typical value.

The model is executed by varying each parameter in turn and selecting values from selected ranges. The value for the other parameters should be the 'best estimate' for the value of that parameter. This will allow the model to be tested over the range of possible field conditions as well as the range of variation in the variables themselves.

Construction of representative scenarios for French regions

Realistic scenarios (i.e. observed combinations of values for the input variables) are created allowing a more meaningful interpretation of the results of the model analysis. In this feasibility study, we focus on the maize crop cultivated in two French territories Brittany and Île-de-France to test the methodology before applying it on the other main crops and whole France.

Choice of the statistical method to use for the analysis

For a complex model like Volt'Air, it is not possible to calculate the probability distribution analytically and other approaches should be used. We plan to use the four-step approach, based on Monte Carlo simulations: (i) define probability distributions for the uncertain model inputs and parameters, (ii) generate values from the distributions defined at (i); (iii) compute the model output(s) for each generated input set and (iv) describe/approximate the distributions of the model output(s) [8]. For the sensitivity analysis, we plan to use the multivariate global sensitivity analysis [8]. This paper presents the first attempt of using those methods for Volt'Air and evaluating the number of simulations needed.

Expected results
The expected results of the study are:
(1) determine which parameters need to be collected more accurately;
(2) determine possible simplification of the model: we try to take the opportunity of those analyses with a huge number of simulations to generate functions of ammonia volatilization, like for example (i) response curves of ammonia volatilization to parameters and variables having the greatest influence, sometimes depending on regional environmental and management specificities, and/or (ii) tables of country-specific or region-specific "Emission factors". Those relationships will be based on the underlying physical, chemical or biological processes leading to ammonia volatilization.

Conclusion and perspectives
This feasibility study will help us to calibrate and refine the databases needed, the simulations to perform, and the analysis to carry out in order to perform complete uncertainty and sensitivity analyses.
We can generalize the generation of simple volatilization functions in a metamodeling approach. This should help (i) producing system diagnosis and advice for a sustainable agriculture, helping to reduce N losses to the environment and avoiding pollution swapping, (ii) improving the quality of the French National Inventory of ammonia emissions, by taking into account country or region-specific emission factors and specific abatement technique effect, (iii) improving the quality of the prediction of particulate formation.

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