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Abstract

Estimation of nitrous oxide (N_2O) emissions from arable soils, in relation to crop fertilization, is essential to devise strategies to mitigate the impact of agriculture on global warming. This paper presents the development and test of a N_2O model resulting from the linkage of a dynamic soil-crop simulation model (CERES) with two sub-models of N_2O production and reduction in soils. These sub-models (NOE and NGAS) account for both the nitrification and denitrification pathways. The resulting models (CERES-NOE and CERES-NGAS) were tested against experimental data collected on three contrasting wheat-cropped soils representative of the Beauce agricultural region in France.

Although the input variables for the N_2O modules were correctly simulated, CERES-NGAS was over-responsive to soil water content in a Haplic Calcisol, and strongly over-estimated the N_2O fluxes as a result. On the other hand, CERES-NOE predicted correct mean N_2O emission levels for all sites, but failed to simulate the peak fluxes observed in the weeks following fertilizer application in the most N_2O-productive soil. Both models achieved root mean squared errors in the 23 to 26 g N-N_2O ha^{-1} d^{-1} range, significantly higher than the average experimental error on the measurements. On the other hand, their mean deviations were acceptable, being lower than 2.2 g N-N_2O ha^{-1} d^{-1}, compared with a mean observed flux of 7.9g N-N_2O ha^{-1} d^{-1}. Overall, the response of CERES-NOE to soil type was more accurate, but this came at the cost of costly, site-specific characterization on the soils' biological properties. The development of pedo-transfer functions to infer these parameters from basic soil characteristics appears as a pre-requisite for the use of CERES-NOE on a wider scale.

Keywords

CERES, Fertilization, Greenhouse gases, Modelling, Nitrous oxide

Introduction

Emissions from arable soils are a key item in the global nitrous oxide (N_2O) budget, making up about half of the terrestrial biogenic emissions (Mosier et al., 1998). Since agricultural activities are gradually coming into focus in the greenhouse gases budget calculations, precise estimates of current N_2O emissions from arable land are being sought, along with possible means of abatement. However, compared to other greenhouse gases such as CO_2, N_2O fluxes are of small magnitude and highly variable in space and time (Duxbury and Bouldin, 1982), being tightly linked to the local climatic sequence and soil properties. This variability makes it it is difficult to discriminate the effect of agricultural management *per se* (Mosier, 1994). The prediction of N_2O emissions within agro-ecosystem models appears as a promising route to deal with this issue, using scenario analysis to single out the effect of crop management practices such as fertilizer applications.

Nitrous oxide is evolved by soils as the result of two micro-biological processes: nitrification and denitrification, which occur mostly in the soil surface. Theses processes are controlled by variables such as water content, temperature, concentrations of inorganic N and soil C respiration rates, most of which are simulated by currently-available process-based agro-ecosystem models. Some of these models were thus adapted to simulate the emissions of N_2O as part of the nitrogen cycle in agro-ecosystems. They range from complex models simulating the dynamics of water, solutes, microbial processes on a fine-scale to simple, empirical tools based on statistical inference (Frolking et al., 1998). Examples include DNDC (Li et al., 1992), *ecosys* (Grant et al., 1992) on the complex end of the spectrum, and NGAS (Parton et al., 1996) or (Muller et al., 1997)'s model at the other end. As a general rule, complex models involve many parameters and require a lot of *a priori* knowledge on the system under study, whereas simpler models are easier to use and more robust. As a result, none of the above-cited approaches clearly emerged as best at predicting N_2O fluxes (Frolking et al., 1998). It was nevertheless shown that the use of simple denitrification equations without prior site-specific calibration yielded rather poor results (Marchetti et al., 1997).

Current N_2O models generally use a crude representation of crop growth, whereby dry matter accumulation or N uptake is a function of simple driving variables such as air temperature (Frolking et al., 1998). Thus, they are hardly able to simulate the interactions of crop growth and yield with the dynamics of soil water and nitrogen, and ultimately crop management. Such capacity is however a pre-requisite to the definition of practices minimizing N_2O losses, essentially N fertilization. On the other hand, agronomic models simulating the growth of crops as a function of management and environmental conditions generally do not account for N_2O losses. It is thus important that agronomic models incorporate such major environmental processes as those governing N_2O emissions. Also, N_2O mitigation scenarios should consider the consequences on other environmental terms, such as nitrate leaching or NH_3 volatilization.

Here, we set out to link up a soil-crop model derived from the CERES family (Jones and Kiniry, 1986) with two stand-alone modules of N_2O emissions from soil: NOE (Hénault et al., 2005), and NGAS (Parton et al., 1996, Parton et al., 2001). We tested the resulting models (CERES-NOE and CERES-NGAS) under contrasting environments, using experimental data collected in Central France.

Material and Methods

The CERES, NOE and NGAS models

NOE

NOE is a semi-empirical model simulating the production and reduction of N_2O in agricultural soils through both the denitrification and nitrification pathways. The denitrification component of NOE is based on NEMIS (Hénault and Germon, 2000), a model that expresses total denitrification of soil NO_3^- as the product of a potential rate with three unitless factors related to soil water content, nitrate content, and temperature. The fraction of denitrified nitrate that evolves as N_2O is then considered as constant for a given soil type.

In a similar fashion, nitrification is modelled as a Michaëlis-Menten reaction, with NH_4^+ as substrate. The corresponding rate is multiplied by unitless modifiers related to soil water content and temperature. As for denitrification, a soil-specific proportion of total nitrification evolves as N_2O. The two pathways are connected in that NO_3^--derived N_2O may be reduced to N_2 by denitrification, should the two processes be simultaneously active. This linkage between the two processes has a micro-biological basis, but has not yet been introduced in N_2O models. NOE is described in details elsewhere (Hénault et al., 2005).

NGAS

Similarly to NOE, NGAS is a stand-alone model that calculates N_2O emissions from nitrification and denitrification (Parton et al., 1996, Parton et al., 2001). It operates on a daily time step, and is driven by surface soil temperature, NO_3^- and NH_4^+ content, and heterotrophic C respiration rate. Like NOE, NGAS predicts total nitrification and denitrification rates as the product of various response functions to the above inputs. The fraction of N_2O evolved as a result of these processes is either fixed (set to 2% for nitrification), or increases as soil water content increases (for denitrification-mediated N_2O). Compared to NOE, the main specific features of NGAS are: its using C respiration as an indicator of the microbiolgical demand for electron acceptors (including O_2 and NO_3^-); its assuming denitrification to be controlled both by environmental conditions (soil O_2 concentration) and molecular species (labile C and available NO_3^-); and its using soil pH to control nitrification. Here, we used the equations currently implemented in the nitrification and denitrification routines of the ecosystem model DAYCENT (Grosso et al., 2001), which incorporates NGAS.

CERES

CERES comprises sub-models for the major processes governing the cycles of water, carbon and nitrogen in soil-crop systems. A physical module simulates the transfer of heat, water and nitrate down the soil profile, as well as soil evaporation, plant water uptake and transpiration in relation to climatic demand. Water infiltrates down the soil profile following a tipping-bucket approach, and may be redistributed upwards after evapo-transpiration has dried some soil layers. In both of these equations, the generalized Darcy's law has subsequently been introduced in order to better simulate water dynamics in fine-textured soils (Gabrielle et al., 1995).

Next, a micro-biological module simulates the turnover of organic matter in the plough layer, involving both mineralization and immobilisation of inorganic N. In this version, the NCSOIL model (Molina et al., 1983) was substituted for the original CERES-module. NCSOIL comprises three OM pools, decomposing at a fixed rate and recycling into the microbial biomass. Nitrification and denitrification are part of the N_2O modules NOE and NGAS, which were detailed in the above paragraphs. The linkage of these modules within the CERES shell are described in the next paragraph.

Lastly, crop net photosynthesis is a linear function of intercepted radiation according to the Monteith approach, with interception depending on leaf are index based on Beer's law of diffusion in turbid media. Photosynthates are partitioned on a daily basis to currently growing organs (roots, leaves, stems, fruit) according to crop development stage. The latter is driven by the accumulation of growing degree days, as well as cold temperature and day-length for crops sensitive to vernalization and photoperiod. Lastly, crop N uptake is computed through a supply/demand scheme, with soil supply depending on soil nitrate and ammonium concentrations and root length density.

CERES runs on a daily time step, and requires daily rain, mean air temperature and Penman potential evapo-transpiration as forcing variables. The CERES models are available for a large number of crop species, which share the same soil components (Jones and Kiniry, 1986).

Linkage of CERES with NOE and NGAS

Input variables for the N_2O modules NOE and NGAS include surface soil moisture content, temperature, NO_3^- and NH_4^+ content, and heterotrophic carbon respiration rate. These inputs were supplied by the physical and micro-biological modules of CERES, independently of NOE and NGAS. However, there was one process common to the three models, namely nitrification. Both NOE and NGAS indeed incorporate nitrification as part of the sequence of calculations leading to the prediction of N_2O emissions. Nitrification is also required to predict the fate of ammonium in the soil micro-biological module of CERES. Here, we chose to use the nitrification routine of NOE because its parameters had been estimated from site-specific incubation data for the three soils. In the NGAS routine implemented within the CERES-NGAS model, the nitrification rate was thus only used as an intermediate variable in the calculation of N_2O production via nitrification. This raises a consistency problem between the nitrification rate actually used in the model to simulate the fate of ammonium N, and the virtual one calculated in NGAS. Comparison of the two nitrification estimates showed that the rates calculated by NGAS were surprisingly small, being about an order of magnitude than those calculated with the NOE routine. Thus, the NGAS routine was driven with ammonium data characterized by a higher turnover-rate than the stand-alone model would have predicted. On the other hand, it is reassuring that the amount of NH_4^+-N evolved as N_2O, as calculated by NGAS, never exceeded the total amount of NH_4^+ nitrified, as calculated in the common NOE nitrification routine.

Another coupling issue involves the spatial resolution of CERES and the N_2O modules. Since

NOE was initially developed for on 20-cm intact topsoil cores, it was run within CERES only down to the 20 cm depth. Because CERES uses 10-cm thick soil layers in the soil surface, NOE was thus run for each of the two top layers, and the resulting predicted N_2O fluxes were compounded to yield the total flux evolved from the soil. As regards NGAS, previous tests against field emission data involved calculations over the 0-15 cm depth (Parton et al., 1996, Parton et al., 2001). We thus used the NGAS equations to predict N_2O fluxes from the top two 10-cm layers of soil, and weighted them with coefficients of 1 (for the 0-10 cm layer) and 0.5 (for the 10-20 cm layer) to obtain the total emission flux.

For both N_2O modules, the above procedures reflect a choice consisting in running the module in each of the soil layers used by CERES, and subsequently summing the fluxes so that the overall soil depth involved be consistent with that originally used by the modules' authors. An alternative method would have consisted in averaging the input variables first over the total depth considered (*i.e.* 0-20 cm for NOE and 0-15 cm for NGAS), and then running the modules to directly obtain the total emission fluxes. However this solution yielded quite different estimates from the first one, due to the strong non-linearity of the models. We therefore chose to ignore it, as described in the Discussion section.

Data sets

Three sites were set up in 1998-99 under conventionally-managed wheat in 3 locations with contrasting soils in the Beauce region (Central France). Following the FAO classification (FAO-UNESCO-ISRIC, 1989), the soils involved were a Haplic Calcisol (site name: Villamblain), a Haplic Luvisol (at La Saussaye), and a Gleyic Luvisol (at Arrou).

N_2O emissions were monitored by the static chamber method using circular chambers (0.5 m in diameter and 0.15 m in height), with 8 replicates. On each sampling date, the chambers were closed with an airtight lid, and the head space was sampled 4 times over a period of 2 hours. The gas samples were stored in 3-mL Vacutainer tubes (Terumo Europe N.V., Leuven, Belgium), and analysed in the laboratory by gas chromatography (Hénault et al., 2005).

Soil nitrogen content in the soil profile was monitored every month. Nine soil cores were taken by manual augering, and subsequently cut in 30-cm increments which were pooled layer-wise. Upon each gas sampling date, three cores from the 0-20 cm layer were also taken every three weeks, and pooled into one composite sample with no replicates. The resulting samples were analysed for moisture content and inorganic N using colorimetric methods in the laboratory. Soil temperature and moisture content were also continuously monitored using thermocouples and a time domain reflectometry (TDR) probes (Tektronix, Beaverton, USA; Imko, Müncheberg, Germany). Plants were also sampled and analysed for aerial dry matter, leaf area and nitrogen content using the Dumas method (combustion-based).

Parameterization and running of CERES

The objective of this stage was to calibrate the components of CERES other than its N_2O modules to make sure the latter were supplied with correct simulated inputs. The calibration was run with NOE as the N_2O module. In principle, the calibration may have been influenced by the particular N_2O module used, whether NOE or NGAS. However, the only N flux that differed between both modules was total denitrification, since the nitrification routine was common to the two models. Over the simulation time-frame, the cumulative denitrification fluxes simulated by NGAS and NOE were of the same magnitude, ranging from 1 to 10 kg N ha^{-1}. These fluxes were negligible compared to the magnitude of the fluxes involved in the other model components on which the calibration was done, essentially plant N uptake which totalled more than 200 kg N ha^{-1}. The calibration was thus relatively independent of the particular N_2O module selected. The inputs required by CERES include soil parameters, plant cultivar-specific parameters (qualified as genetics), and daily weather data as forcing variables. The latter data were measured on-site by means of standard meteorological stations. All soils were analysed for their physico-chemical properties (pH, $CaCO_3$, particle-size distribution, organic C and N contents) in the laboratory. Bulk density was measured on undisturbed samples taken to the laboratory. The other physical parameters (water retention and hydraulic conductivity curves) were measured on intact cores taken to the laboratory. To measure retention properties, large undisturbed clods (50 to 100 cm^3 in volume) were collected in winter when soil water content was close to field capacity, and for hydraulic conductivity measurements, soil cylinders (7 cm in diameter, 15 cm in length) were collected at the same period. Water retention properties were determined using a pressure membrane apparatus (Klute, 1986). Unsaturated hydraulic conductivity (K) was assessed using the Wind inverse method (Wind, 1968), while saturated K was estimated with the constant-head method (Klute and Dirksen, 1986). The soil micro-biological parameters involved in the soil organic matter model were set to their default values, as related to total soil organic C content (Houot et al., 1989). Inputs of fresh organic matter from the preceding crops were estimated from the harvested yields. Some soil-specific parameters required by NOE were measured in the laboratory: a potential denitrification rate, measured on intact soil cores (10 cm in diameter and 20 cm in depth), and coefficients of nitrification response to soil moisture content, measured on sieved soil samples (Hénault et al., 2005). Thus, none of the parameters of either N_2O modules were pre-calibrated against field data.

In Arrou where the presence of free water was noted upon soil sampling in wintertime, a water table was simulated at the 120 cm depth from January to mid-March. Lastly, the crop genetic parameters related to phenological development were calibrated against crop biomass data (Gabrielle et al., 2002).

Model evaluation

The simulations of CERES-NOE and CERES-NGAS were compared to field observations using graphics to capture dynamic trends, and statistical indicators gave an idea of the model's mean error. Regarding the latter we used two standard criteria (Smith et al., 1996) : the mean deviation (MD) and the root mean squared error (RMSE). Here, they are defined as: $MD = E(S_i - O_i)$ and $RMSE = (E[(S_i - O_i)^2])^{1/2}$, where S_i and O_i are the time series of the simulated and observed data, and E denotes the expectancy. MD indicates an overall bias with the predicted variable, while RMSE quantifies the scatter between observed and predicted data, which is readily comparable with the experimental error on the observed data.

Results

Water and nitrogen balance

In general, CERES provided satisfactory predictions of the major crop variables, as exemplified in Figure 1 for the Villamblain site. Dynamics of leaf area growth and subsequent senescence was well reproduced, along with the accumulation of biomass and nitrogen in the plant shoots. However, Figure 1 reveals a problem with the crop phenology modules which could not be solved by tuning the genetic coefficients specific to the cultivars used in the experiments. Although final N uptake and crop biomass were generally well predicted, there was a 15-day lag between the observed and simulated cumulative uptake or biomass curves in spring. Correcting for this lag through the genetic coefficients resulted in an anticipation of leaf senescence and a strong under-estimation of final grain yields. This denotes an intrinsic shortcoming in the phenological module of CERES-Wheat.

The effect of this discrepancy on the prediction of water and nitrate contents in the soil profile was however very limited, as can be seen on Figure 2. The relatively good match between simulated and observed nitrate data did not require further calibration, and a similar fit was also noted in the other two sites. The model's RMSE for the prediction of nitrate over the three soil profiles ranged between 7.2 and 12.8 kg N ha^{-1}. CERES tended to under-estimate nitrate content over the soil profile, especially in Arrou (not shown). It may be linked to its rather conservative simulation of net mineralization fluxes, which ranged between 30 and 40 kg N ha^{-1} over the 10 months of the simulation. A two-fold increase in these fluxes would indeed be more typical of the arable soils of this area (Gabrielle et al., 2002). On the other hand, the simulation of soil water content required to increase the field-capacity water content in the topsoil, in Villamblain and La Saussaye, otherwise soil moisture was systematically under-estimated by CERES. Thus, field-capacity contents were incremented by 2% of volumetric water content in the two soils, relative to the estimates derived from the laboratory-determined retention curves. As noted by (Ratliff et al., 1983), the field-capacity content used by tipping-bucket models such as CERES to govern water infiltration may be somewhat different from the estimates obtained by physical characterization of soil water retention. Thus, this calibration was acceptable given the uncertainty in measuring this parameter.

Simulation of inputs for the NOE and NGAS models

Figure 3 provide a visual assessment of the simulation by CERES of four input variables common to the N_2O emission modules, NOE and NGAS. Following the conclusions of the above paragraph, there appears a generally good agreement between the simulated and observed dynamics of the soil state variables involved. Surface temperature is the least problematic variable, with a mean deviation of less than 0.5°C and a mean error (RMSE) ranging from than 1.5 to 2.1°C across the three sites. It should be noted that, over the period considered, soils froze only for a few days and that no significant snowfalls were recorded, which made the energy balance of the soil surface easier to predict. Soil moisture content proved more difficult to simulate, and TDR monitoring enabled a more thorough test of the simulated dynamics in the soil surface. Overall, the wet periods which were particularly relevant to the denitrification process were quite well mimicked by the model. The simulation of drier spells proved was less successful, as may be noted in March and June 1999 in all sites. CERES did not offer a consistent pattern across the soils and dry periods. Soil moisture was slightly over-estimated in Villamblain and Arrou over the May-June time interval. In March through April, it was under-predicted in La Saussaye but over-estimated in Arrou. The latter discrepancies proved quite critical to the prediction of N_2O emissions since it coincided with the fertilizer applications, resulting in conditions particularly conducive to denitrification. Unfortunately, they could not be corrected by adjusting soil hydrodynamic properties since it resulted in larger discrepancies in the rest of the simulation period.

Dynamics of surface nitrate and ammonium contents were essentially driven by the applications of fertilizers in spring. Both mineral forms of nitrogen did not persist for more than a few weeks after fertilizer application, especially ammonium which was rapidly nitrified. In all sites, CERES appeared to over-estimate the rate of this transformation, anticipating the decrease of topsoil NH_4^+ while over-predicting NO_3^- content. Unfortunately it is rather difficult to infer the true dynamics of nitrate at that time since fertilizer applications make it highly variable in the field. This shows in the wide error bars associated with the average NO_3^- and NH_4^+ contents in Fig. 3. Over the rest of the season, CERES failed to reproduce the background topsoil NH_4^+ stock of about 5 kg N ha^{-1}, due to its quickly nitrifying all the NH_4^+ pool. Whether this residual NH_4^+ participates in the dynamics of N as a transient pool, or is somehow withheld by the soil matrix remains open to debate, but presumably it did not influence the N_2O emissions.

Prediction of N_2O fluxes

Figure 4 provides a comparison of the observed N_2O emissions at the three sites and the simulations by CERES-NOE and CERES-NGAS, while Table 2 gives quantitative indicators of models' performance.

The magnitude of the observed N_2O fluxes varied markedly among the soils, with the highest emissions occurring with the Gleyic Luvisol at Arrou (range: 0 to 100 g N-N_2O ha^{-1} d^{-1}), and the lowest with the Haplic Luvisol at La Saussaye (range: 0-5 g N-N_2O ha^{-1} d^{-1}). The Haplic Calcisol at Villamblain presented an intermediate situation, with low background fluxes and two peaks after fertilizer applications rising to 30 g N-N_2O ha^{-1} d^{-1}. According to the laboratory micro-biological studies, the three soils had the similar nitrification and denitrification potentials. Only the Arrou soil was singled out because of the high fraction (64%) of denitrified N it evolved as N_2O, compared to the other two soils for which this fraction was measured as 20%. This explains why the highest emissions occurred in Arrou. Otherwise, the water regime was the predominant factor behind the emissions, as it determined the frequency of anoxic periods conducive to denitrification. As an indicator of this behaviour, we computed the percentage of days in which the average reading from the TDR probes was above the threshold used by NOE to trigger denitrification, corresponding to a water-filled pore space of 62%. Over the *circa* 200 days of TDR monitoring, the percents were 73%, 76% and 87% for the Villamblain, La Saussaye and Arrou soils, respectively. This reflects the ranking mentioned for the mean N_2O fluxes earlier, and shows the influence of surface hydrodynamic properties. Over the season, the time distribution of N_2O emissions were also modulated by NO_3^- content, with the highest rates concentrated in the spring period. The effect of temperature appeared essentially in winter, when it drastically hampered microbial activity and hence the production of N_2O.

The two N_2O models responded to variability across soils and over time with various degrees of success. They simulated a broad range of emission rates across sites and throughout the season - albeit with different patterns. CERES-NGAS strongly over-estimated the fluxes in Villamblain, where it simulated the highest emissions. These may be explained by the higher simulated WFPS values in Villamblain, where topsoil WFPS averaged 80% over the simulation period, compared to 66% in Arrou and 69% in La Saussaye. CERES-NGAS predicted much lower fluxes in the other two sites, especially in Arrou where it under-estimated the flux by 17 g N-N_2O ha^{-1} d^{-1} on average. CERES-NGAS thus failed to predict the observed ranking of sites in terms of N_2O emissions. However, its errors compensated across the three sites, and it achieved a mean deviation of only -1.5 g N-N_2O ha^{-1} d^{-1}, which compares well with a mean observed flux of 7.9 g N-N_2O ha^{-1} d^{-1}. On the other hand, CERES-NOE achieved more acceptable mean deviations for all the three sites, ranging from 0.2 to 5.4 g N-N_2O ha^{-1} d^{-1}, and correctly predicted the ranking of the three sites (Table 2).

In Arrou, CERES-NOE anticipated the emission peaks observed in early spring by about three weeks, while CERES-NGAS did not predict any peak at all. These peaks occurred from three to five weeks following fertilizer application. Because the soil was relatively dry in that period, the models simulated very little denitrification activity or none. Nitrification was quite active on the other hand, with simulated rates ranging from 3 to 6 kg N ha^{-1}. However, they translated only as a few g N-N_2O ha^{-1} d^{-1} in the CERES-NOE simulations because in the parameterisation for Arrou only 0.06% of the nitrified N was evolved as N_2O (Hénault et al., 2005). CERES-NGAS simulated a higher proportion of nitrified N converted to N_2O, but its calculated nitrification rates were an order of magnitude lower than those calculated by CERES. The reason for the low nitrification rates with NGAS is that the latter used a maximum nitrification rate of 6 kg N ha^{-1} d^{-1} over the 0-15 cm depth, and that this rate was multiplied it by an overall modifier ranging between 0.1 and 0.2. This modifier compounded the effects of various abiotic factors such as soil water content, temperature, and pH, which were moderately conducive to nitrification. As a result, the nitrification-N_2O fluxes predicted by CERES-NGAS did not exceed 7 g N-N_2O ha^{-1} d^{-1} over the spring period considered.

The fact that none of the models could predict the peak emission data in Arrou was especially critical since these data points were the maximum measured values, and thus played an important role in the statistical performance criteria. As a consequent, CERES-NOE and CERES-NGAS achieved similar RMSEs across the three sites, ranging from 23 to 26 g N-N_2O ha^{-1} d^{-1}. Both RMSEs were significantly greater than the experimental error on the measurements (Table 2).

According to both models, denitrification was responsible for most of the emissions, with a fraction ranging from 93.7 to 98.1% for CERES-NOE and from 96.7 to 99.5% for CERES-NGAS (Fig. 5). It is also noticeable that, although the models predicted various magnitudes of denitrification-N_2O fluxes, they simulated similar levels of nitrification-mediated N_2O emissions.

Discussion

Coupling issues

This paper presents an attempt at linking stand-alone gas emission modules with a more global ecosystem model. In this phase, care was taken so that, once integrated into the CERES environment, the original modules would not be made to function under a set of conditions too remote from their development context. However, some degree of liberty was necessary to maintain some coherence among the resulting two models. The use of the heterotrophic C respiration and nitrification rates output by CERES provides two illustrations. Regarding the former, NGAS originally included a simple equation to predict them from soil temperature and water content

(Parton et al., 1996). In our case, this equation produced values an order of magnitude higher than the CERES estimates. However, it is interesting to note that the use of these values instead of the CERES simulations resulted in a strong over-estimation of N_2O fluxes in all sites (not shown). This implies that using the CERES estimates was the soundest option, altogether with being more consistent. On the other hand, the CERES nitrification rates were much higher than those calculated by NGAS. As a result, NGAS was supplied with soil ammonium contents that decreased quicker over time than would have been predicted from the NGAS nitrification rates themselves. It follows that the use of the NGAS rates instead of the CERES simulations would have resulted in sustaining significant nitrification-N_2O emissions longer after the applications of fertilizer in spring. This option proves however irrelevant since the measured dynamics of ammonium content actually fitted the pattern predicted by CERES (Fig. 3).

The integration of the N_2O modules within the vertical soil layering scheme of CERES proved a more sensitive issue. Two questions needed to be addressed in the linkage: i/ the depth over which to calculate the gaseous fluxes, and ii/ the procedure for averaging over the various soil layers involved.

As regards the first item, Fig. 6a compares two calculation depths in Villamblain in the case of CERES-NOE: 20 cm and 30 cm. The former depth was taken as our baseline given that NOE was developed using soil data measured in the 0-20 cm layer. However, in an arable soil subjected to regular ploughing, it is likely that denitrification and nitrification occurs deeper than 20 cm (Iqbal, 1992). The use of the 20 cm depth, and likewise of the 0-15 cm layer by NGAS reflects more the experimental conditions particular to the development of the N_2O modules than the actual vertical extension of N_2O production and diffusion in soils. Thus, while the question of integration depth remains open, it is notable that it did not make such a dramatic difference in the simulated fluxes (Fig. 6a). Should the emissions have been proportional to soil depth, there would have been a factor of 3/2 between the 0-20 cm and 0-30 cm calculations, respectively. The fact that this was clearly not the case shows that the physical characteristics of the 20-30 cm soil layer were less conducive to denitrification than those in the above layers.

As for the second coupling issue, Fig. 6b compares a procedure in which NOE was run on input data averaged over the 0-20 cm depth with one in which NOE was run for each the top two 10-cm layers, prior to summing the resulting individual fluxes over the 0-20 cm layer. It shows that averaging the NOE soil input data before calculating the N_2O emissions yielded markedly higher fluxes throughout the simulation. This increase relative to the ’simulate and average’ option probably stems from the strong non-linearity of the NOE equations, and the vertical gradients in moisture content and temperature in the surface layers. From a mathematical point of view, the second procedure is more rigorous (Addiscott et al., 1995), and was selected here. However, one may note that the first procedure was more consistent with the data used in the development of NOE (based on bulk data taken on the 0-20 cm soil cores).

Performance of CERES-NOE and CERES-NGAS

In the testing phase, we made use of all the available data to ensure a correct simulation of the input data for the N_2O modules. Thus, no striking discrepancies appeared in the simulation of topsoil physical and chemical variables. Such conditions were usually not met in previous N_2O models tests or comparisons (Frolking et al., 1998, Smith et al., 2002), despite their being a pre-requisite to the discussion of the relative merits of individual trace-gas modules. Only the simulated soil microbial respiration rates, which were used as input to the NGAS denitrification component, were not checked against field data.

The two models nonetheless experienced some difficulties in predicting either the mean magnitude of N_2O emissions across soils, or their time course over the season investigated. They failed under different sets of experimental conditions: CERES-NGAS was over-responsive to water content in Villamblain, and under-responsive to soil nitrate content in Arrou. In the latter site, CERES-NOE was also incapable of reproducing the high emission rates, being under-responsive to water content in the weeks following fertilizer application.

A key issue faced by both models was the scaling from laboratory to field conditions. Both models based on laboratory data to derive the equations for denitrification- and nitrification-mediated N_2O, since this partitioning is hardly accessible *in situ*. Except for the nitrification component of NOE, the two models were developed from incubations of intact soil cores (Parton et al., 2001) as opposed to disturbed soil samples, which is clearly a progress compared to earlier models (Parton et al., 1996). The use of sieved soil indeed would have implied ignoring the structure and dynamics of soil aggregates, which are a predominant control of denitrification in the field (Vinten et al., 1996, Renault et al., 1994). Thus, some of the controls occurring in the field were already active in the laboratory experiments used to develop NOE and NGAS. However it seems that this did not suffice in ensuring correct predictions in all soil types.

From a more general prospective, the chances of success when applying a model to a new field situation depend on the degree of similarity between the set of situations used in model development, and the particular situation at stake. Here, NOE evidently stood better chances since some of its parameters had been measured in the laboratory for the three sites tested here. Also, it has been developed from data on similar soils in France. On the other hand, NGAS did not require site-specific parameters. Besides, it was originally developed with data from soils from the US Mid-West, which were likely to behave differently from the European soils, in terms of trace-gas production. This was exemplified in the case of the Villamblain soil, for which CERES-NGAS strongly over-estimated the N_2O emissions. However, it is interesting to note that CERES-NGAS gave good predictions for the other two soils, without requiring specific laboratory measurements.

In conclusion regarding the two N_2O modules, CERES-NOE was more accurate in its response to soil properties, but required a significant share of costly, site-specific information. On the other hand, CERES-NGAS was easier to operate - but gave erroneous estimates in one out of the three sites. Prospects for improving the prediction of N_2O using soil-crop models should thus focus on the role of physical and biological controls on the processes of denitrification and nitrification, such as soil structure or the capacity of soils to reduce N_2O. Both properties account for much of the variability in soil N_2O emissions, and do not readily relate to basic soil characteristics (Hénault et al., 2005). The development of pedo-transfer functions, based on a wider sample of soil conditions, to infer these parameters from routinely available soil information appears as a pre-requisite for the use of CERES-NOE or CERES-NGAS on a wider scale.

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References

Addiscott, T. M., Smith, J. U., and Bradbury, N. J. (1995). Critical evaluation of models and their parameters. J. Env. Qual. 24:803-807.

Duxbury, J. M. and Bouldin, D. R. (1982). Emission of nitrous oxide from soils. Nature 298: 462-464.

FAO-UNESCO-ISRIC (1989). Carte mondiale des sols, légende révisée. In *Rapport sur les ressources en sols du monde*, volume 60. Food and Agriculture Organization, Rome.

Frolking, S. E., Mosier, A. R., Ojima, D. S., Li, C., Parton, W. J., Potter, C. S., Priesack, E., Stenger, R., Haberbosch, C., Dörsch, P., Flessa, H., and Smith, K. A. (1998). Comparison of N2O emissions from soils at three temperate agricultural sites: simulations of year-round measurements by four models. Nutri. Cycl. Agroecosys. 52: 77–105.

Gabrielle, B., Mary, B., Roche, R., Smith, P., and Gosse, G. (2002). Simulation of carbon and nitrogen dynamics in arable soils: a comparison of approaches. Eur. J. Agron. 18: 107-120.

Gabrielle, B., Menasseri, S., and Houot, S. (1995). Analysis and field-evaluation of the CERES models' water balance component. Soil Sci. Soc. Am. J. 59:1402-1411.

Grant, R. F., Nyborg, M., and Laidlaw, J. W. (1992). Evolution of nitrous oxide from soil: I. Model development. Soil Sci. 156: 259-277.

Grosso, S. J. D., Parton, W. J., Mosier, A. R., Hartman, M. D., and Keough, C. A. (2001). *Simulated effects of land use, soil texture, and precipitation on N gas emissions using DAYCENT*, pages 413–431. Elsevier Science Publishers, The Netherlands.

Hénault, C., Bizouard, F., Laville, P., Gabrielle, B., Nicoullaud, B., Germon, J. C., and Cellier, P. (2005). Predicting *in situ* soil N2O emissions using NOE algorithm and soil data base. Global Change Biol. 11: 115-127.

Hénault, C. and Germon, J. C. (2000). NEMIS, a predictive model of denitrification on the field scale. Eur. J. Soil Sci. 51: 257-270.

Houot, S., Molina, J., Chaussod, R., and Clapp, C. E. (1989). Simulation by NCSOIL of net mineralization in soils from the Deherain 36 Parcelles plots at Grignon. Soil Sci. Soc. Am. J. 53: 451-455.

Iqbal, M. (1992). Potential rates of denitrification in two field soils in southern England. J. Agric. Sci. 118: 223-227.

Jones, C. A. and Kiniry, J. R. (1986). *Ceres-N Maize: a simulation model of maize growth and development*. Texas A&M University Press, College Station, Temple, TX.

Klute, A. (1986). Water retention : laboratory methods. In Klute, A., editor, *Methods of soil analysis. Part 1 - Physics and Mineralogical Methods*, number 9 in Agron. Monogr., pages 635–660. ASA and SSSA, Madison, 2nd edition.

Klute, A. and Dirksen, C. (1986). Hydraulic conductivity and diffusivity : laboratory methods. In Klute, A., editor, *Methods of soil analysis. Part 1 - Physics and Mineralogical Methods*, number 9 in Agron. Monogr., pages 687–734. ASA and SSSA, Madison, 2nd edition.

Li, C., Frolking, S. E., and Frolking, T. A. (1992). A model of nitrous oxide evolution from soils driven by rainfall events: 1. Model structure and sensitivity. J. Geophys. Res. 97: 9759-9776.

Marchetti, R., Donatelli, M., and Spallacci, P. (1997). Testing denitrification functions of dynamic crop models. J. Env. Qual. 26–:394-401.

Molina, J. A. E., Clapp, C. E., Shaffer, M. J., Chichester, F. W., and Larson, W. E. (1983). NCSOIL, a model of nitrogen and carbon transformation in soil: description, calibration and behavior. Soil Sci. Soc. Am. J. 47: 85-91.

Mosier, A. R. (1994). Nitrous oxide emissions from agricultural soils. Fert. Res. 37:191-200.

Mosier, A. R., Kroeze, C., Nevison, C., Oenema, O., Seitzinger, S., and Cleemput, O. V. (1998). Closing the global N2O budget: nitrous oxide emissions through the agricultural nitrogen cycle. Nutri. Cycl. Agroecosys. 52: 225-248.

Muller, C., Sherlock, R. R., and Williams, P. H. (1997). Mechanistic model for nitrous oxide emissions via nitrification and denitrification. Biol. Fertil. Soils 24: 231-138.

Parton, W. J., Holland, E. A., Grosso, S. J. D., Hartman, M. D., Martin, R. E., Mosier, A. R., Ojima, D. S., and Schimel, D. S. (2001). General model for NO_x and N_2O emissions from soils. J. Geophys. Res. 106: 17,403:17,419.

Parton, W. J., Mosier, A. R., Ojima, D. S., Valentine, D. W., Schimel, D. S., Weier, K., and Kulmala, A. E. (1996). Generalized model for N_2 and N_2O production from nitrification an denitrification. Global Biogeochem. Cycles 10: 401-412.

Ratliff, L. F., Ritchie, J. T., and Cassel, D. K. (1983). Field-measured limits of soil water availability as related to laborayory measured properties. Soil Sci. Soc. Am. J. 47: 770-775.

Renault, P., Sierra, J., and Stengel, P. (1994). Transfert d'oxygène et anoxie dans les sols agrégés: contribution à l'étude de la dénitrification. Agronomie 14:395-409.

Smith, J. U., Smith, P., and Addiscott, T. M. (1996). Quantitative methods to evaluate and compare Soil Organic Matter (SOM) models. In Powlson, D. S., Smith, J. U., and Smith, P., editors, *Evaluation of Soil Organic Matter Models*, pages 181–199, Berlin Heidelberg. Springer-Verlag.

Smith, W. N., Desjardins, R. L., Grant, B., Li, C., Lemke, R., and Rochette, P. (2002). Testing the DNDC model using N2O emissions at two experimental sites in Canada. Can. J. Soil Sci. 82: 365-374.

Vinten, A. J. A., Castle, K., and Arah, J. R. M. (1996). Field evaluation of models of denitrification linked to nitrate leaching for aggregated soil. Eur. J. Soil Sci. 47: 305–317.

Wind, G. (1968). Capillarity conductivity data estimated by a simple method. In Rijtema, P. and Wassink, H., editors, *Water in the saturated zone. Vol. 1. Proceedings of the Wageningen symposium, Wageningen, the Netherlands. 19-23 June 1966*, pages 181–191. IASH, Gentbrugge, the Netherlands and UNESCO, Paris.

List of Figures

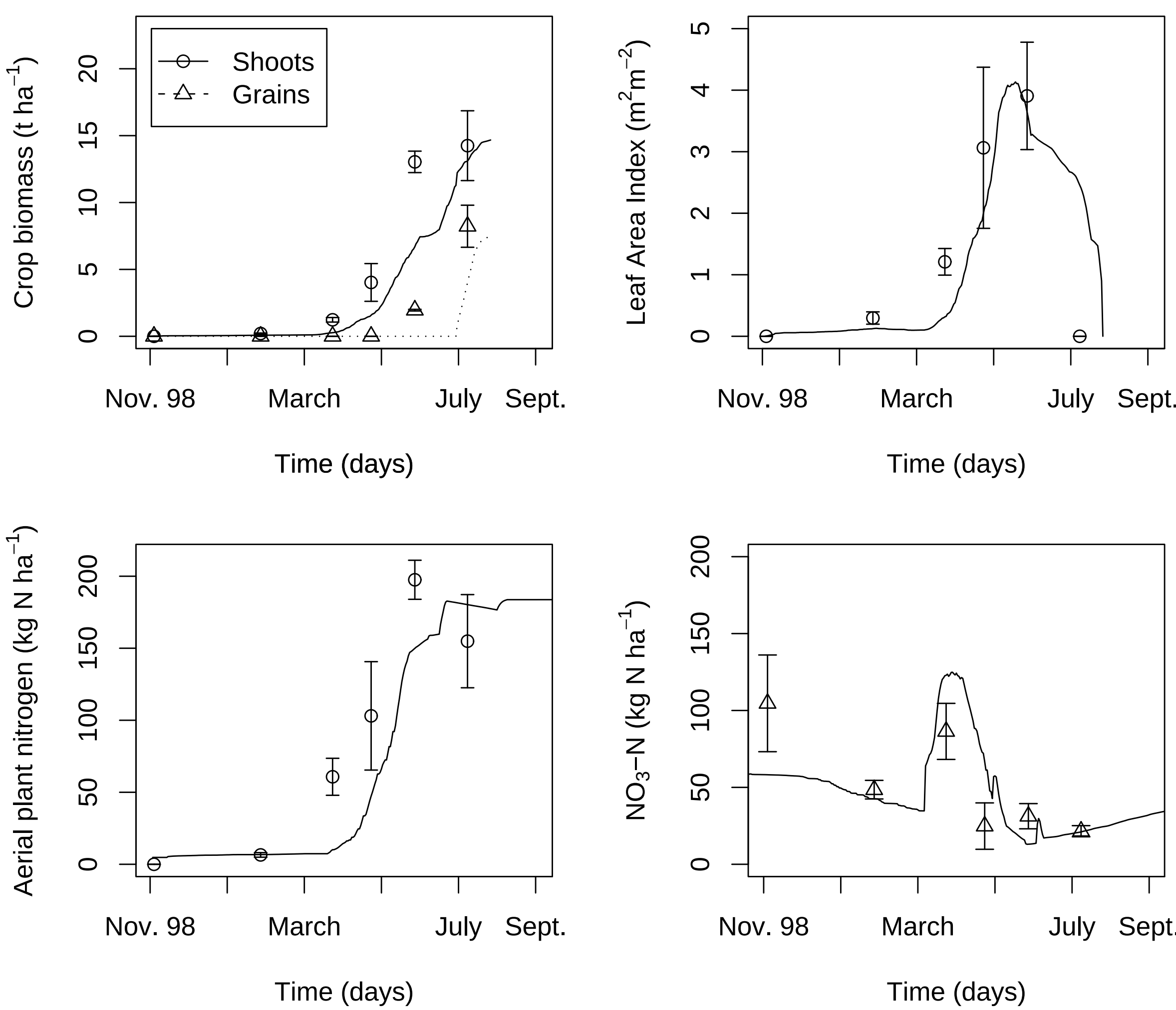


Figure 1: Simulated (lines) and observed (symbols, $\pm$ 1 s.d.) time course of crop shoot and grain dry matter, crop aerial nitrogen content, crop leaf area index, and soil nitrate content over the 0-90 cm profile, at the Villamblain test site.

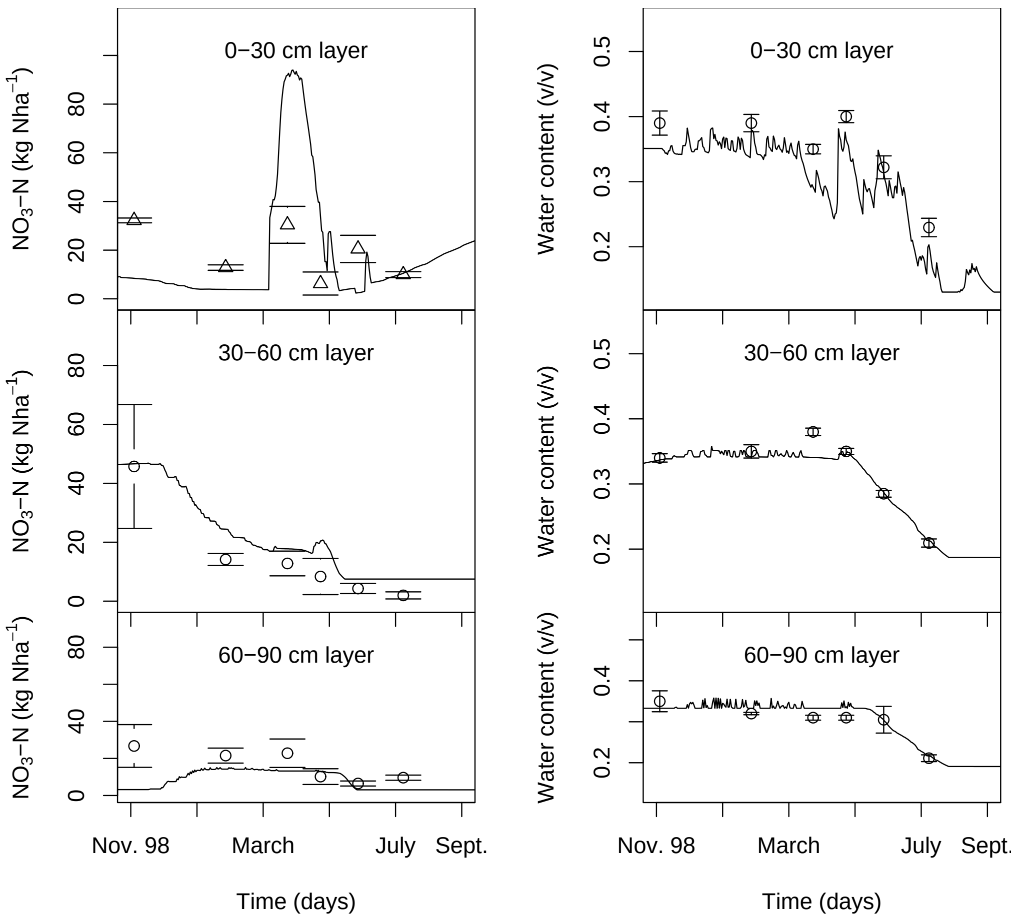
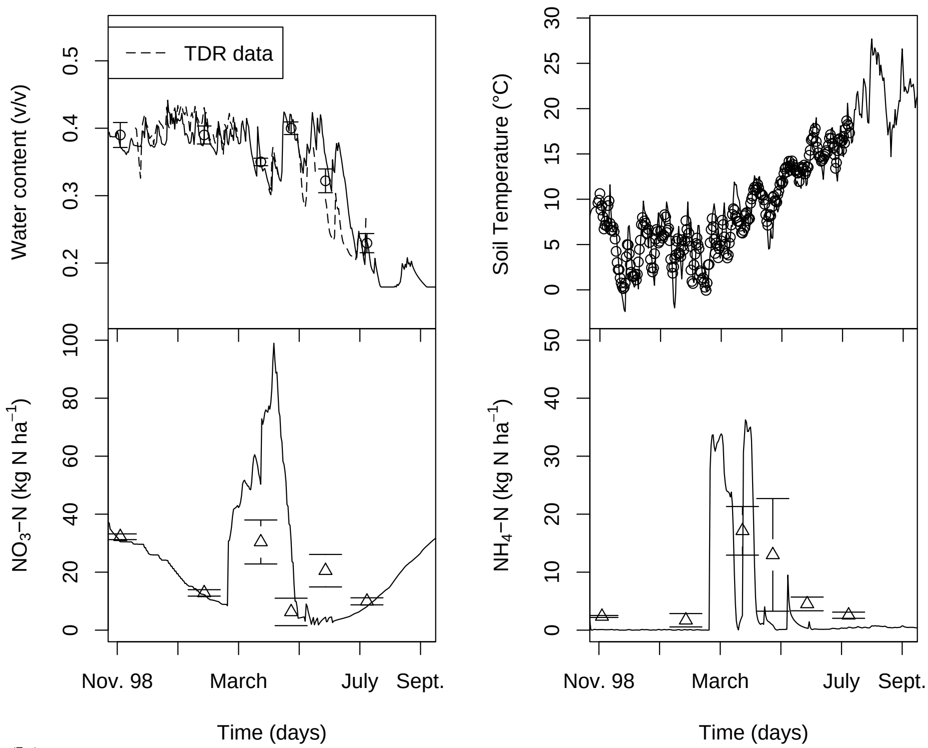


Figure 2: Simulated (lines) and observed (symbols, ± 1 s.d.) time course of soil moisture (right) and nitrate contents (left) in the soil profile at Villamblain.

(a)



(b)

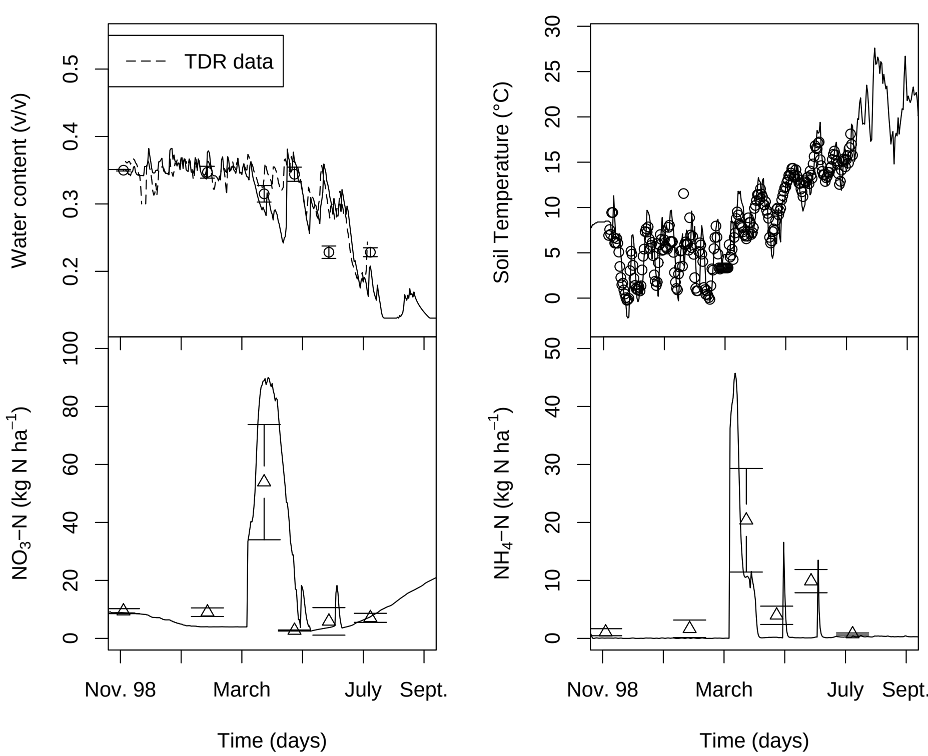


Figure 3: Simulated (lines) and observed (symbols, ± 1 s.d.) time course of input variables to the N_2O modules: topsoil nitrate and ammonium content, moisture content, and temperature (at the 10 cm depth). Graphs are presented for the three sites: Villamblain **(a)**, La Saussaye **(b)**, and Arrou **(c)** (continued on next page).

(c)

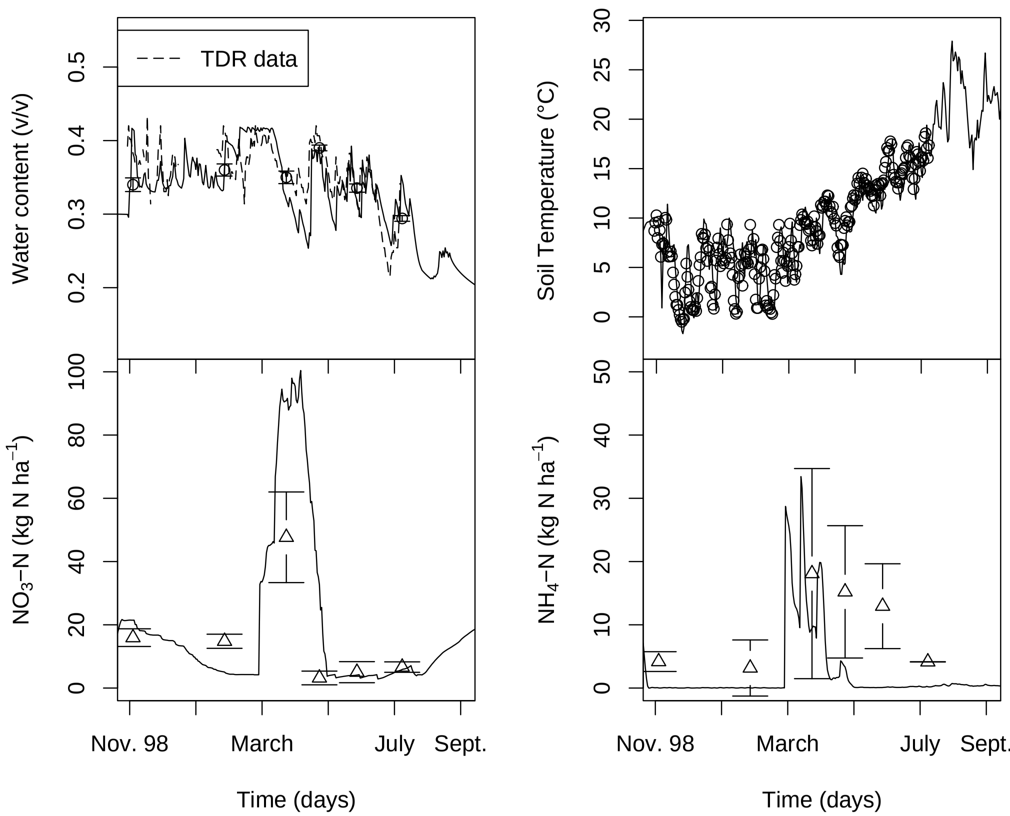


Figure 3: (continued)

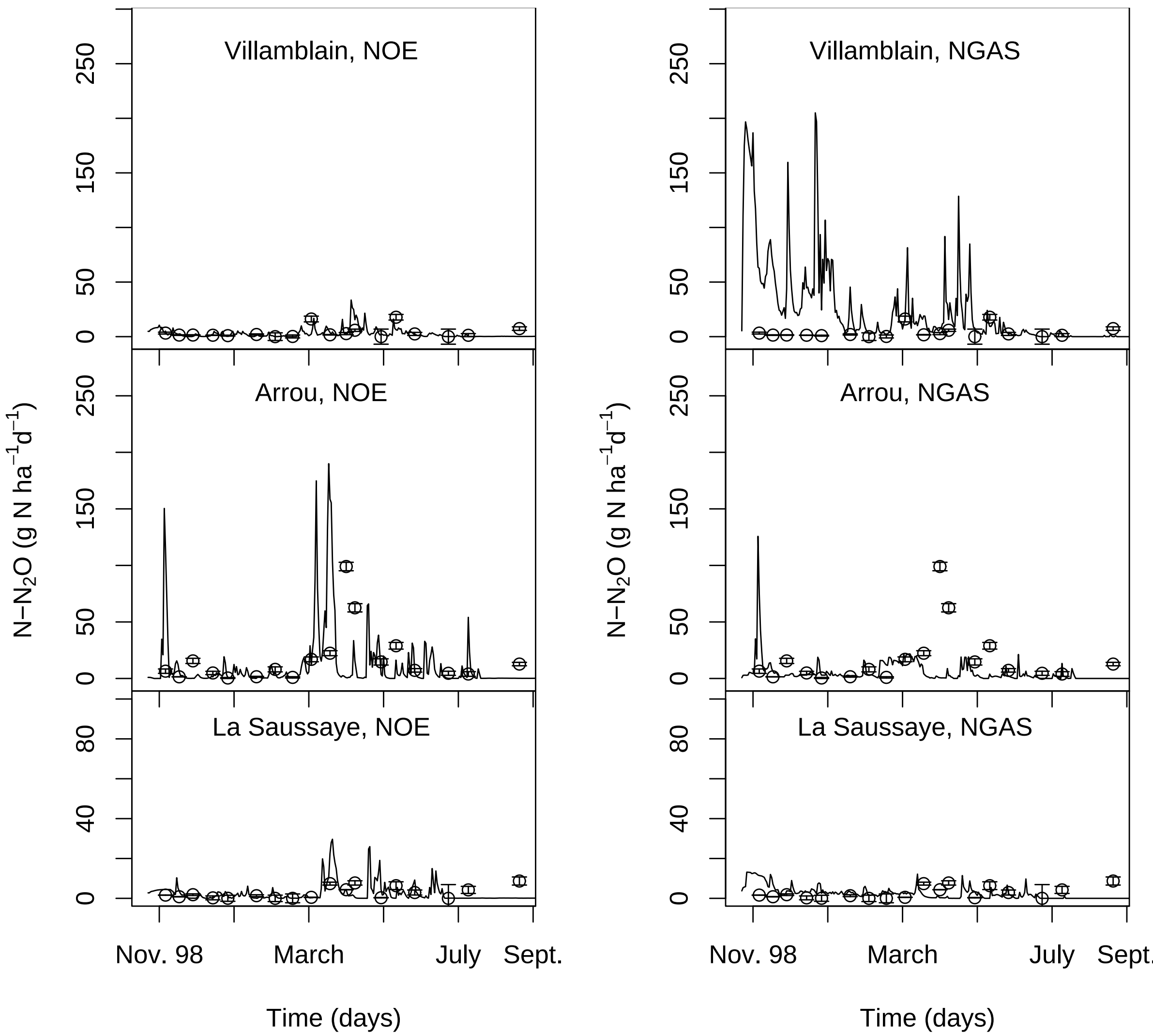


Figure 4: Simulated (lines) and observed (symbols, ± 1 s.d.) time course of N_2O fluxes at the three test sites, and with the two N_2O modules: CERES-NOE (left), and CERES-NGAS (right).

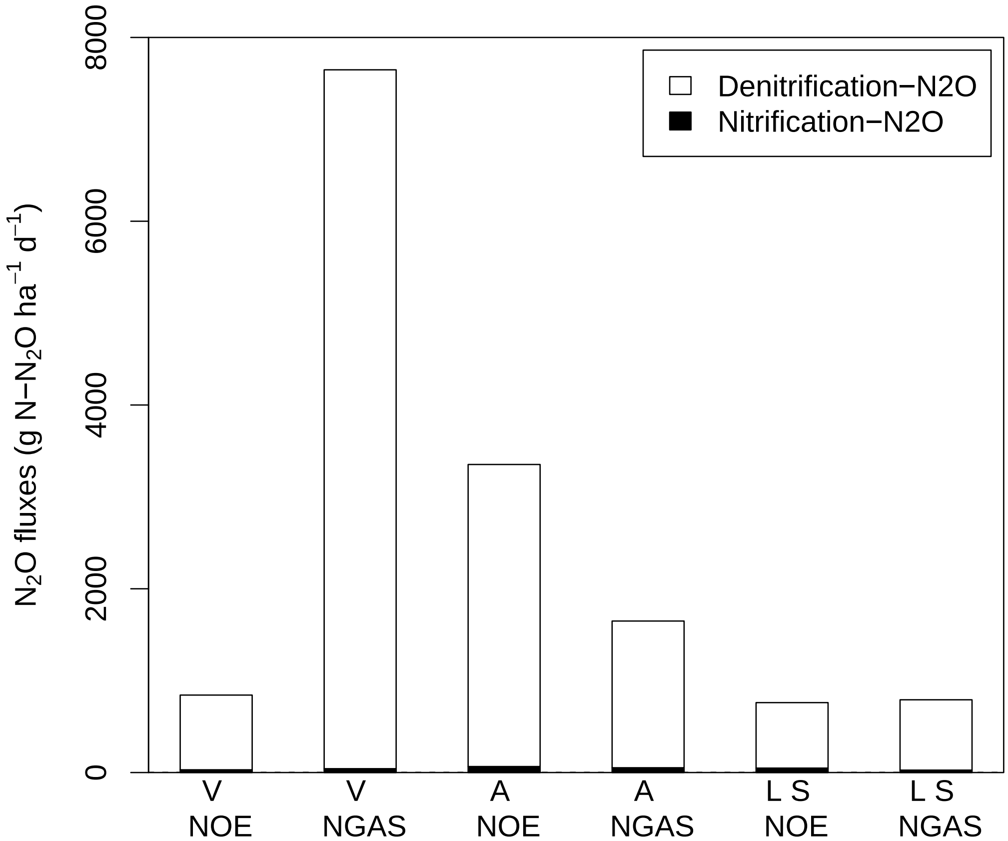
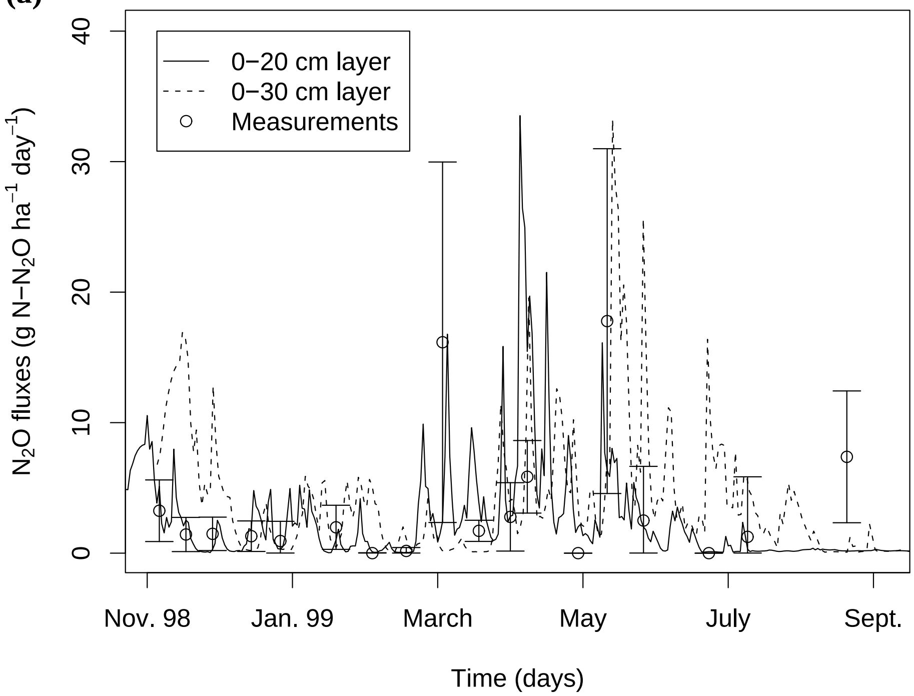


Figure 5: Breakdown of denitrification- and nitrification-N_2O, as simulated by CERES-NOE and CERES-NGAS at the three sites over the one-year simulation period (V = Villamblain; A = Arrou; L S = La Saussaye).

(a)



(b)

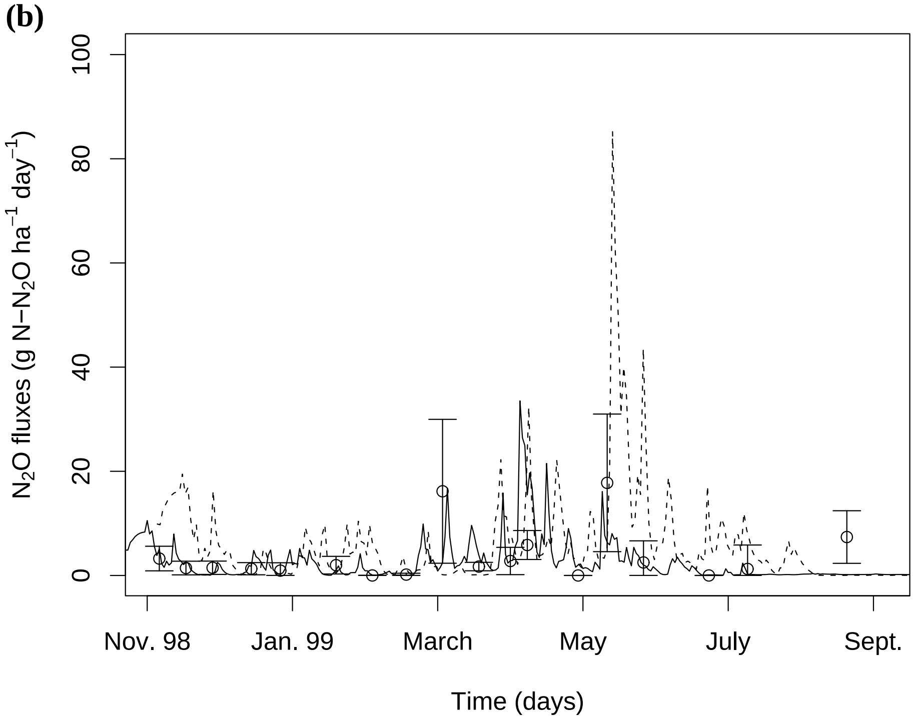


Figure 6: Sensitivity of CERES-NOE-simulated N_2O fluxes (lines) to two coupling hypotheses: calculating the fluxes down to 30 cm instead of 20 cm (**a**); averaging soil input data before running the N_2O module versus calculating N_2O fluxes for each individual soil layer and summing the resulting values (**b**). In both charts, the solid lines correspond to the second option, which is the baseline scenario used in the rest of the paper. The simulations are run for the Villamblain site, and compared to observed data (symbols, $\pm$ 1 s.d.).

List of Tables

Table 1: Selected characteristics of the three experimental sites in the Beauce region.

Location	La Saussaye	Villamblain	Arrou
Soil type[a]	Haplic Luvisol	Haplic Calcisol	Gleyic Luvisol
Surface (0-30 cm) properties:			
Clay content (%)	24	33	14
Sand content (%)	4	3	6
$CaCO_3$ content (%)	0	75	0
pH (water)	6.5	7.9	6.8
Bulk Density (g cm^{-3})	1.32	1.38	1.29
Organic C (%)	1.10	1.47	0.96
C:N ratio	9.75	8.40	9.15
Management:			
Preceding crop	Oilseed rape	Maize	Oilseed rape
Tillage	Conventional	Direct drill	Direct drill
Fertilizer N dose (kg N ha^{-1})	199	230	181

[a]: European classification (FAO-UNESCO-ISRIC, 1989).

Table 2: Statistical indicators for the goodness of fit of CERES+NOE and CERES+NGAS in the three experimental locations. MD and RMSE stand for the models' mean deviation and root mean squared error, respectively. The predicted variable was the daily N_2O flux evolved from the soil surface (unit is g N-N_2O ha^{-1} d^{-1}). The hypothesis that MD is zero was tested using a two-tailed t-Test (p=0.05), and RMSE is compared to mean experimental error using an F variance test (Smith et al., 1996).

Location & soil type			Model						
			CERES-NOE			CERES-NGAS			
	N[1]	Mean observed flux	Mean simulated flux	MD[2]	RMSE[2]	MD	RMSE	Mean simulated flux	Mean observed flux
Villamblain Haplic Calcisol	18	3.7	2.6	1.1[3]	7.2[4]	-16.9	28.6	20.6	3.7
Arrou Gleyic Luvisol	18	17.3	11.9	5.4	38.4	12.0	33.5	5.3	17.3
La Saussaye Haplic Luvisol	18	2.7	2.5	0.2[3]	5.9	0.3[3]	5.6	2.4	2.7
All sites	54	7.9	5.7	2.2	22.8	-1.5[3]	25.6	9.4	7.9

[1]: sample size.
[2]: unit is g N-N_2O ha^{-1} d^{-1}.
[3]: not significantly different from zero (p=0.05).
[4]: not significantly greater than experimental error (p=0.05).