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Process-based modeling of nitrous oxide emissions from wheat-cropped soils at the sub-regional scale

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Abstract. Arable soils are a large source of nitrous oxide (N_2O) emissions, making up half of the biogenic emissions worldwide. Estimating their source strength requires methods capable of capturing the spatial and temporal variability of N₂O emissions, along with the effects of crop management.

Here, we applied a process-based model, CERES, with geo-referenced input 6 data on soils, weather, and land use to map N_2O emissions from wheat-cropped 7 soils in three agriculturally intensive regions in France. Emissions were mostly 8 controlled by soil type and local climate conditions, and only to a minor ex-9 tent by the doses of fertilizer nitrogen applied. As a result, the direct emis-10 sion factors calculated at the regional level were much smaller (ranging from 11 0.0007 to 0.0033 kg kg N₂O-N kg⁻¹ N) than the value of 0.0125 kg N₂O-N kg⁻¹ 12 N currently recommended in the IPCC Tier 1 methodology. Regional emis-13 sions were far more sensitive to the soil microbiological parameters govern-14 ing denitrification and its fraction evolved as N₂O, soil bulk density, and soil 15 initial inorganic N content. Mitigation measures should therefore target a 16 reduction in the amount of soil inorganic N upon sowing of winter crops, and 17 a decrease of the soil N_2O production potential itself. From a general per-18 spective, taking into account the spatial variability of soils and climate thereby 19 appears necessary to improve the accuracy of national inventories, and to 20 tailor mitigation strategies to regional characteristics. 21

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1. Introduction

Emissions from arable soils are a key item in the global nitrous oxide (N_2O) budget, 1 making up about half of the terrestrial biogenic emissions [Mosier et al., 1998]. Since 2 agricultural activities are gradually coming into focus in the greenhouse gas (GHG) bud-3 get calculations, precise estimates of current N_2O emissions from a able land are being 4 sought, along with possible means of abatement. However, compared to other GHG such 5 as CO_2 , N_2O fluxes are of small magnitude and highly variable in space and time [Duxbury 6 and Bouldin, 1982, being tightly linked to the local climatic sequence and soil properties. 7 In national GHG inventories, the default recommended method is that defined by *IPCC* 8 [1997], currently being overhauled. It relates direct N_2O emissions to the amount of ferq tilizer N applied based on a fixed emissions factor, thereafter noted EF_d . Although this 10 method is relatively easy to implement, by combination with nationwide economic statis-11 tics, it ignores the effect of the above-mentioned characteristics. Also, it cannot be used 12 directly to define crop management strategies that would mitigate N_2O emissions, since 13 it does not account for the effect of fertilizer N application (let alone other management 14 practices) on crop growth and yield. 15

In the last ten years, the prediction of N_2O emissions within process-based agro-ecosystem models has emerged as a promising route to deal with these issues, primarily at the local scale to single out the effect of crop management practices [*Li et al.*, 2005]. Application on larger spatial scales has also been demonstrated at the regional, country and subcontinental levels [*Mummey et al.*, 1998; *Li et al.*, 2001; *Butterbach-Bahl et al.*, 2004]. However, it is complicated by the lack of adequate input data and the fact that models

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may not be robust to such upscaling. In terms of spatial resolution, the above examples 1 involved 16 to 400-km²-wide elementary counties or grid squares, implying that models 2 were run on 'average' soils resulting from the combination of the possibly wide range of soil 3 types occurring in the elementary spatial unit considered. Short-range (< 1 km) variability 4 across agricultural fields was therefore likely to be smoothed out in these spatial extrap-5 olations, which precludes a back-tracking of those zones with high emission potentials on 6 which particular measures might be taken to reduce the efflux of N_2O . Also, it makes it 7 impossible to compare the elementary cell-averaged flux with local, ground measurements, 8 the level at which these plot-scale models were generally tested [Butterbach-Bahl et al., 9 2004]. 10

Upscaling to small areas with a much finer grain has also been reported [Grant and Pat-11 tey, 2003]. The latter authors simulated N_2O emissions in a 12-ha landscape by means 12 of 50 m x 50 m grid squares, and showed micro-relief to be responsible for emission 'hot-13 spots' accounting for most of the spatial variability in N_2O efflux. They concluded that 14 aggregation of N₂O emissions at higher scales should be based on 'typical landscapes in 15 which surface topography and soil type is accurately represented'. There is therefore a 16 need for process-based inventories at an intermediate resolution between the field (1-100 17 ha) and county $(10-1000 \text{ km}^2)$ levels, which would explicitly account for heterogeneities 18 between individual soil types. 19

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Here, we report results obtained on such a grain for N_2O emissions from wheat-cropped soils, at the sub-regional level. We used a crop model derived from CERES [Jones and *Kiniry*, 1986], which incorporates a module for N_2O emissions [Gabrielle et al., 2006]. The

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model was run on elementary units (vectorized contours) resulting from the combination of
several information layers in three agricultural sub-regions in Central France. The model
parameterization procedure was checked against ground measurements of N₂O emissions
in three test sites, and its spatial estimates compared to those obtained with the *IPCC*[1997] method. We assessed the sensitivity of the modeled sub-regional estimates to uncertainties in key physical and microbiological parameters, and evaluated their impacts
by means of an uncertainty analysis.

2. Material and Methods

2.1. The CERES-EGC model

CERES-EGC was adapted from the CERES suite of soil-crop models [Jones and Kiniry, 8 1986], with a focus on the simulation of environmental outputs such as nitrate leaching q and gaseous emissions of N_2O , ammonia and nitrogen oxides [Gabrielle et al., 2006]. 10 CERES-EGC comprises sub-models for the major processes governing the cycles of wa-11 ter, carbon and nitrogen in soil-crop systems. A physical module simulates the transfer 12 of heat, water and nitrate down the soil profile, as well as soil evaporation, plant water 13 uptake and transpiration in relation to climatic demand. A microbiological module simu-14 lates the turnover of organic matter in the plow layer, involving both mineralization and 15 immobilization of inorganic N. Lastly, crop net photosynthesis is a linear function of in-16 tercepted radiation according to the Monteith approach, with interception depending on 17 leaf area index based on Beer's law of diffusion in turbid media. Crop N uptake is com-18 puted through a supply/demand scheme, with soil supply depending on soil nitrate and 19 ammonium concentrations and root length density. 20

²¹ CERES-EGC includes NOE [*Hénault et al.*, 2005], a semi-empirical sub-model simulating

the production and reduction of N_2O in agricultural soils through both the denitrifi-1 cation and nitrification pathways. The denitrification component of NOE is based on 2 NEMIS [*Hénault and Germon*, 2000], a model that expresses total denitrification of soil 3 NO_3^- as the product of a potential rate with three unitless factors related to soil water 4 content, nitrate content, and temperature. The fraction of denitrified nitrate that evolves 5 as N_2O is considered as constant for a given soil type, according to the experimental evi-6 dence provided by *Hénault et al.* [2001]. In a similar fashion, nitrification is modeled as a 7 Michaëlis-Menten reaction, with NH_4^+ as substrate. The corresponding rate is multiplied 8 by unitless modifiers related to soil water content and temperature. As for denitrifica-9 tion, a soil-specific proportion of total nitrification evolves as N_2O , following the results 10 of Garrido et al. [2002]. The two pathways are connected in that nitrification-derived 11 N_2O may be reduced to N_2 by denitrification, should the two processes be simultaneously 12 active. Unlike other N₂O emission modules such as NGAS [Parton et al., 2001] or DNDC 13 [Li et al., 2001], NOE does not use the microbial respiration of organic C as a driver for 14 denitrification. 15

¹⁶ CERES-EGC runs on a daily time step, and computes the various transforma-¹⁷ tion rates of N with the following sequence: nitrification, denitrification, mineraliza-¹⁸ tion/immobilization, and crop uptake. This sequence reflects the priority order for possi-¹⁹ bly competing processes, such as denitrification and crop uptake of nitrate.

2.2. Spatial simulations

²⁰ 2.2.1. Information layers

The study area comprised three administrative 'agricultural sub-regions' of the Beauce region, lying approximately 200 km southwest of Paris, France: Beauce Chartraine (74

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000 ha), Beauce Dunoise (61 200 ha), and Faux-Perche (48 200 ha). The sub-regions were 1 delineated by French authorities as relatively homogeneous zones from the point of view 2 of physical characteristics (climate, pedogenesis and geological substrate), and agricul-3 tural production systems. The majority of soils in Beauce Chartraine are thick clay loams 4 (Haplic Luvisols - Isambert [1984]), either permeable upon limestone parent material, or 5 less material developed on a flinty clay substrate. The mean annual rainfall is 600 mm, 6 and mean air temperature is 10.6 °C. Beauce Dunoise comprises mostly thin loamy clay 7 soils (Haplic Calcisols), developed on calcareous layers. Mean annual rainfall is 636 mm. 8 and mean air temperature is 10.8 °C. Lastly, the soils in Faux-Perche are loamy Gleyic q Luvisols, developed on a flint clay substrate. Mean annual rainfall is 783 mm, and mean 10 air temperature is 10.3 °C. Farming systems are based on cereal crops in the first two 11 regions, and include some livestock production in Faux-Perche. 12

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Elementary simulation units were defined by overlaying spatial information soil types, 14 climate, land use and crop management available at various geographical or administra-15 tive levels. Only a fraction of the sub-regions was simulated, since we had chosen to focus 16 on winter wheat. Wheat is the major arable crop in the area, being grown on 30% to 40%17 of total arable land. Each sub-region comprised 4 counties, at which level information 18 on land use was available through agricultural census data and farmers declarations for 19 European subsidies. Typical crop management practices for winter wheat were set based 20 on a survey in the three sub-regions. Soils were parameterized based on a 1:250 000 scale 21 soil map, organized into geographical units (SMU) containing a mixture of soil typological 22 units (STU), following the model of the European Union soil map [King et al., 1994]. The 23

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soil data base attached with the map comprised geographical information (the shape of
the SMUs) and quantitative data for each SMU: the occurrence of particular STUs within
the SMU, and various descriptors characterizing the STUs. The SMUs covered between
3 and 19,000 ha, with an average size of 775 ha. Daily weather data was taken for each
simulation unit from the closest station available, less than 20 km away from the centroid
of the unit.

7 2.2.2. Soil parameterization

Various methods were combined to estimate the soil parameters of CERES-EGC. Some 8 were readily-available as thematic fields in the soil data base: depth to parent material 9 (down to 2 m), which was used to set the simulation depth; maximum rooting depth 10 (with an upper limit of 1.5 m); the thickness of the various soil horizons along with 11 their particle-size distribution and bulk density. Soil water contents at wilting point and 12 field-capacity were estimated with pedo-transfer functions developed on a collection of c. 13 600 samples, mostly taken from the Paris basin, with contrasting textures [Bastet et al., 14 1998]. The saturation water content, also required by CERES-EGC as input, was esti-15 mated with the pedo-transfer function originally proposed by CERES [Jones and Kiniry, 16 1986]. Topsoil organic matter content was also included based on a nationwide survey 17 [Arrouays et al., 1999], and updated in the course of this study. Surface pH and $CaCO_3$ 18 contents were added to the data base using local references and expertise, and the same 19 went with saturated hydraulic conductivity. The latter was estimated using only three 20 classes centered on the following values: 0.02, 0.08, and 0.3 m d^{-1} , respectively. 21

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erning the processes of N_2O production and reduction in soils, as detailed in *Hénault* et al. [2005]. They were measured in the laboratory in each test site of the sub-regions, 2 as follows: potential denitrification rates were measured by acetylene blocking of undis-3 turbed soil cores taken from the top 20 cm of soil, saturated with water and incubated 4 with an ample supply of nitrate [Hénault and Germon, 2000]; the fraction of denitrified 5 nitrate that evolves as N_2O was determined as the difference between the N_2O production 6 rates of soil cores incubated with and without acetylene [Hénault et al., 2001]; lastly, the 7 fraction of nitrification evolved as N_2O was measured on sieved soil samples incubated 8 with increasing soil moisture content and non-limiting NH₃ supply, using the methodology 9 proposed by *Garrido et al.* [2002]. Table 1 lists the parameter values obtained in the three 10 sites. 11

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¹³ Unfortunately, the limited size of the data base currently available for these parameters ¹⁴ precludes the definition of pedo-transfer functions for their spatial extension [*Hénault* ¹⁵ *et al.*, 2005]. We thus simply applied the values obtained in the test site to the whole sub-¹⁶ region, considering these sites representative of this area. The influence of this hypothesis ¹⁷ on the final results was tested in the uncertainty analysis.

¹⁸ 2.2.3. Model running

¹⁹ CERES-EGC was run in each of the elementary simulation units for a reference period ²⁰ running from mid-September, 1998, to mid-September, 1999. Initial moisture content was ²¹ set at 90% of the field-capacity content throughout the soil profile, based on simulations ²² of the preceding cropping season. Initial nitrate and ammonium concentrations in the soil ²³ were set at 5 and 1 mg N kg⁻¹ soil, respectively, throughout the profile. It corresponds to

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a total residual N content of 80 kg N ha⁻¹ in the top 1 m of soil, which is the average of
N stocks measured in the region at that time of year (B. Nicoullaud, unpublished data,
2003). Annual N deposition was neglected, being less than 4 kg N ha⁻¹ in the area [*Ulrich and Willot*, 1993]. Since the focus was on wheat-cropped soils, the area of the simulation
units were corrected for the fraction of land cropped to wheat in these units. Aggregation
of elementary fluxes within each sub-region yielded the total N₂O efflux estimated from
winter wheat crops over this sub-region.

⁸ Wheat management data was set according to the recommendations made by local advi-⁹ sory services [Germon et al., 2003]. The mean doses of fertilizer N were 195 kg N ha⁻¹ in ¹⁰ Beauce Dunoise and 215 kg N ha⁻¹ in Faux-Perche and Beauce Chartraine, split into ¹¹ three applications in spring. Only mineral fertilizers were considered (in the form of am-¹² monium nitrate and urea), since organic forms are applied on only 2% of the cropland area ¹³ in the region studied here, and make up less than 2 % of the total amounts of fertilizer N ¹⁴ applied.

¹⁵ 2.2.4. Sensitivity and uncertainty analysis

Extrapolating model simulations from plot to regional scale involves two main sources of uncertainty [*Butterbach-Bahl et al.*, 2004], which may be considered independent: i/ uncertainties in model inputs, including parameters, driving variables (climate and crop management), and initial conditions, and ii/ model prediction error.

To address the first source, we ran a simple, local sensitivity test in which the inputs were varied one-at-a-time over their plausible range while keeping the others at their nominal value. We subsequently estimated a probability density functions (pdfs) for the most sensitive inputs, and evaluated their combined effect on the variance of model predictions

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using winding stairs sampling [Jansen et al., 1994]. The method is a modified Latin 1 Hypercube sampling which makes it possible to estimate the contribution of individual 2 inputs (X_i) to the total variance in model output (Y) using variance ratios. For instance, 3 the 'top marginal variance' (TMV) is defined as: $TMV = Var(E(Y \mid X_i = x_i))/Var(Y)$, 4 where Var and E denote the variance and expectancy, respectively. The TMV indicates 5 the mean reduction of Var(Y) made possible by setting input X_i at its nominal value x_i , 6 *i.e.* imposing $Var(X_i) = 0$. 7

All analyses were done at the sub-regional scale, the output variable of interest (Y) being 8 the simulated N_2O efflux. 9

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The second source of uncertainty (model error) was estimated as mean squared error 11 achieved by CERES-EGC in the prediction of annual N_2O fluxes in the three test sites, 12 using the regional parameterization (see below section). Ultimately, the total uncertainty 13 on the predicted sub-regional efflux was calculated as the sum of the variances related to 14 input uncertainties and to model error. 15

2.3. Local test sites

One test site was set up in each sub-region to check the simulations of N_2O emissions 16 obtained with the regional parameterization procedure detailed in section 2.2.2. The sites 17 were selected as representative of the sub-region, and involved a Haplic Luvisol in Beauce 18 Chartraine (site name: La Saussaye; 4824'N, 134'E), a Haplic Calcisol in Beauce Dunoise 19 (at Villamblain; 4798'N, 134'E), and a Gleyic Luvisol in Faux-Perche (at Arrou; 4808'N, 20 106'E) - FAO classification [ISSS/ISRIC/FAO, 1998]. 21

 N_2O emissions were monitored by the static chamber method using circular chambers (0.5) 22

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m in diameter and 0.15 m in height), with 8 replicates [*Hénault et al.*, 2005]. Other outputs were also monitored to test the simulation of intermediate variables. Topsoil water
content was continuously recorded using TDR probes, soil nitrogen content was measured
every two weeks in the topsoil and every month in the subsoil, and plants were regularly
sampled and analyzed for aerial dry matter, leaf area and nitrogen content. Lastly, a
weather station was set up to record the data required by CERES-EGC (rainfall, air temperature and solar radiation), along with soil temperature.

⁸ Detailed information was also collected to supply the soil parameters of CERES-EGC.
⁹ Hydrodynamic parameters (water retention and hydraulic conductivity curves) were mea¹⁰ sured on intact cores taken to the laboratory. Site-specific parameters required by the
¹¹ N₂O module were also measured in the laboratory, following the procedures given in sec¹² tion 2.2.3.

These data sets were used to test the implementation of the N₂O modules within CERES-13 EGC in a previous paper *Gabrielle et al.* [2006]. Here, they served to test the 'regional' 14 parameterization method described in section 2.2.2, against the baseline, more detailed 15 'local' parameterization resulting from the above measurements. In the test sites, model fit 16 to observed data was evaluated by calculating the mean deviation (MD) and the root mean 17 squared error (RMSE), defined as: $MD = E(O_i - S_i)$ and $RMSE = (E[(O_i - S_i)^2])^{1/2}$, 18 where S_i and O_i are the time series of the simulated and observed data. Model error in 19 the prediction of yearly cumulative (as opposed to daily instantaneous) N_2O fluxes was 20 assumed proportional to the simulated flux, and estimated as [Smith et al., 1996]: 21

²² $RMSE_{yr} = 100/E(O_{i,s}) \times [E(MD_s^2)]^{1/2},$

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where MD_s are the mean deviations in the test sites, and $O_{i,s}$ the daily observations in these sites.

3. Results

3.1. Simulations in the three test sites

Figure 1 compares the simulations obtained with the regional parameterization procedure in the three test sites with those resulting from the detailed soil characterization, which was used to implement the N₂O module of CERES-EGC [*Gabrielle et al.*, 2006]. In one of the sites (Villamblain), the potential denitrification rate had to be reduced by a factor of 5 in order to obtain an acceptable fit to observed emission rates. Thus, this parameter was set at 3.4 kg N₂O-N ha⁻¹ yr⁻¹ in the surrounding sub-region, namely Beauce Dunoise.

¹⁰ The local and regional parameterization scenarios yielded similar temporal dynamics in ¹¹ all sites. However, closer examination revealed some differences in the magnitude of the ¹² emission peaks simulated. Compared to the local parameterization, the regional one re-¹³ sulted in lower fluxes after spring fertilization at Arrou and Villamblain, and higher fluxes ¹⁴ in La Saussaye. As a result, the N₂O emissions predicted by the regional parameteri-¹⁵ zation scenarios differed by -40% to +130% relative to the local parameterization, when ¹⁶ accumulated over the simulation period (Table 2).

These discrepancies were mostly due to differences regarding soil water retention properties and bulk density, to which the model proved very sensitive. At La Saussaye, for instance, topsoil bulk density differed by only 0.08 g cm⁻³ between the two parameterizations, but this was enough to create a 30% deviation in terms of simulated N₂O efflux.

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¹ Despite these discrepancies, the mean deviations (MD) and root mean squared errors ² (RMSE) achieved by the two parameterization scenarios were generally close, the only ³ notable difference being that the RMSE was significantly higher with the regional param-⁴ eterization than with the local one at Arrou. The mean deviation was also relatively high ⁵ for this site (amounting to 8 g N₂O-N ha⁻¹ d⁻¹), compared to the other two sites in which ⁶ it was negligible. As a result, the estimated relative error for the annual simulated flux ⁷ (RMSE_{yr}) amounted to 64%.

3.2. Regional simulations

Table 3 summarizes the simulation outputs for the three sub-regions, while Figure 2 8 provides a geographical mapping of the emissions. In terms of spatial distribution, there 9 were no marked differences between the sub-regions, which all presented a wide range of 10 emission rates. Beauce Chartraine exhibited a longitudinal gradient with lower N₂O fluxes 11 to the East and higher fluxes to the West, whereas in Faux-Perche the emission levels were 12 vertically stratified from North to South. Conversely, Beauce Dunoise was rather homo-13 geneous and centered in the mid-range values of N₂O fluxes. When expressed per unit 14 area, the mean N_2O fluxes varied markedly across the regions, from 0.63 kg N_2O -N ha⁻¹ 15 yr^{-1} in Beauce Dunoise to 2.23 kg N₂O-N ha⁻¹ yr^{-1} in Faux-Perche. This range was 16 much lower than the 3.85 - 5.45 kg N_2 O-N ha⁻¹ yr⁻¹ simulated in the test sites with the 17 regional parameterization. 18

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Within the sub-regions, the western half of Beauce Chartraine appeared particularly sensitive in the regional balance of N_2O emissions. Other zones prone to N_2O emissions zones could also be delineated, such as the northernmost and southernmost tips of Faux-Perche.

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Spatial structures in the other parts of the map were mostly determined by the spatial 1 resolution of the soil map units (SMU), some of which were rather large with sizes ranging 2 up to 19,000 ha. In addition, SMUs were made up of two to five different soil type units 3 (STUs), with possibly contrasting potentials for N_2O emission. On the other hand, emis-4 sions were much less variable within a given STU when it occurred across several map 5 units and thereby climatic conditions. Figure 3 shows the distribution of fluxes across the 6 various STUs to be strongly skewed, with an extended tail in the higher range of emissions 7 $(> 5 \text{ kg N ha}^{-1} \text{ yr}^{-1})$. However, the weight of this upper-tail was very limited, comprising 8 only 11 STUs out of a total of 230, and making up 0.7% of the total area simulated. 9

3.3. Sensitivity analysis

Table 4 lists the parameters included in the sensitivity analysis, along with their standard deviations or variation ranges. Model response to changes in these inputs is given only in the case of Beauce Chartraine, but similar patterns were noted in the other two sub-regions (not shown).

Overall, the two microbiological parameters governing N_2O emissions (PDR and r_D) were 14 among the three most sensitive inputs. When varied across their inter-regional range, 15 they introduced a one- to three-fold variation in the predicted N_2O efflux. This could 16 be expected since there was a factor of 5 between the minimum and maximum values of 17 PDR, and a factor of 3 for r_D . Also, given the nature of the denitrification equations, the 18 model responded linearly to changes in these parameters. Soil bulk density (BD) was the 19 next most influential parameter, as already noted in the local test sites. A 10% relative 20 variation of BD entailed more than much higher relative changes in model output, ranging 21 from -80% to 320%. This is due to the markedly convex power function used in the model 22

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to relate the water-filled pore space (WFPS) to denitrification [Hénault and Germon, 2000]. Increasing bulk density decreases soil porosity and thereby the threshold moisture 2 content above which denitrification is activated, which corresponds to 62% WFPS. It 3 therefore increases the probability of moisture conditions conducive to denitrification and 4 N_2O emissions. For the same reason, the field-capacity water content (θ_{fc}) also proved 5 sensitive, but to a lesser extent. Surprisingly, the saturated hydraulic conductivity had 6 very little effect, despite being varied over a wide range $(\pm 50\%)$. It is probably because 7 the dynamics of topsoil water were mostly governed by the field-capacity content, at least 8 for water contents close to saturation, as previously reported with the CERES water bal-9 ance routine [Gabrielle and Kenqni, 1996]. 10

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The model was unsensitive to topsoil organic C content and pH, because unlike other 12 models [Parton et al., 2001; Li et al., 2001], it does not explicitly include these factors as 13 controls in the production and reduction of N_2O . Their influence is only indirect, via the 14 processes of ammonia volatilization (for soil pH) and the mineralization/immobilization 15 of soil N (for soil organic C). Initial soil water and N content appeared little to mod-16 erately sensitive, respectively. There was a -21% to +31% change in the sub-regional 17 N_2O flux over the range of initial N contents. The influence of initial water content was 18 more marginal, probably because the simulations started two months ahead of the wetter 19 winter season. On the other hand, changes in annual rainfall affected soil water content 20 throughout the simulation period, and rainfall appeared as sensitive as initial N content 21 as a result. 22

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3.4. Uncertainty analysis

Based on the above results, 5 parameters were selected for the uncertainty analysis: PDR, r_D , BD, θ_{fc} , and initial soil N content (I_N). We used truncated Gaussian pdfs ($0.025 \le p \le 0.975$) for the last 3 inputs, considered site-specific, and uniform pdfs for the first two, considered as constant within each sub-region. A correlation coefficient of -0.52 between the field-capacity water content and bulk density was introduced, according to the finding of *Bastet et al.* [1998].

The distributions of N_2O fluxes generated with the winding stairs sampling (WSS) of these 7 inputs were log-normal, with an extended tail in the higher range of values and a large 8 variance (Figure 4). Table 5 shows the median and 95% confidence intervals calculated q in the three sub-regions. In all of them, the median fluxes were larger than the baseline 10 values of Table 3. This was expected in Beauce-Chartraine and Beauce Dunoise, given 11 that in the baseline parameterization they were ascribed the lowest values for r_D and/or 12 PDR. Since the pdfs of these two parameters were centered on the mid-range estimates 13 of these parameters, the fluxes generated by sampling in these pdfs could only be higher 14 than with the baseline parameterization. However, this is not true of Faux-Perche, and 15 in fact the opposite since the baseline value of r_D in Faux-Perche was the higher bound of 16 its sampling range (64%). The fact that the WSS-generated median flux was still higher 17 than its baseline value evidences the influence of the site-specific parameters (θ_{cf} , I_N and 18 BD), and also strong non-linearity with the model. 19

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There was ample variation around the median: the lower and upper 95% confidence
limits corresponded to 18-20% and 420-450% of the median, respectively, and the coeffi-

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cients of variations ranged from 109% to 123%. Compounding this variability with the 1 estimated model prediction error (assuming both variates to be log-normal), the lower 2 and upper limits of the 95% confidence were estimated as 33% and 300% of the predicted 3 flux, respectively. Lastly, the calculation of top marginal variances (TMV) made it pos-4 sible to estimate the contribution of individual inputs to the total variance. Soil physical 5 parameters (BD and $\theta_f c$) explained 62% to 75% of the total variance, while the microbi-6 ological parameters (PDR and r_D) had a contribution ranging from 12% to 30%, and the 7 initial nitrate content only had a marginal role. This ranking differs from that output by 8 the one-at-a-time sensitivity test (Table 4), evidencing interactions between inputs that 9 amplified model response to physical parameters while drastically reducing the influence 10 of initial conditions. 11

3.5. Sensitivity to fertilizer N

At the sub-regional level, the model-based estimates of direct N₂O emissions from wheat-12 cropped fields were 10% to 70% lower than the IPCC ones. The deviation was strongest 13 in Beauce Dunoise and smallest in Faux-Perche, reflecting the ranking of the sub-regions 14 respective to N_2O emissions on a per hectare basis. The background emissions simulated 15 by CERES-EGC were also lower than the IPCC default value of 1 kg N_2 O-N ha⁻¹, but to 16 a lesser extent than the total emissions, and ranged from 0.52 to 1.02 kg N₂O-N ha⁻¹. As 17 a result, model-based EF_d estimates were extremely low compared to the IPCC default 18 $(0.0125 \pm 0.01 \text{ kg N}_2\text{O-N kg}^{-1} \text{ N})$, ranging from 0.0007 to 0.0033 kg N₂O-N kg⁻¹ N. This 19 low sensitivity of model results to fertilizer N essentially arose from the fact that a major 20 fraction of the emissions happened outside the spring season during which fertilizer was 21 applied. Some emissions occurred prior to wheat planting in the fall of 1998, as may be 22

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seen on Figure 1, or in the late summer and fall of 1999. Because wheat crops actively
took up soil N during their growing season, fertilization actually had little influence on
the soil inorganic content upon harvest in summer, and on the subsequent emissions of
N₂O.

5

Secondly, N_2O emissions were generally proportional to the amount of fertilizer N applied to crops, whatever the range of fertilizer doses (Figure 5). As a result, the average EF_{ds} estimated by fitting a straight line to the response curve provided estimates nearly identical to those obtained by using emissions data only for the nominal and zero doses of fertilizer N, as is usually done in the IPCC method.

4. Discussion

4.1. Uncertainty and validity of regional estimates

Extrapolating model simulations from plot to regional scale involves some degree of uncertainty in spatialized inputs as well as model robustness to spatial extension. The uncertainties of a range of inputs could be quantified prior to extrapolation, and their effects approached via sensitivity and uncertainty analyses (UA).

The setting of microbiological parameters (PDR and r_D) proved most crucial in the regional extension, being both sensitive and highly uncertain. Unfortunately, they could not be spatialized based on the available soil information because they do not yet appear to be related to particular physico-chemical properties, such as soil texture or organic matter content [*Hénault et al.*, 2005]. For lack of an alternative method, we assumed in the baseline parameterization that the values of PDR and r_D measured in each test site could apply to the entire surrounding sub-region. This hypothesis of a strong spatial structure

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in the distribution of soil microbiological properties was based on the pedoclimatic zoning 1 of the sub-regions. However, it may appear somewhat arbitrary, and was actually tested 2 against a null hypothesis by which microbiological properties were randomly distributed 3 across the sub-regions within their overall variation ranges. The difference between the 4 two parameterizations turned out to be extremely large: the median N_2O effluxes cal-5 culated in the UA were 1.2- to 8-fold higher than with the baseline parameterization. 6 Better knowledge of the spatial determinants of those parameters is therefore paramount 7 to reducing the uncertainty of such model-based estimates. 8

9

Topsoil bulk density was also very sensitive, but its contribution to the total variance 10 was somewhat reduced because of its correlation with the field-capacity water content. 11 Although the wide body of literature currently available on the estimation of these param-12 eters makes it possible to narrow down their range of uncertainty, it is notable that they 13 contributed nearly as much variance to the N₂O fluxes as the microbiological parameters. 14 This contribution of water content was also noted by Mummey et al. [1998], who reported 15 a 1.3- to 2-fold increase in N_2O emissions from a able crops when increasing soil water 16 content by 40%. In addition, because the variation ranges chosen for these parameters 17 fall within their spatial variations at the field-scale [Yanai et al., 2003], it is likely that 18 this source of error will remain as a background noise in the predictions of N_2O . 19

Lastly, the fact that the model was sensitive to the initial soil N content points at a possible strategy for reducing N₂O emissions. A target initial content of 40 kg N ha⁻¹ (down to 1 m) would indeed make it possible to reduce the emissions by 25%, which is more than what could be achieved by a drastic reduction of fertiliser N application to the following

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crop. Best management practices may in principle make it possible to reach such a target
 [Loyce et al., 2002].

3

4

The second major source of uncertainty (model robustness to spatial extension) could 5 be judged from the mean deviations achieved by CERES-EGC in the test sites with the 6 regional parameterization. These errors ranged from 0.5 to 8.4 g N₂O-N ha⁻¹ d⁻¹, which 7 represents 7% to 50% of the mean observed fluxes (Table 2). This range may be taken as 8 the error margin associated with the simulation of the annual N_2O efflux by the model. 9 When compounded over the three sites, the average relative prediction error was esti-10 mated at 64%, because one of the test sites (Arrou) had much higher fluxes than the 11 other two. From a more qualitative viewpoint, the extent to which CERES-EGC could 12 be extrapolated to new field situations may be judged based on its N₂O sub-model, NOE. 13 The latter was successfully tested in 3 field sites in France, other the 3 test sites involved 14 here, along with 3 field sites in Central America [Hénault et al., 2005]. In these sites the 15 mean daily emission rates varied between 2 to 50 g N₂O-N ha⁻¹ d⁻¹, thus encompassing 16 the 6-7 g N₂O-N ha⁻¹ d⁻¹ range that could be expected in the sub-regions based on the 17 IPCC approach (Table 3). 18

19

Regional estimates based on bottom-up aggregation of plot-scale fluxes generally involve
model testing in a few test sites, and direct extrapolation to the area of interest [*Li et al.*,
2001; *Mummey et al.*, 1998]. Because testing usually involves site-specific calibration of
some model parameters [*Frolking et al.*, 1998; *Gabrielle et al.*, 2002], we included here

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an intermediate phase in which the default parameterization procedure applied at the regional scale was compared with a more detailed, site-specific parameterization. Of course, 2 this comparison also involves a scaling issue, since the soil typological units (STUs) used 3 in the regional parameterization were much larger than the area covered by the measure-4 ments in the test sites. As a result, the discrepancies between the model outputs using 5 whether the site-specific or the regional parameterization should not be taken as a failure 6 of the model, but rather as an indication of the degree of uncertainty associated when 7 downscaling from the mapping unit (SMU) to the plot-scale. It is also noticeable that 8 they produced an acceptable fit to the measurements (Table 2). g

Overall, combining the unknowns mentioned above resulted in 95% confidence limits representing 33% and 300% of the mean simulated estimates, respectively. This is much larger than the $\pm 80\%$ confidence interval of the IPCC methodology, and the $\pm 50\%$ interval reported by *Li et al.* [2001] in their inventory based on the DNDC model, but it encompasses more sources of uncertainty - including, most notably, model prediction error.

4.2. Empirical and model-based emission factors

There is a growing body of literature on the determination of direct emission factors (EFds) from field measurements at the plot-scale. These factors have been shown to be extremely variable from one field to the other, ranging from 0.0003 to 0.068 kg N₂O-N kg⁻¹ N [*Flessa et al.*, 2002; *Velthof et al.*, 2003; *Kaiser et al.*, 1998; *Zheng et al.*, 2004]. There are many sources of uncertainty behind these empirical estimates: quantification of background emissions, spatial and temporal coverage, and time-frame on which the measurements are carried out, which all warrant corrections [*Zheng et al.*, 2004]. Ac-

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¹ cording to the latter, the absence of background emissions data is expected to lead to ² an over-estimation of EF_d s, by 15% to 110% under Chinese conditions. Conversely, a ³ shortage of temporal coverage (insufficient frequency of measurements) would lead to an ⁴ under-estimation by 19% to 30%.

Process-based models should not require any such corrections since they simulate 5 N_2O emissions continuously over time, and can predict fertilized as well as unfertilized 6 crops. Thus, they may be expected to supply EF_d values up to 80% lower than the empir-7 ical estimates listed above, among which the IPCC methodology. Such was the case with 8 the EF_ds simulated with CERES-EGC, which fell in the lower range of the IPCC valg ues. Similarly, another modeling study reported an average EF_d of 0.008 kg N₂O-N kg⁻¹ 10 N with a 0.0025-0.04 kg N₂O-N kg⁻¹ N range for cropland in China [Zheng et al., 2004]. 11 The same tendency was reported in another modeling study: Li et al. [2001] estimated 12 Calculation of EF_d s without the control term (ie assuming zero emissions for unfertilized 13 crops), as was done in a number of studies for lack of background emissions data [Zheng 14 et al., 2004], resulted in EF_ds ranging between 0.0033 and 0.0104 kg N₂O-N kg⁻¹ N. This 15 falls within the lower half of the IPCC range (0.0025 to 0.0225 kg N₂O-N kg⁻¹ N). 16

Fertilizer type is also mentioned to affect the values of EF_d , although there is a lack of sufficient data to derive generic, fertilizer-specific figures [*Bouwman*, 1996; *Mosier et al.*, 1996]. *Bouwman* [1996] reported EF_d values of 0.003 ± 0.003 kg N₂O-N kg⁻¹ N for ammonium nitrate and urea, the two types of fertilizers used in the sub-regions simulated here.

22

 $_{23}$ Lastly, EF_ds should capture some range of inter-annual variability. It is in principle

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¹ possible with a model like CERES-EGC, but we considered it beyond scope here since we ² focused on spatial extension from plot-scale to regional scale. However, our results are to a ³ large extent conditioned by the growing season in which the experiments and simulations ⁴ were run. Investigating the effect of inter-annual climate variability is therefore a major ⁵ prospect for future work on N_2O simulations.

4.3. Factors controlling N_2O emissions at the regional scale

Two major differences occured between the model-based and IPCC estimates of 6 N_2O emissions at the sub-regional scale: the magnitude of the emissions, and the response to fertiliser N. Both appeared much weaker with the model, and are discussed below. The lack of response to fertilization essentially occured because the simulated 9 N_2O emissions were not concentrated in the spring season when fertilizer was applied. 10 However, it may also be a result of the upscaling from field- to regional-scale. The lit-11 erature on spatial extension of N₂O fluxes, whether using process-based models or more 12 empirical methods, shows the 'fertilizer dose' factor to lose some influence in favor of envi-13 ronmental characteristics, as the spatial area increases. At the European scale, *Freibauer* 14 [2003] modeled N₂O emissions based on pedological and agronomic factors, and found a 15 coefficient of only 0.4% in the correlation between these emissions and fertilizer doses. In 16 a review of emission data covering a wide range of crop management and geographical 17 locations, Kaiser et al. [1998] report a similar coefficient with a value of 0.6%. These 18 figures could be interpreted as an average EF_d of 0.004 to 0.006 kg N₂O-N kg⁻¹ N for 19 Europe. The apparent discrepancy between the ranges of EF_d s obtained at the plot and 20 regional scales may be due to an uneven sampling of field sites biased towards the more 21 N_2O -productive sites, when establishing empirical EF_ds , and these sites might turn out 22

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to represent only a small proportion of total arable land. Such was the case in our study since the test sites were actually above average in terms of N₂O emissions. The frequent lack of background data in these experiments is also a source of bias since a significant part of the emissions attributed to fertilizer use might actually be related to the soil potential per se, as happened in our simulations. For urea and ammonium-nitrate type fertilizers, *Bouwman* [1996] reported relative differences as high as 100% between EF_d estimates including or not an unfertilized control.

8

Regarding the magnitude of the simulated fluxes, the study by $Li \ et \ al.$ [2001] at the 9 country level revealed a clustered spatial pattern for N_2O emissions, with contrasting ef-10 flux rates between groups of counties (equivalent to our sub-regions). It is thus probable 11 that some sub-regions would contribute significantly less N_2O than others, which seems 12 to be the case with those we had selected here. On the other hand, the IPCC EF_d are 13 representative at a global or continental scale, as they were obtained from observations 14 worldwide, rather than at the sub-regional level. Overall, in our sub-regions, N_2O emission 15 levels primarily depend on a local potential set by climatic conditions combined with soil 16 microbiological and physical properties, with the influence of crop management appearing 17 somewhat minor in the expression of this potential. As a consequence, reducing fertilizer 18 N would seemingly have little effect on abating N_2O fluxes. However, the fertilizer dose 19 also influences the residual N content upon sowing of the proceeding crop, which signifi-20 cantly affected the sub-regional N_2O efflux. 21

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²³ As a conclusion, under such mild temperate climatic conditions as investigated here,

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mitigation measures should target a reduction in the amount of soil mineral N in autumn,
and a decrease of the soil N₂O production potential itself. While there is a range of
best management packages available to address the first point, there is a need for future
research on the microbial and physical determinants of soil emission potentials, and how
they may be affected by crop management.

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 Table 1.
 Soil microbiological parameters of NOE measured at the three test sites.

 Symbol Description (Unit)
 Parameter value

 La Saussaye Villamblain Arrou

PDR	Potential denitrification rate (kg N ha ⁻¹ yr ⁻¹)	15.7	16.9	9.4
r_D	Fraction of denitrification evolved as $N_2O(\%)$	20	20	64
r_N	Fraction of nitrification evolved as $N_2O(\%)$	0.06	0.06	0.06

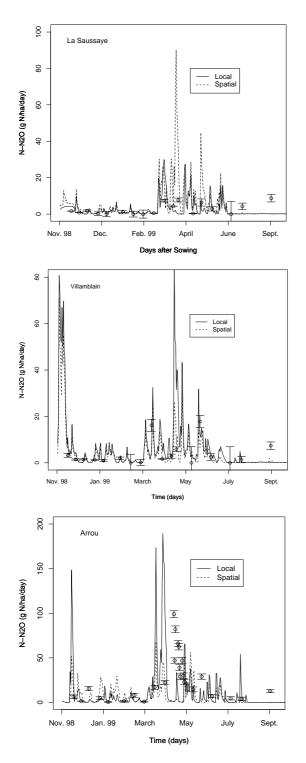


Figure 1. Simulated (lines) and observed (symbols) emissions of N_2O in the three test sites. In the local parameterization scenario, detailed, site-specific information on soil properties was used, whereas the regional scenario involved only information derived from the soil map.

Table 2. Cumulative annual N₂O emissions (kg N₂O-N ha⁻¹ yr⁻¹) simulated with the local and regional regional parameterization procedures, along with statistical indicators of model fit to observed data. The hypothesis that the mean deviation is zero was tested using a two-tailed t-Test, and the root mean squared error is compared to mean experimental error using an F variance test [*Smith et al.*, 1996].

	La Saussaye		Villamblain		Arrou	
Parameterization	Regional	Local	Regional	Local	Regional	Local
scenario						
Annual	5.08	3.29	5.45	2.39	3.85	6.64
N_2O flux						
$(\text{kg N}_2\text{O-N ha}^{-1} \text{ yr}^{-1})$						
Mean deviation	0.61^{a}	-0.95 ^a	0.56^{a}	-1.24 ^a	8.84^{a}	5.57^{a}
(g N ₂ O-N ha ⁻¹ d ⁻¹)						
Root mean squared error	4.99^{b}	8.04	6.43^{b}	$9.00^{\rm b}$	34.1	38.4
$(g N_2O-N ha^{-1} d^{-1})$						

 $^{\rm a}$ not significantly different from zero (p=0.05)

^b not significantly greater than experimental error (p=0.05)

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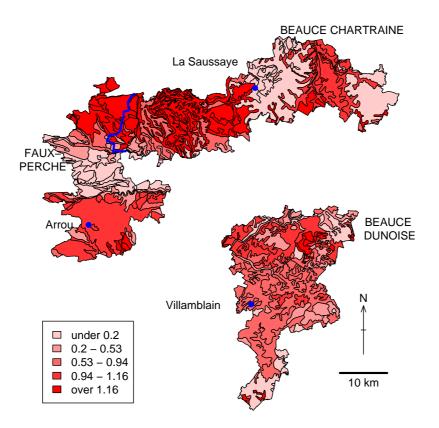


Figure 2. Simulation of N_2O emissions from wheat-cropped land in three agricultural sub-regions of the Beauce region. The fluxes are expressed in kg N_2O -N ha⁻¹.

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Table 3. Emissions of N_2O simulated within each sub-region (total and average per hectare), with a standard or zero dose of fertilizer N. Regional estimates obtained with the IPCC methodology are also reported (corresponding to the emissions due to fertilizer application).

Sub-region	Total area	Fertilizer N	Mean annual	Regional flux	Regional Emission
	simulated	dose	N_2O flux		Factor
	ha	kg N ${\rm ha^{-1}}$	kg N ₂ O-N ha ⁻¹	kg N ₂ O-N	kg N ₂ O-N kg ⁻¹ N
Beauce	31,927	215	1.37	42,887	0.0016
Chartraine		0	1.02	31,868	
IPCC	31,927	215	2.42	85,804	0.0125
Beauce	23,474	195	0.65	15,384	0.0007
Dunoise		0	0.52	12,165	
IPCC	23,474	195	2.13	57,218	0.0125
Faux-	16,578	215	2.23	37,010	0.0033
-Perche		0	1.51	25,062	
IPCC	16,578	215	2.42	44,553	0.0125

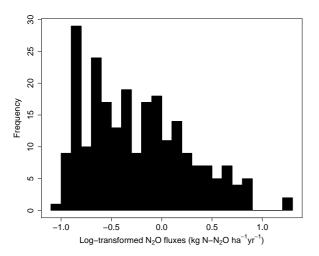


Figure 3. Histogram of log-transformed simulated fluxes across the various soil type units in the three sub-regions.

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Table 4. Sensitivity of model-predicted N_2O efflux in the Beauce Dunoise sub-region to selected inputs. Soil parameters pertain to the top layer (0-30 cm). Site-specific inputs were assigned a fixed coefficient of variation (CV, in %), and varied within their 95% confidence interval, while inputs considered constant at the sub-regional level were given an overall variation range. Model response is expressed as changes in model output relative

to	the	baseline	input	setting.

Symbol	Description (Unit)	Variation	Source	Model response		
		range / CV		(change relative		
				to baseline)		
SOIL P.	ARAMETERS					
OC	organic carbon content (g g^{-1} soil)	15%	1	-1.7% to $+2.2%$		
рН	pH in water	8%	1	-0.3% to $+2.1\%$		
BD	Topsoil bulk density (g $\rm cm^{-3}$)	5%	2	-80% to $+321%$		
K_{sat}	Saturated hydraulic conductivity (m $\mathrm{d}^{-1})$	50%	3	-1.3% to +1.9%		
$ heta_{fc}$	Soil water content at field-capacity (g g^{-1} soil)	10%	4	-72.5% to +250%		
PDR	Potential denitrification rate (kg N ₂ O-N ha ⁻¹ yr ⁻¹)	3.4 - 15.7	5	-71% to $0%$		
r_D	Fraction of denitrification evolved as N ₂ O (%)	20 - 64	5	0% to $+290%$		
DRIVIN	DRIVING VARIABLES					
R	Annual rainfall (mm yr^{-1})	10%	6	-22.3% to +27.2%		
INITIAL CONDITIONS						
\mathbf{I}_N	Mineral N in soil profile (top 1 m; kg N ha^{-1})	40 - 125	6	-24.1% to +31.4%		
I_w	Moisture content in soil profile (top 1 m; mm)	50 - 150	6	-6.7% to +1.8%		

1: Variability within soil type units; 2: Measurement error; 3: Range covered by each K_{sat} class; 4: Prediction error of pedo-transfer function [*Bastet et al.*, 1998]; 5: Range across the 3 test sites; 6: Intra-regional variability [Nicoullaud, B. (unpublished data, 2003)].

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Table 5. Statistics of the sub-regional N₂O fluxes generated by winding stairs sampling of 5 parameters. The coefficient of variation (CV) was estimated on the truncated distribution $(0.025 \le p \le 0.975)$.

Sub-region	Median	95% confidence	CV
		interval	
	Mg	$N_2O-N yr^{-1}$	%
Beauce Chartraine	118.1	21.2 - 497.2	109%
Beauce Dunoise	125.0	15.0 - 561.2	123%
Faux-Perche	49.4	9.8 - 213.0	113%

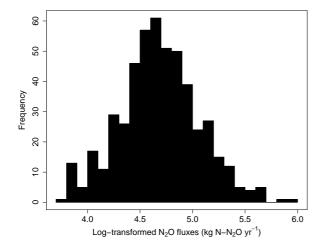


Figure 4. Log-transformed frequency distribution of the total N_2O efflux in Faux-Perche obtained by winding stairs sampling of model inputs.

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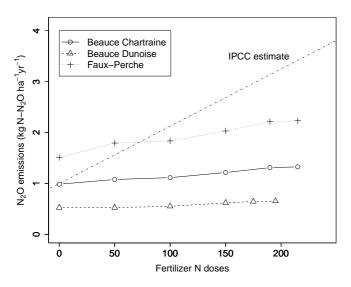


Figure 5. Simulated relationships between fertilizer N dose and year-round N_2O emissions at the sub-regional level. The straight line corresponds to the *IPCC* [1997] relationship.