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Benoit Gabrielle, Patricia Laville, Odile Duval, Bernard Nicoullaud, Jean-Claude Germon, et al..
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2006. hal-00017134v1

HAL Id: hal-00017134

<https://hal.science/hal-00017134v1>

Preprint submitted on 17 Jan 2006 (v1), last revised 22 Dec 2006 (v3)

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

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1 **Abstract.** Arable soils are a large source of nitrous oxide (N₂O) emis-
2 sions, making up half of the biogenic emissions worldwide. Estimating their
3 source strength requires methods capable of capturing the spatial and tem-
4 poral variability of N₂O emissions, along with the effects of crop manage-
5 ment.

6 Here, we applied a process-based model, CERES, with geo-referenced input
7 data on soils, weather, and land use to map N₂O emissions from wheat-cropped
8 soils in three agriculture intensive regions in France. Emissions were mostly
9 controlled by soil type and local climate conditions, and only to a minor ex-
10 tent by the doses of fertilizer nitrogen applied. As a result, the direct emis-
11 sion factors calculated at the regional level were much smaller (ranging from
12 0.0005 to 0.0016 kg kg N₂O-N kg⁻¹ N) than the value of 0.01125 kg N₂O-
13 N kg⁻¹ N currently recommended in the IPCC Tier 1 methodology. How-
14 ever, regional emissions were highly sensitive to the soil inorganic N content
15 at the beginning of the simulation in late summer. Mitigation measures should
1 therefore target a reduction in the amount of soil inorganic N upon sowing
2 of winter crops, and a decrease of the soil N₂O production potential itself.
3 From a general perspective, taking into account the spatial variability of soils
4 and climate thereby appears necessary to improve the accuracy of national
5 inventories, and to tailor mitigation strategies to regional characteristics.

1. Introduction

6 Emissions from arable soils are a key item in the global nitrous oxide (N₂O) budget,
7 making up about half of the terrestrial biogenic emissions [*Mosier et al.*, 1998]. Since
8 agricultural activities are gradually coming into focus in the greenhouse gases budget cal-
9 culations, precise estimates of current N₂O emissions from arable land are being sought,
10 along with possible means of abatement. However, compared to other greenhouse gases
11 such as CO₂, N₂O fluxes are of small magnitude and highly variable in space and time
12 [*Duxbury and Bouldin*, 1982], being tightly linked to the local climatic sequence and soil
13 properties. In national inventories of greenhouse gas emissions, the default recommended
14 method is that defined by *IPCC* [1997], currently being overhauled. It relates direct
15 N₂O emissions to the amount of fertilizer N applied based on a fixed emissions factor,
16 thereafter noted EF_d. Although this method is relatively easy to implement, by combi-
17 nation with nationwide economic statistics, it ignores the effect of the above-mentioned
18 characteristics. Also, it cannot be used directly to define crop management strategies
19 that would mitigate N₂O emissions, since it does not account for the effect of fertilizer N
20 application (let alone other management practices) on crop growth and yield.

21 In the last ten years, the prediction of N₂O emissions within process-based agro-ecosystem
1 models has emerged as a promising route to deal with these issues, primarily at the local
2 scale by using scenario analysis to single out the effect of crop management practices
3 [*Li et al.*, 2005]. Application on larger spatial scales has also been demonstrated at
4 the regional, country and sub-continental levels [*Mummey et al.*, 1998; *Li et al.*, 2001;
5 *Butterbach-Bahl et al.*, 2004].

6 However, it is complicated by the lack of adequate input data and the fact that models
7 may not be robust to such upscaling. The spatial resolutions involved in the above ex-
8 amples involved 16 to 400-km²-wide elementary counties or grid squares, implying that
9 models were run on 'average' soils resulting from the combination of the possibly wide
10 range of soil types occurring in the elementary spatial unit considered. Short-range (<
11 1 km) variability across agricultural fields was therefore likely to be smoothed out in
12 these spatial extrapolations, which precludes a back-tracking of those zones with high
13 emissions potentials on which particular measures might be taken to reduce the efflux of
14 N₂O. Also, it makes it impossible to compare the elementary cell-averaged flux with local,
15 ground measurements, the level at which these site-scale models were generally tested
16 [*Butterbach-Bahl et al.*, 2004].

17 On the other end of the spectrum, upscaling to small areas with a much finer grain has
18 also been reported [*Grant and Pattey*, 2003]. The latter authors simulated N₂O emissions
19 in a 12 ha landscape by means of 50 m x 50 m grid squares, and showed micro-relief to
20 be responsible for emission 'hot-spots' accounting for most of the spatial variability in
21 N₂O efflux. They concluded that aggregation of N₂O emissions at higher scales should
22 be based on 'typical landscapes in which surface topography and soil type is accurately
23 represented'. There is therefore a need for process-based inventories at an intermediate
1 resolution between the field (1-100 ha) and county (10-1000 km²) levels, which would
2 explicitly account for heterogeneities between individual soil types.

3
4 Here, we report results obtained on such a grain for N₂O emissions from wheat-cropped
5 soils, at the sub-regional level, based on a 1:250 000 vectorized soil map. We used a crop

6 model derived from the CERES family [*Jones and Kiniry, 1986*], in which two different
7 modules of N₂O emissions from soil were integrated [*Gabrielle et al., 2006b*]. The model
8 was run on elementary units (vectorized contours) resulting from the combination of sev-
9 eral information layers (soil survey map, weather stations, land use and crop management
10 practices), in three administrative agricultural sub-regions in Central France. The model
11 parameterization procedure was checked against ground measurements of N₂O emissions
12 in three test sites, and its spatial outputs compared to those obtained with the *IPCC*
13 [1997] method.

2. Material and Methods

2.1. The CERES-EGC model

14 CERES-EGC was adapted from the CERES family of soil-crop models [*Jones and*
15 *Kiniry, 1986*], with a focus on the simulation of environmental outputs such as nitrate
16 leaching and gaseous emissions of N₂O, ammonia and nitrogen oxides [*Gabrielle et al.,*
17 *2005a, 2006b*]. CERES-EGC comprises sub-models for the major processes governing the
18 cycles of water, carbon and nitrogen in soil-crop systems. It runs on a daily time step,
19 and requires daily rain, mean air temperature and Penman potential evapo-transpiration
20 as forcing variables. CERES-EGC includes NOE [*Hénault et al., 2005*], a semi-empirical
21 sub-model simulating the production and reduction of N₂O in agricultural soils through
1 both the denitrification and nitrification pathways. The denitrification component of NOE
2 is based on NEMIS [*Hénault and Germon, 2000*], a model that expresses total denitrifi-
3 cation of soil NO₃⁻ as the product of a potential rate with three unitless factors related to
4 soil water content, nitrate content, and temperature. The fraction of denitrified nitrate
5 that evolves as N₂O is then considered as constant for a given soil type. In a similar fash-

ion, nitrification is modeled as a Michaëlis-Menten reaction, with NH₄⁺ 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 N₂O. The two pathways are connected in that NO₃⁻-derived N₂O may be reduced to N₂ by denitrification, should the two processes be simultaneously active.

2.2. Spatial simulations

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 (74 000 ha), Beauce Dunoise (61 200 ha), and Faux-Perche (48 200 ha). The sub-regions were delineated by French authorities as relatively homogeneous zones from the point of view of physical characteristics (climate, pedogenesis and geological substrate) and production systems. The majority of soils in Beauce Chartraine are thick clay loams (Haplic Luvisols - *Isambert* [1984]), either permeable upon limestone parent material, or less material developed on a flinty clay substrate. The mean annual rainfall is 600 mm, and mean air temperature is 10.6 °C. Beauce Dunoise comprises mostly thin loamy clay soils (Haplic Calcisols), developed on calcareous layers. Mean annual rainfall is 636 mm, and mean air temperature is 10.8 °C. Lastly, the soils in Faux-Perche are loamy Gleyic Luvisols, developed on a flint clay substrate. Mean annual rainfall is 783 mm, and mean air temperature is 10.3 °C. Farming systems are based on cereal crops in the first two regions, and include some livestock production in Faux-Perche.

Elementary simulation units were defined by overlaying spatial information soil types,

6 climate, land use and crop management available at various geographical or administra-
7 tive levels (Table 1). Only part of the sub-regions were simulated, since we had chosen to
8 focus on winter wheat. Wheat is the major arable crop in the area, being grown on 30% to
9 40% of total arable land. Each sub-region comprised 4 counties, at which level information
10 on land use was available through agricultural census data. Typical crop management
11 practices for winter wheat were set based on a survey in the three sub-regions. The soil
12 map was organized into soil map units (SMU) containing a mixture of soil typological
13 units (STU), following the model of the soil map of the European Union [*King et al.*,
14 1994]. The soil data base attached with the map comprised geographical information (the
15 shape of the SMUs) and quantitative data for each SMU: the occurrence of particular
16 STUs within the SMU, and various descriptors characterizing the STUs. The SMUs cov-
17 ered between 3 and 19 000 ha, with an average size of 775 ha. Daily weather data was
18 taken for each simulation unit from the closest station available, less than 20 km away
19 from the centroid of the unit.

20 **2.2.2. Soil parameterization**

21 Various methods were combined to estimate the soil parameters of CERES-EGC. Some
22 were readily-available as thematic fields in the soil data base: depth to parent material
23 (down to 1.5 m), the thickness of the various soil horizons along with their particle-size
1 distribution and bulk density. Soil water content at wilting point and field-capacity were
2 estimated with pedo-transfer functions developed on a collection of *c.* 600 samples mostly
3 taken from the Paris basin, with contrasting textures [*Bastet et al.*, 1998]. The satu-
4 ration water content, also required by CERES-EGC as input, was estimated with the
5 pedo-transfer function originally proposed by CERES [*Jones and Kiniry*, 1986]. Topsoil

6 organic matter content was also included based on a nationwide survey [*Arrouays et al.*,
7 1999], and updated in the course of this study. Surface pH and CaCO₃ contents were
8 added to the data base using local references and expertise, and the same went with sat-
9 urated hydraulic conductivity. The latter was estimated using only three classes centered
10 on the following values: 20, 80, and 300 cm d⁻¹, respectively.

11
12 The N₂O module of CERES-EGC involves a set of 5 microbiological parameters gov-
13 erning the processes of N₂O production and reduction in soils, as detailed in *Hénault*
14 *et al.* [2005]. They were measured in the laboratory in each test site of the sub-regions.
15 Unfortunately, the limited size of the data base currently available for these parameters
16 precludes the definition of pedo-transfer functions for their spatial extension [*Hénault*
17 *et al.*, 2005]. We thus simply applied the values obtained in the test site to the whole
18 sub-region, considering these sites representative of this area.

19 **2.2.3. Model running and data analysis**

20 CERES-EGC was run in each of the elementary simulation units for a reference period
21 running from mid-September 1998 to mid-September 1999. Initial moisture content was
22 set at 90% of the field-capacity content throughout the soil profile, based on simulations
23 of the preceding cropping season. Initial nitrate and ammonium concentrations in the soil
1 were set at 5 and 1 mg N kg⁻¹ soil, respectively, throughout the profile. It corresponds
2 to a total residual N content of 80 kg N ha⁻¹ down to 100 cm, which corresponds to
3 the average of N stocks measured in the region at that time of year (ranging from 40
4 to 125 kg N ha⁻¹ on deep loams - provided by B. Nicoullaud, unpublished data, 2003).
5 Annual N deposition was neglected, being less than 4 kg N ha⁻¹ in the area [*Ulrich and*

6 *Willot*, 1993]. Since the focus was on wheat-cropped soils, the area of the simulation
7 units were corrected for the fraction of land cropped to wheat in these units. Aggregation
8 of elementary fluxes within each sub-region yielded the total N₂O efflux estimated from
9 winter wheat crops over this sub-region.

2.3. Local test sites

10 One test site was set up in each sub-region to check the simulations of N₂O emissions
11 obtained with the regional parameterization procedure detailed above. The sites were
12 selected as representative of the sub-region, and involved a Haplic Luvisol in Beauce
13 Chartraine (site name: La Saussaye; 4824'N, 134'E), a Haplic Calcisol in Beauce Dunoise
14 (at Villamblain; 4798'N, 134'E), and a Gleyic Luvisol in Faux-Perche (at Arrou; 4808'N,
15 106'E) - FAO classification [*ISSS-ISRIC-FAO*, 1998].

16 N₂O emissions were monitored by the static chamber method using circular chambers, and
17 other outputs were also monitored to test the other components of CERES-EGC. Topsoil
18 water content was continuously recorded using TDR, soil nitrogen content was measured
19 every two weeks in the topsoil and every month in the subsoil, and plants were regularly
20 sampled and analyzed for aerial dry matter, leaf area and nitrogen. Lastly, a weather
21 station was set up to record the data required by CERES-EGC (rainfall, air temperature
22 and solar radiation), along with soil temperature.

1 Detailed information was also collected to supply the soil parameters of CERES-EGC.
2 Hydrodynamic parameters (water retention and hydraulic conductivity curves) were mea-
3 sured on intact cores taken to the laboratory. Some soil-specific parameters required by
4 the N₂O module were also measured in the laboratory: a potential denitrification rate,
5 measured on intact soil cores, and coefficients of nitrification response to soil moisture

6 content, measured on sieved soil samples [*Hénault et al.*, 2005]. These data sets were then
7 used to test the implementation of the N₂O modules within CERES-EGC. The procedure
8 for this detailed parameterization are described in *Gabrielle et al.* [2006b], and will be
9 referred to as the 'local' parameterization in the following, as opposed to the regional
10 parameterization described earlier.

11 In the test sites, model fit to observed data was evaluated by calculating the mean devia-
12 tion (MD) and the root mean squared error (RMSE), defined as: $MD = E(O_i - S_i)$ and
13 $RMSE = (E[(O_i - S_i)^2])^{1/2}$, where S_i and O_i are the time series of the simulated and
14 observed data, and E denotes the expectancy.

2.4. The IPCC methodology

15 The CERES-EGC predictions of N₂O efflux resulting from the application of fertilizer
16 N correspond to the direct emissions of the IPCC methodology [*IPCC*, 1997]. By default,
17 they are calculated as the product of the amount of fertilizer applied and the direct
18 N₂O emission factor, noted EF_d in the following. In the IPCC inventory for the three
19 sub-regions, we used an average fertilizer dose following the recommendations made by
20 local advisory services [*Germon et al.*, 2003]. The mean doses were 195 kg N ha⁻¹ in
21 Beauce Dunoise and 215 kg N ha⁻¹ in Faux-Perche and Beauce Chartraine, split into
1 three applications in spring. Only mineral fertilizers were considered (in the form of
2 ammonium nitrate and urea), since organic forms are applied on only 2% of the cropland
3 area in the region studied here, and make up less than 2 % of the total amounts of fertilizer
4 N applied.

5 The default IPCC methodology [*IPCC*, 1997] calculates direct emissions from mineral

6 fertilizers as follows:

$$E_{N_2O} = EF_d \times Nfert \times (1 - Frac_{GASF})$$

7 where E_{N_2O} is the N₂O emission in kg N₂O-N ha⁻¹, $Nfert$ is the fertilizer dose (kg N
8 ha⁻¹), and $Frac_{GASF}$ is the fraction of fertilizer N volatilized as NH₃. By default, EF_d is
9 set at 0.0125 ± 0.01 kg N₂O-N kg⁻¹ N, and $Frac_{GASF}$ at 0.1.

10 In order to derive EF_d from CERES-EGC, the model was run for various doses of fertilizer
11 N ranging from 0 to the nominal doses mentioned above. Simulated EF_d was calculated
12 as:

$$EF_d = (E_{N_2O}(Nfert) - E_{N_2O}(N_0))/Nfert \quad (1)$$

13 where $E_{N_2O}(Nfert)$ and $E_{N_2O}(N_0)$ are the emission rates simulated with the nominal
14 and zero fertilizer doses, respectively. Since CERES-EGC simulates NH₃ volatilization,
15 the EF_d values of the above equation should be directly compared to the IPCC EF_d
16 estimates of $(0.0125 \pm 0.01 \text{ kg N}_2\text{O-N kg}^{-1} \text{ N}) \times 0.9 = (0.01125 \pm 0.009 \text{ kg N}_2\text{O-N kg}^{-1}$
17 $\text{N})$. Simulations were run over an annual period ranging September, 1998 (prior to the
18 planting of wheat) to September, 1999, whether at the local or sub-regional levels.

3. Results

3.1. Simulations in the three test sites

1 Figure 1 compares the simulations obtained with the regional parameterization proce-
2 dures with those resulting from the detailed soil characterization in the three test sites,
3 which was used as to test the N₂O module of CERES-EGC [*Gabrielle et al.*, 2006b]. In
4 all sites, the local and regional parameterization scenarios yielded similar temporal dy-
5 namics. However, closer examination revealed notable differences in the magnitude of

6 simulated emission peaks. For instance, the regional scenario resulted in systematically
7 lower fluxes than the local one in all sites. When accumulated over the simulation period,
8 the N₂O emissions predicted by the two parameterization scenarios differed by 30% as a
9 result (Table 2).

10 These discrepancies were mostly due to differences regarding soil water retention prop-
11 erties and bulk density, to which the model proved very sensitive. At La Saussaye, for
12 instance, topsoil bulk density differed by only 0.08 g cm⁻³ between the local and regional
13 parameterizations, but this was enough to create a 30% deviation in terms of simulated
14 N₂O efflux. Despite these discrepancies, the mean deviations (MD) and root mean squared
15 errors (RMSE) achieved by the two parameterization scenarios were generally close, the
16 only notable difference being that the RMSE was significantly higher with the regional
17 parameterization than with the local one at Arrou.

3.2. Regional simulations

18 Table 3 summarizes the simulation outputs for the three sub-regions, while Figure 2
19 provides a geographical mapping of the emissions. In terms of spatial distribution, there
20 were no marked differences between the sub-regions, which all presented a wide range of
21 emission rates. Beauce Chartraine exhibited a longitudinal gradient with lower N₂O fluxes
22 to the East and higher fluxes to the West, whereas in Faux-Perche the emission levels were
1 vertically stratified from North to South. Conversely, Beauce Dunoise was rather homo-
2 geneous and centered in the mid-range values of N₂O fluxes. In terms of total N₂O efflux,
3 the ranking of the sub-regions did not reflect that of the test sites, since Beauce Char-
4 traine came up with as the highest contributor (Table 3), despite being characterized
5 by significantly lower emission rates at the plot scale compared to the Faux-Perche area

6 (Table 2).

7 Within the sub-regions, the western half of Beauce Chartraine appeared particularly sen-
8 sitive in the regional balance of N₂O emissions. Other zones prone to N₂O emissions zones
9 could also be delineated, such as the northernmost and southernmost tips of Faux-Perche.
10 Spatial structures in the other parts of the map were mostly determined by the spatial
11 resolution of the soil map units (SMU), some of which were rather large with sizes ranging
12 up to 19 000 ha. In addition, SMUs were made up of two to five different soil type units
13 (STUs), with possibly contrasting potentials for N₂O emission. On the other hand, emis-
14 sions were much less variable within a given STU when it occurred across several map
15 units and thereby climatic conditions. Figure 3 shows the distribution of fluxes across
16 the various STUs to be strongly skewed, with an extended tail in the higher range of
17 emissions ($> 5 \text{ kg N}_2\text{O-N ha}^{-1}$). However, the weight of this upper-tail was very limited,
18 comprising only three STUs out of a total of 230, and making up 0.5% of the total area
19 simulated.

3.3. Comparison with IPCC estimates

20 At the sub-regional level, the model-based estimates of direct N₂O emissions from wheat-
21 cropped fields were 60% to 85% lower than the IPCC ones. The deviation was strongest
22 in Beauce Dunoise and smallest in Beauce Chartraine, reflecting the ranking of the sub-
1 regions respective to N₂O emissions on a per hectare basis. The background emissions
2 simulated by CERES-EGC were also lower than the IPCC default value of 1 kg N₂O-N
3 ha⁻¹, but to a lesser extent than the total emissions, and ranged from 0.29 to 1.02 kg
4 N₂O-N ha⁻¹. As a result, model-based EF_d estimates were extremely low compared to
5 the IPCC default ($0.01125 \pm 0.01 \text{ kg N}_2\text{O-N kg}^{-1} \text{ N}$), ranging from 0.0004 to 0.0012 kg

6 N₂O-N kg⁻¹ N. They were also much lower than the plot-scale estimates found in the three
7 test sites, which varied between 0.008 and 0.005 kg N₂O-N kg⁻¹ N ((Figure 4). The test
8 sites were actually located in zones with a higher than average potential for N₂O emissions
9 (Figure 2), especially in Faux-Perche.

10
11 Secondly, N₂O emissions were generally proportional to the amount of fertilizer N applied
12 to crops, on a sub-regional scale. Annual N₂O emissions were linearly related to N fertil-
13 izer inputs with little dependency on the range of fertilizer doses. As a result, the average
14 EF_{dS} estimated by fitting a straight line to the response curve provided estimates nearly
15 identical to those obtained from eq. 1 for the nominal dose of fertilizer N. Howevern, there
16 was a field site (La Saussaye) in which N₂O emissions reached a maximum for a dose of
17 150 kg N ha⁻¹, and decreased thereafter. This surprising result actually stemmed from a
18 change in the first fertilizer application for doses above 150 kg N ha⁻¹, which increased
19 from 70 to 80 kg N ha⁻¹. As a consequence, the crop growth potential was improved,
1 resulting in better fertilizer use efficiency and lower soil mineral contents throughout the
2 simulation. Unfertilized controls emitted only slightly less N₂O than the crops receiving
3 the nominal N dose (Figure 4), and simulated emission factors were extremely low as a
4 result.

5

4. Discussion

4.1. Uncertainty and validity of regional estimates

6 Extrapolating model simulations from plot to regional scale involves some degree of
7 uncertainty in spatialized inputs as well as model robustness to spatial extension.

8
9 The uncertainties of some inputs could be quantified prior to extrapolation, and their
10 effects approached via sensitivity analysis. These include soil water retention properties
11 and initial conditions in the soil profile, as discussed in the next paragraph. Other inputs
12 could not be associated with a range of uncertainty, most notably soil bulk density, to
13 which denitrification is very sensitive [*Hénault and Germon, 2000*]. Also, microbiological
14 parameters could not be spatialized based on the available soil information because they
15 do not appear to be related to particular physico-chemical properties such as soil texture
16 or organic matter content [*Hénault et al., 2005*]. For lack of an alternative method, we
17 assumed that the microbiological parameter sets measured in each test site could apply
18 to the entire surrounding sub-region.

19
20 The pedo-transfer functions used to derive soil water retention properties had a RMSE
21 ranging from 0.02 to 0.05 g g⁻¹ soil, depending on texture class and parent material
22 [*Bastet et al., 1998*]. This range of error falls within the spatial variations of such physical
1 properties at the field-scale [*Yanai et al., 2003*]. However, it had a marked influence on
2 model outputs, since an increase of 0.04 g g⁻¹ in the soil water content at field-capacity
3 and saturation resulted in a relative increase of 85%, 40% and 150% in the simulated sub-
4 regional N₂O efflux in Beauce Chartraine, Beauce Dunoise and Faux-Perche, respectively.
5 Conversely, a decrease of the same parameters by 0.04 g g⁻¹ resulted in a 40-80% decrease

6 in the N₂O efflux. Soil water content is known to be a major control of denitrification
7 via the water-filled pore space, to which this process is exponentially-related [*Hénault*
8 *and Germon, 2000; Hénault et al., 2005*]. The initial conditions at the beginning of the
9 simulations (ie, soil water and inorganic N content) were also varied based on the range
10 of values recorded in the sub-regions. Initial soil N was relatively sensitive: there was a
11 33-48% increase in the sub-regional fluxes between the minimum and maximum values of
12 initial N contents. The influence of initial water was marginal influence: setting it at 50%
13 of maximum plant available water instead of 90% (baseline value) induced only a 5-10%
14 decrease in the N₂O fluxes, probably because the simulations started two months ahead
15 of the wetter (winter) season.

16

17 The second major source of uncertainty (model robustness to spatial extension) could
18 be judged from the mean deviations achieved by CERES-EGC in the test sites with the
19 regional parameterization. These errors ranged from 0 to 8 g N₂O-N ha⁻¹ d⁻¹, which
20 represents 0 to 50% of the mean observed fluxes (Table 2). This range may be taken as
21 the error margin associated with the simulation of the annual N₂O efflux by the model.
22 From a more qualitative viewpoint, the extent to which CERES-EGC could be extrap-
23 olated to new field situations may be judged based on its N₂O sub-model, NOE. The
1 latter was successfully tested in 3 field sites in France, other the 3 test sites involved here,
2 along with 3 field sites in Central America [*Hénault et al., 2005*]. In these sites the mean
3 daily emission rates varied between 2 to 50 g N₂O-N ha⁻¹ d⁻¹, thus encompassing the 6-7
4 g N₂O-N ha⁻¹ d⁻¹ range that could be expected in the sub-regions based on the IPCC
5 approach (Table 3).

6

7 Regional estimates based on bottom-up aggregation of site-scale fluxes generally involve
8 model testing in a few test sites, and direct extrapolation to the area of interest [*Li et al.*,
9 2001; *Mummey et al.*, 1998]. Because testing usually involves site-specific calibration of
10 some model parameters [*Frolking et al.*, 1998; *Gabrielle et al.*, 2002], we included here
11 an intermediate phase in which the default parameterization procedure applied at the re-
12 gional scale was compared with site-specific parameterization. Of course this comparison
13 also involves a scaling issue, since the soil typological units (STUs) used in the regional
14 parameterization were much larger than the area covered by the measurements. As a con-
15 sequence, the properties of the STU corresponding to the test sites differed to some extent
16 from those actually measured on the experimental plots. However, in practice the soil
17 properties differed by less than 10%, which well within the range of variability that may
18 be expected at the field-scale itself [*Yanai et al.*, 2003]. Also, N₂O emissions are known to
19 be extremely variable spatially at the field scale, with coefficients of variations sometimes
20 exceeding 100% [*Hénault and Germon*, 1995]. As a result, the divergences between the
21 model outputs using whether the site-specific or the regional parameterization should not
22 be taken as a failure of the model, but rather as an indication of the degree of uncertainty
23 associated when downscaling from the mapping unit (SMU) to the site-scale. It is also
1 noticeable that the SMU-based simulations achieved an acceptable fit to the plot-scale
2 measurements (Table 2).

3 Overall, combining the unknowns mentioned above (including soil parameters, initial
4 conditions, and model error) result in an uncertainty of 50-100% around our mean simu-
5 lated estimates, which is rather large but comparable with the uncertainties of the IPCC

6 methodology and the $\pm 50\%$ margin reported by *Li et al.* [2001] in their inventory based
7 on the DNDC model.

8
9 Regional estimates may be verified against independent data, such as other inventories
10 or inverse atmospheric modeling [*Freibauer*, 2003]. Here, we investigated the first option
11 through the discussion on the emission factors, in the next paragraph. The alternative (at-
12 mospheric models) could not be applied since source strength estimates are only available
13 for much larger areas than the sub-regions considered here. Also, our estimates covered
14 only *c.* 40% of total arable land. Integration of other crops is therefore a pre-requisite for
15 such comparison to take place.

4.2. Empirical and model-based emission factors

16 There is a growing body of literature on the determination of direct emission factors
17 (EF_{ds}) from field measurements at the plot-scale. These factors have been shown to be
18 extremely variable from one field to another, ranging from 0.0003 to 0.068 kg N₂O-N kg⁻¹
19 N [*Flessa et al.*, 2002; *Velthof et al.*, 2003; *Kaiser et al.*, 1998; *Zheng et al.*, 2004]. There
20 are many sources of uncertainty behind those empirical estimates: quantification of back-
21 ground emissions, spatial and temporal coverage, and time-frame on which measurements
22 are carried out, which all warrant corrections [*Zheng et al.*, 2004]. Correcting for the ab-
1 sence of background emissions data is expected to lead to an over-estimation of EF_{ds}, by
2 a margin estimated at 15% to 110% under Chinese conditions [*Zheng et al.*, 2004]. Con-
3 versely, a shortage of temporal coverage (insufficient frequency of measurements) leads to
4 an under-estimation by 19% to 30% .

5 In principle, process-based models should not require any such corrections since they

6 simulate N₂O emissions continuously over time, and can predict fertilized as well as un-
7 fertilized crops. Thus, they may be expected to supply EF_d values up to 80% lower than
8 the empirical estimates listed above, among which the IPCC methodology. Such was the
9 case with the EF_ds simulated with CERES-EGC, which fell in the lower range of the val-
10 ues cited above. Calculation of EF_ds without the control term (ie assuming E_{N₂O}(N₀)=0
11 in eq. 1, as was done in a number of studies for lack of background emissions data [*Zheng*
12 *et al.*, 2004]), resulted in EF_ds ranging between 0.0016 and 0.0047 kg N₂O-N kg⁻¹ N,
13 closer to but still partly outside the IPCC range (0.00225 to 0.0202 kg N₂O-N kg⁻¹ N).
14 The same tendency was reported in another modeling study, but to a smaller extent: *Li*
15 *et al.* [2001] estimated an average EF_d of 0.008 kg N₂O-N kg⁻¹ N using the DNDC model
16 in China, with a 0.0025 to 0.04 kg N₂O-N kg⁻¹ N range.

17 Fertilizer type is also mentioned to affect the values of EF_d, although there is a lack of
18 sufficient data to derive generic, fertilizer-specific figures [*Bouwman*, 1996; *Mosier et al.*,
19 1996]. *Bouwman* [1996] reported EF_d values of 0.003 ± 0.003 kg N₂O-N kg⁻¹ N for am-
20 monium nitrate and urea, the two types of fertilizers used in the sub-regions simulated
21 here.

22
23 Lastly, EF_ds should capture some range of inter-annual variability. It is in principle
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 N₂O simulations.

4.3. Factors controlling N₂O emissions at the regional scale

6 The literature on spatial extension of N₂O fluxes, whether using process-based models
7 or empirical methods, shows the 'fertilizer dose' factor to lose some influence in favor of
8 environmental characteristics such as soil type and functional characteristics. At the Eu-
9 ropean scale, *Freibauer* [2003] modeled N₂O emissions based on pedological and agronomic
10 factors, and found a coefficient of only 0.4% in the correlation between these emissions and
11 fertilizer doses. In a review of emission data covering a wide range of crop management
12 and geographical locations, *Kaiser et al.* [1998] report a similar coefficient with a value
13 of 0.6%. These figures could be interpreted as an average EF_d of 0.004 to 0.006 kg N₂O-
14 N kg⁻¹ N for Europe. The apparent discrepancy between the ranges of EF_ds obtained at
15 the plot and regional scales may be due to an uneven sampling of field sites biased towards
16 the more N₂O-productive sites, when establishing empirical EF_ds, and these sites might
17 turn out to represent only a small proportion of total arable land. Such was the case
18 in our study since the test sites were actually above average in terms of N₂O emissions.
19 The frequent lack of background data in these experiments is also a source of bias since
20 a significant part of the emissions attributed to fertilizer use might actually be related to
21 the soil potential per se, as happened in our simulations. For urea and ammonium-nitrate
22 type fertilizers, *Bowman* [1996] reported relative differences as high as 100% between
1 EF_d estimates including or not an unfertilized control.

2

3 Lastly, the study by *Li et al.* [2001] at the country level revealed a clustered spatial pattern
4 for N₂O emissions, with contrasting efflux rates between groups of counties (equivalent to
5 our sub-regions). It is thus probable that some sub-regions would contribute significantly

6 less N₂O than others, which seems to be the case with those we had selected here. In such
7 sub-regions, N₂O emission levels primarily depend on a local potential set by climatic
8 conditions combined with soil microbiological and physical properties, with the influence
9 of crop management appearing somewhat minor in the expression of this potential. This
10 was evidenced by the low values of emission factors deduced from model output, im-
11 plying that a reduction in fertilizer application doses would have little effect on abating
12 N₂O fluxes. However, the fertilizer also influences the residual N content upon sowing of
13 the proceeding crop, which had a significant influence on the sub-regional N₂O efflux.
14 As a conclusion, mitigation measures should target a reduction in the amount of soil min-
15 eral N upon sowing of winter crops, and a decrease of the soil N₂O production potential
16 itself. While there is a range of best management packages available to address the first
17 point, there is a need for future research on the determinants of soil emission potentials.

18 **Acknowledgments.** Financial support from the French Ministry for the Environment
19 (through its GESSOL grant program) is acknowledged .

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Table 1. Spatial format of the various information layers used in the simulations

Type of information	Geographical format	Spatial level	Source
Soil types	Shapefile (contours of soil map units)		French Soil Survey
Weather data	Local meteorological stations	County	French Met Office
Crop management	Average per sub-region	Sub-region	Survey by advisory services
Land use	Average per county	County	Census data (1988), CAP declarations

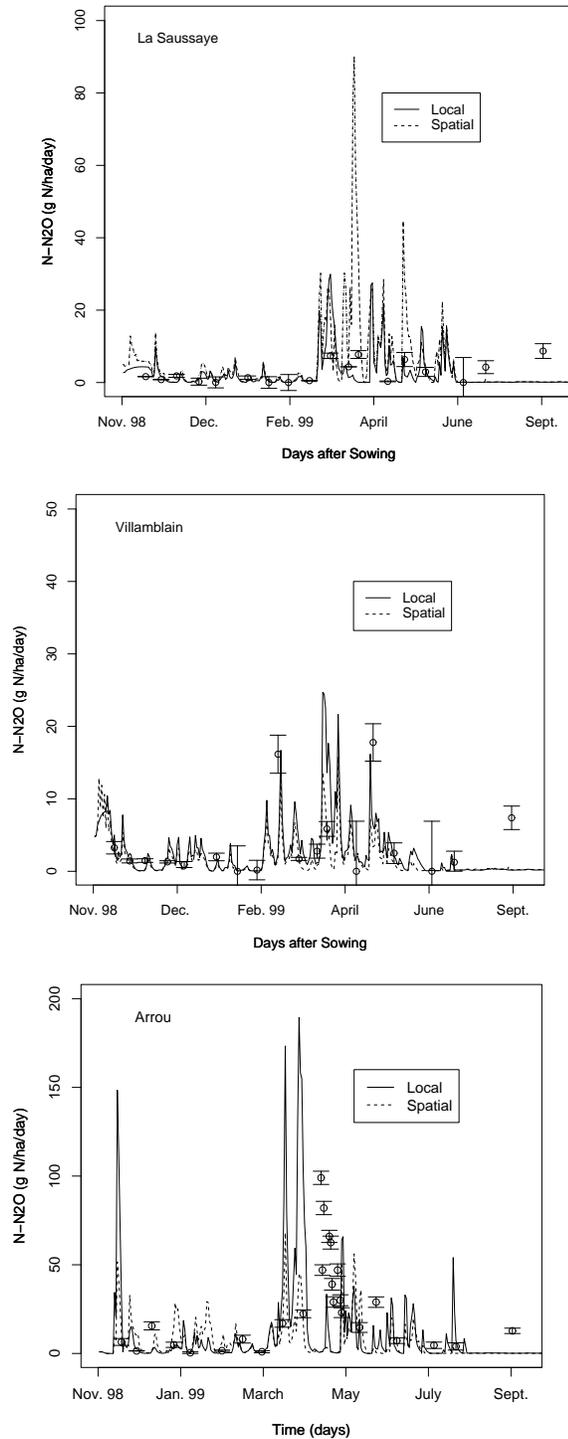


Figure 1. Simulated (lines) and observed (symbols) emissions of N₂O in the three test sites: an Haplic Luvisol at La Saussaye, an Haplic Calcisol at Villamblain, and a Redoxic Luvisol at Arrou. In the local parameterization scenario, detailed, site-specific information on soil properties was used, whereas the regional scenario involved only information

derived from the soil map.

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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 (p=0.05), and the root mean squared error is compared to mean experimental error using an F variance test [Smith *et al.*, 1996].

Parameterization scenario	La Saussaye		Villamblain		Arrou	
	Regional	Local	Regional	Local	Regional	Local
Cumulative N ₂ O flux (kg N ₂ O-N ha ⁻¹ yr ⁻¹)	2.16	3.10	1.23	1.79	3.51	5.10
Mean deviation (g N ₂ O-N ha ⁻¹ d ⁻¹)	0.00 ^a	0.19 ^a	2.00 ^a	0.78 ^a	8.03	6.26 ^a
Root mean squared error (g N ₂ O-N ha ⁻¹ d ⁻¹)	5.33 ^b	4.95 ^b	6.88 ^b	7.16 ^b	34.5	39.5

^a not significantly different from zero (p=0.05)

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

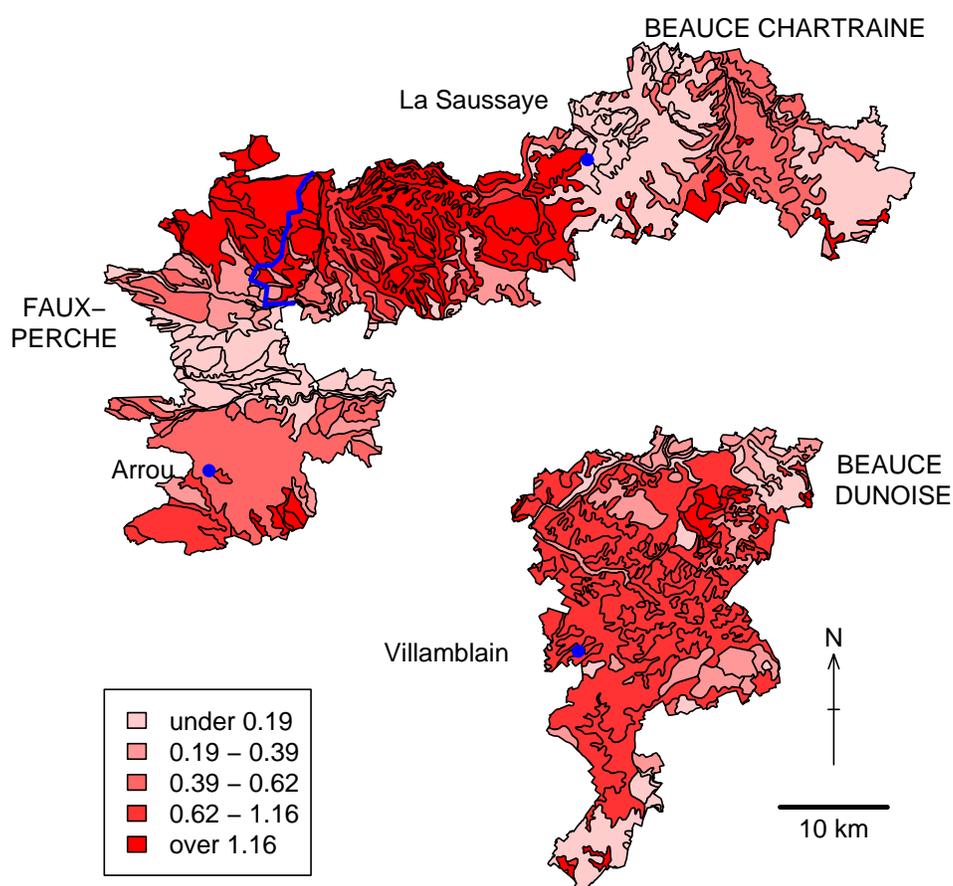


Figure 2. Simulation of N₂O emissions from wheat-cropped land in three agricultural sub-regions of the Beauce region. The fluxes are expressed in kg N₂O-N ha⁻¹.

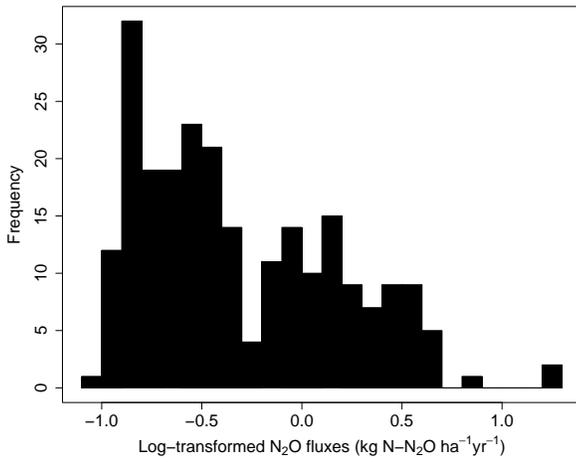


Figure 3. Histogram of log-transformed simulated fluxes across the various soil type units in the three sub-regions.

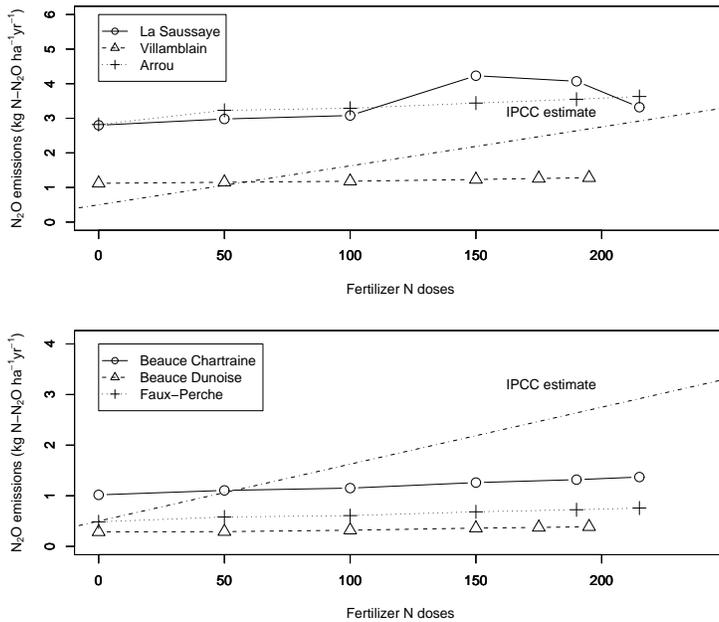


Figure 4. Simulated relationships between fertilizer N dose and year-round N₂O emissions at the local (top) and sub-regional (bottom) levels. The straight line corresponds to the *IPCC* [1997] relationship.

Table 3. Emissions of N₂O 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 simulated	Fertilizer N dose	Mean annual N ₂ O flux	Regional flux	Regional Emission Factor
	ha	kg N 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	77 223	0.01125
Beauce	23 474	195	0.39	9 108	0.0005
Dunoise		0	0.29	6 733	
IPCC	23 474	195	2.13	51 496	0.01125
Faux-	16 578	215	0.76	12 567	0.0013
-Perche		0	0.49	8 049	
IPCC	16 578	215	2.42	40 098	0.01125