

1 **Modelling nitrous oxide emissions from mown-grass and grain-cropping systems: Testing and**
2 **sensitivity analysis of DailyDayCent using high frequency measurements**

3 Nimai Senapati ^{a,b,*}, Abad Chabbi ^{a,b,*}, André Faé Giostri ^c, Jagadeesh B. Yeluripati ^d, Pete Smith ^e

4 ^a French National Institute for Agricultural Research (INRA), Poitou-Charentes, URP3F, 86600 Lusignan, France

5 ^b French National Institute for Agricultural Research (INRA), Versailles-Grignon, UMR- ECOSYS, 78850 Thiverval-Grignon, France

6 ^c Federal University of Parana, Rua XV de Novembro, 1299 – Centro, Curitiba – PR, 80060-000, Brazil

7 ^d The James Hutton Institute, Craigiebuckler, Aberdeen AB15 8QH, Scotland, UK

8 ^e Institute of Biological and Environmental Sciences, University of Aberdeen, 23 St Machar Drive, Aberdeen AB24 3UU, UK

9 Corresponding author Email: nimai_senapati@yahoo.com; nimaisenapati@gmail.com; abad.chabbi@lusignan.inra.fr

10 **Abstract**

11 The DailyDayCent biogeochemical model was used to simulate nitrous oxide (N₂O) emissions from
12 two contrasting agro-ecosystems *viz.* a mown-grassland and a grain-cropping system in France.
13 Model performance was tested using high frequency measurements over three years; additionally a
14 local sensitivity analysis was performed. Annual N₂O emissions of 1.97 and 1.24 kg N ha⁻¹ yr⁻¹ were
15 simulated from mown-grassland and grain-cropland, respectively. Measured and simulated water
16 filled pore space ($r = 0.86$, $ME = -2.5\%$) and soil temperature ($r = 0.96$, $ME = -0.63^\circ\text{C}$) at 10 cm soil
17 depth matched well in mown-grassland. The model predicted cumulative hay and crop production
18 effectively. The model simulated soil mineral N concentrations, particularly NH₄⁺, reasonably, but
19 the model significantly underestimated soil NO₃⁻ concentration under both systems. In general, the
20 model effectively simulated the dynamics and the magnitude of daily N₂O flux over the whole
21 experimental period in grain-cropland ($r = 0.16$, $ME = -0.81 \text{ g N ha}^{-1} \text{ day}^{-1}$), with reasonable
22 agreement between measured and modelled N₂O fluxes for the mown-grassland ($r = 0.63$, $ME = -$
23 $0.65 \text{ g N ha}^{-1} \text{ day}^{-1}$). Our results indicate that DailyDayCent has potential for use as a tool for
24 predicting overall N₂O emissions in the study region. However, in-depth analysis shows some
25 systematic discrepancies between measured and simulated N₂O fluxes on a daily basis. The current
26 exercise suggests that the DailyDayCent may need improvement, particularly the sub-module

1 responsible for N transformations, for better simulating soil mineral N, especially soil NO_3^-
2 concentration, and N_2O flux on a daily basis. The sensitivity analysis shows that many factors such
3 as climate change, N-fertilizer use, input error and parameter value could influence the simulation of
4 N_2O emissions. Sensitivity estimation also helped to identify critical parameters, which need careful
5 estimation or site-specific calibration for successful modelling of N_2O emissions in the study region.

6 **1. Introduction**

7 Nitrous oxide (N_2O) is a potent greenhouse gas (GHG), with a 100-year global warming
8 potential, nearly 300 times that of carbon dioxide (CO_2) on a mass basis, contributing 6.24% (third
9 most important contributor after CO_2 and methane) to overall global radiative forcing (Forster et al.,
10 2007; WMO, 2010). N_2O has a critical role in the global energy balance, earth surface temperature
11 and global climate change (IPCC, 2006). N_2O is also the single-most important contributor to
12 stratospheric ozone depletion, and a doubling of the atmospheric N_2O concentration could decrease
13 the ozone layer by 10%, which ultimately would increase harmful ultra-violet radiation reaching the
14 earth by 20% (Crutzen and Ehhalt, 1977; Ravishankara et al., 2009). The atmospheric N_2O
15 concentration has increased nearly 21% from a pre-industrial level of about 270 ppbv to 325.9 ppbv
16 in 2013, with an average increase rate of about $0.82 \text{ ppbv yr}^{-1}$ for the last decade (WMO, 2014).
17 With a relatively long atmospheric life-time of about 114 years, the increasing atmospheric N_2O
18 concentration is a global concern (IPCC, 2007). Of the approximately $19 \text{ Tg N}_2\text{O-N yr}^{-1}$ emitted
19 globally, 40-50% of total emissions derive from anthropogenic activities, (Forster et al., 2007; EPA,
20 2010; Syakila and Kroeze, 2011). Agriculture is the single biggest source of anthropogenic N_2O ,
21 contributing approximately 60–80% of global anthropogenic N_2O emissions (Denman et al., 2007;
22 Syakila and Kroeze, 2011). Expansion of agricultural land area, widespread use of nitrogenous (N)
23 fertilizers, and increased manure application are the main drivers of enhanced N_2O emissions from
24 agricultural systems (IPCC, 2007; Davidson, 2009). With an increasing human population, and the

1 consequent demand for higher food production, N₂O emissions are likely to continue to rise in the
2 coming decades (Mosier and Kroeze, 2000; Davidson, 2009; EPA, 2012). Important current
3 challenges are the development of robust N₂O inventories at national, regional and global scales,
4 understanding of climate change impact of N₂O emissions, and the definition of cost-effective
5 potential mitigation options across different agro-ecosystems.

6 The predominant microbial processes of N₂O emissions from agricultural soils are
7 nitrification and denitrification, which are regulated by different climatic drivers (temperature,
8 precipitation) (Liu et al., 2006, 2011), and soil physical (texture, structure, density, aeration, soil
9 water properties, water filled porosity) and chemical (pH, soil C and N availability) properties
10 (Čuhel et al., 2010; Signor and Cerri, 2013). Human induced activities, which affect soil
11 temperature, moisture and aeration regimes, along with the availability of soil C and mineral N, also
12 influence N₂O emissions under different agro-ecosystems. Significant emissions have been observed
13 after tillage (Omonode et al., 2011), N-fertilizer and manure application (Das and Adhya, 2014),
14 irrigation (Trost et al., 2013), and incorporation of crop residues (Shan and Yan, 2013). Across
15 different cropping systems, choice of crops, types of crop rotations and crop growth stages also have
16 an impact on N₂O emissions (Jeuffroy et al., 2013). Intensive grassland management practices, such
17 as mowing (cutting and subsequent harvesting) with frequent fertilization, have been reported to
18 enhance N₂O emissions (Rafique et al., 2011). However, underlying processes of N₂O production,
19 consumption and exchange between soil-atmosphere interface, and their interactions with biotic
20 (*e.g.*, plant species, microbial composition and diversity) and abiotic (*e.g.* climate, soil and
21 management practices) factors are yet to be fully understood (Butterbach-Bahl et al., 2013). Again,
22 variabilities in different controlling factors, both in space and time, result into enormous spatial and
23 temporal variations in N₂O emissions, adding uncertainty to efforts to upscale field measurements to
24 national/regional/global N₂O inventories (Mathieu et al., 2006; Groffman et al., 2009; Butterbach-

1 Bahl et al., 2013). Future global warming or climate change feedbacks on N₂O emissions are also
2 uncertain (Butterbach-Bahl et al., 2013).

3 Process-based dynamic models, such as DailyDayCent (Parton et. al., 1998; Del Grosso et
4 al., 2001, 2011) can be used not only to reduce the uncertainty/error originating from contrasting
5 agro-ecosystems or spatio-temporal variability, but also help in testing scientific hypotheses,
6 projecting N₂O emissions under future land uses and climate change scenarios, and investigating
7 potential mitigation strategies (Abdalla et al., 2010; Del Grosso et al., 2010; Kim et al., 2014). In
8 recent decades, many process-based models have been developed to simulate N₂O emission,
9 describing different biotic and abiotic processes, along with different factors that control emissions,
10 at differing levels of complexity. Although there is a need for simplicity in models, different
11 ecosystem processes need to be simulated in sufficient detail. The model DailyDayCent was selected
12 for simulation of daily N₂O emission in our present study as because a) DailyDayCent is a generic
13 model, thus can be used in different ecosystems including grassland and cropping systems, b) the
14 model is of intermediate complexity, but important processes are represented mechanistically and
15 are sufficiently detailed, c) required input data are often readily available, and d) the model
16 performed at least reasonably across different regions (Stehfest and Müller, 2004; Jarecki et al.,
17 2008; Del Grosso et al., 2008a, 2011; Abdalla et al., 2010; Scheer et al., 2014). The model is
18 currently used to estimate N₂O emissions for the U.S. National GHG Inventory conducted annually
19 and reported to the United Nations Framework Convention on Climate Change (UNFCCC) (EPA,
20 2013). DailyDayCent is also being increasingly used for projection of N₂O emission under various
21 climate and land use change scenarios, and investigation potential mitigation options globally (Del
22 Grosso et al., 2009; Abdalla et al., 2010). However, there is still considerable uncertainty in model
23 simulation and further model improvement is needed for higher precision and accuracy (Del Grosso
24 et al., 2010). Although the model has been tested under a range of agricultural systems around the

1 world (Stehfest and Müller, 2004; Jarecki et al., 2008; Abdalla et al., 2010; Scheer et al., 2014),
2 before using the model in new environments, the model needs to be tested carefully. Further, more
3 model testing and improvement will ultimately help to improve our current understanding of
4 underlying process of N₂O emissions and reduce uncertainty. Rigorous, in-depth model testing with
5 high frequency data of different streams, linked with different process information on nitrification
6 and denitrification, is important to make sure that the model simulates the dynamics of other
7 variables correctly along with N₂O emissions, otherwise there could be apparent good model
8 performance for the wrong reasons and *vice-versa* (Del Grosso et al., 2011). However, these types of
9 studies are limited, particularly for the DailyDayCent model (Del Grosso et al., 2008a; Jarecki et al.,
10 2008; Scheer et al., 2014).

11 Analysis of model sensitivity to different parameters is an important task to assess how the
12 model will behave in a different environment other than the one in which it was developed (Smith
13 and Smith, 2007). Sensitivity analysis identifies critical inputs or model internal parameters, which
14 are the most influential on the model outputs, and also determines correlations between model
15 results and a given parameter (Smith et al., 2012). It is also important to identify sensitive
16 parameters so that uncertainty bounds for model simulations can be reduced with careful
17 consideration of those critical parameters. A local or a global sensitivity analysis has its own
18 advantages and disadvantages. Although few global sensitivity analysis of the
19 DayCent/DailyDayCent model for N₂O emissions have been performed recently, either using an
20 inverse modelling approach for mostly internal model parameters (Rafique et al., 2014; Nécipálová et
21 al., 2015), or applying a Monte Carlo-based simulation for model input parameters (Fitton et al.,
22 2014a, b), a systematic local sensitivity analysis changing one parameter at a time is rare,
23 particularly for model inputs and internal model parameters in contrasting agro-ecosystems. A local

1 sensitivity analysis was performed to assess parameter sensitivity to model simulations in our
2 present study. The main objectives of the present study were -

3 a) to test the ability of the model for simulation of N₂O emissions under mown-grass and
4 grain-cropping systems, using high frequency measurements, along with model testing for soil
5 temperatures, soil water contents (water filled pore space), soil mineral nitrogen, soil organic
6 carbon (SOC) and plant production,

7 b) to analyse sensitivity of the model towards different inputs and model parameters, along
8 with their influence on model performance.

9 **2. Material and Methods**

10 *2.1. Experimental site and treatments*

11 The experimental site is located in Lusignan (46°25'12,91" N; 0°07'29,35" E) at the national
12 long-term experimental observatory, Poitou-Charentes, France. The experimental site is about 22 ha,
13 and is part of a long-term observatory for environmental research (Agroecosystems, Biogeochemical
14 Cycles and Biodiversity, SOERE-ACBB; <http://www.soere-acbb.com>) (Fig. 1). Average air
15 temperature and annual precipitation during the experimental period March 2011 to February 2014
16 were 12.3°C and 950 mm, respectively (Fig. 2). Summer was hot and dry, whereas winter was cold
17 and moist. August was the hottest month (average maximum temperature ~ 25.7°C) and the coldest
18 month was February (average minimum temperature ~ 0.6°C). December received the highest
19 precipitation (159 mm month⁻¹), whereas March and August received the lowest precipitation (33-40
20 mm month⁻¹). The most favourable climatic conditions for plant growth, in terms of average air
21 temperature and precipitation, were found in spring followed by autumn, summer and winter. The
22 experimental site was designed conjointly by INRA and CNRS research organisation institutes to
23 increase understanding of the effects of temporary grassland management and mixed arable

1 cropping/grassland systems on environmental outputs. The original experiment was established in
2 spring (March-April), 2005. Before 2005, part of the observatory was under either managed
3 grassland, grain-cropping or ley-arable rotations for at least 17 years. The soil profile can be divided
4 into two main domains: upper soil horizons are characterized by a loamy texture, classified as
5 Cambisol, whereas lower soil horizons are clayey rubefied horizons, rich in kaolinite and iron
6 oxides, classified as a Paleo-Ferralsol. A detailed description of the study site can be found
7 elsewhere (Chabbi et al., 2009; Moni et al., 2010; Senapati et al., 2014). Two paddocks (P1/T3 and
8 P2/T5), each about 3 ha in size and almost rectangular in shape, were selected from the original
9 experiment for the present study (Fig. 1). Temporary C_3 -grass was sown in both the paddocks during
10 spring in 2005. The herbaceous layer in the grassland consisted of a mixture of three grass species
11 *viz. Lolium perenne* L., *Festuca arundinacea* Schreb. and *Dactylis glomerata* L. Each of these two
12 paddocks was subject to equal treatment *viz.* regular mowing (cutting) and hay harvesting with
13 application of nitrogen (N) fertilizer without returning any off-site animal excreta for the time period
14 2006-2010. As a part of the original experiment of the ley-arable system (6-yrs. Grassland – 3-yrs.
15 cropping), one mown-grass paddock (P1/T3) was converted to grain cropping in March, 2011, with a
16 summer-corn (*Zea mays* L.) – winter-wheat (*Triticum* sp) – winter-barley (*Hordeum vulgare* L.)
17 rotation till February, 2014, hereafter referred to as the “grain-cropland”. The sown corn, wheat and
18 barley varieties were PR38V12 PIONER, Caphorn and Limpid, respectively. The second mown-
19 grass paddock (P2/T5) was continued with the same grass mowing treatment from March 2011 to
20 February 2014, hereafter referred to as the “mown-grassland”. Fertilizer N application rate and the
21 timing of crop sequences were adjusted every year using the PC-AZOTE software program for near
22 maximum plant production (Angevin, 1999; Kunrath et al., 2015). Nitrogen Nutrition Index (NNI)
23 was estimated regularly according to the method described by Farruggia et al. (2004) and Duru
24 (2004). The timing and rate of fertilizer applications were regulated to maintain an NNI of between

1 0.9 and 1.0, i.e. close to a non-limiting N nutrition allowing for potential herbage production
2 (Lemaire et al., 2008). N₂O emission was measured in the mown-grassland and grain-cropland
3 continuously for three years from March 2011 to February 2014, completing a full cycle of grain-
4 cropping and grass-mowing. The details of the management practices of the two treatments during
5 2011-2014 are summarized in Table 1.

6 *2.2. Meteorological measurements*

7 Daily weather parameters were measured on the site of the experiment and available on the
8 data base Climatik, maintained by INRA AgroClim. Daily maximum and minimum air temperature
9 and precipitation for the period 2005-2014 were used as climatic driving variables for the
10 DailyDayCent model. For the model spin-up run, similar past weather data of 30 years (1975-2004)
11 were used.

12 *2.3. Soil moisture and temperature measurements*

13 Volumetric soil water content was measured in the mowing paddock with TDR probes
14 continuously from 2011-2013 at half-hourly intervals at 6 soil depths (10, 20, 30, 60, 80 and 100
15 cm), whereas soil temperature was measured with temperature probes at 7 soil depths (5, 10, 20, 30,
16 60, 80 and 100 cm). Water filled pore space (WFPS) was estimated from soil moisture
17 measurements by using the equation:

$$18 \text{ WFPS (\%)} = [\theta_v / (1 - \text{bulk density} / \text{particle density})] \times 100 \quad (\text{Linn and Doran, 1984})$$

19 where θ_v is the percent volumetric water content. We used both WFPS and soil temperature data on
20 daily time scale at the 10 cm depth for model testing in mown-grassland. However, soil water and
21 temperature were not measured in the cropping paddock due to resource constraints.

22 *2.4. Soil organic carbon and mineral nitrogen measurements*

1 Total SOC stocks in the top 30 cm soil layer were measured in both mown-grassland and
2 cropland in the year 2005, 2008, 2011 and 2014. Although our present study of the N₂O emissions
3 was for the period 2011-2014, we used all the available SOC measurements from 2005-2014 for
4 model evaluation. To match with the model output for SOC, since DailyDayCent simulates SOC
5 only for the top 20 cm soil layer, measured SOC stocks in the 0-30 cm soil layer were converted into
6 SOC stocks of the 0-20 cm soil layer by assuming a minimum and maximum distribution of 60 and
7 90% of total SOC in the top 20 cm soil layer. However, for simplification, we used SOC stock for
8 the top 20 cm soil layer as an average of 75% of the top 30 cm soil layer. Soil mineral nitrogen
9 concentrations (NO₃⁻ and NH₄⁺) were measured from fresh soil samples during 2011-2013. Briefly,
10 25 g soil sample was extracted with 1M KCl (1:3 soil: solution ratio). The extract was centrifuged
11 for 15 min at 5800 g and filtered through a No.3 Durieux paper disc. The mineral nitrogen
12 concentrations in the soil extract were analysed by continuous flow colorimetry (TRAACS 2000,
13 Irama corp, Milwaukee,WI, USA). The NO₃⁻ concentration was determined as described by
14 Kamphake et al. (1967).

15 *2.5. Plant production*

16 Harvested hay production from the mown-grassland was measured as megagram of dry
17 matter (DM) per hectare (Mg DM ha⁻¹) after each mowing event. There were 3-4 mowing events
18 annually on irregular dates (Table 1). Cumulative harvested hay production was used for testing
19 model performance over the three year cycle. Similarly, total above ground biomass, grain and straw
20 yield were estimated in the units of Mg DM ha⁻¹ after harvesting events on cropland.

21 *2.6. Flux measurement*

22 N₂O and CO₂ flux were measured simultaneously using six automatic chambers from 2011-
23 2014 in both mown-grassland and grain-cropland. We used the same automatic chamber and method

1 for flux measurements in our experiment as described in detail by Laville et al. (2011). Briefly, the
2 automatic chambers, with dimensions of 0.7m × 0.7m × 0.30m, were made of stainless steel to
3 prevent air constituents such as ozone and nitrogen dioxide reacting with the chamber walls. Each
4 chamber frame was pressed into the earth to a depth of 9 cm, giving an effective height above
5 ground of around 20 cm and headspace of 98 L. A cover mounted on pivot arms was moved by an
6 electric actuator to open and close the chamber. A small vent of 4-mm in diameter provided the
7 pressure equilibrium between the inside and outside of the chamber. The N₂O and CO₂ gas analysers
8 were connected serially and their outlet flow was fed back into the chamber. The N₂O and CO₂
9 concentrations were measured by infrared absorption spectrometry (Thermo-Environmental
10 Instruments Inc., model 46C, Franklin, Massachusetts; and LI-COR Inc., model Li-840, Lincoln,
11 Nebraska, respectively). The sensitivity thresholds (noise level) of the analysers were around 10 ppb
12 for N₂O and 1.5ppm for CO₂. The gas analysers were calibrated once a month, using certified gas
13 tanks. Each chamber was sampled in 10 seconds intervals, for 15 minutes, through the analysers, and
14 the outflow of the N₂O and CO₂ analysers was fed back to the chamber. Raw concentrations were
15 recorded every 10 seconds using a data logger (CR1000, Campbell Scientific, Inc, US). Each
16 chamber was closed for 15-min periods, and with 6 chambers the complete measurement cycle thus
17 lasted for 90 minutes. The six chambers device therefore allowed 96 flux measurements per day or
18 16 mean fluxes per day for each of the 6 chambers. N₂O and CO₂ fluxes were calculated from the
19 variations over time in the slopes of the gas outlet concentration (C_{out}), using the following equation:

$$20 \quad F = (V/A) \times (dC_{out} / dt)$$

21 where F is the flux (in ppb s⁻¹), V is the chamber headspace volume (m³), A is the ground area
22 covered by the chamber (m²) and dC_{out} / dt is the time derivative of the outlet concentration (ppb
23 s⁻¹). Fluxes were converted from ppb s⁻¹ to ng N m⁻² using the following equation:

1 $\text{ng N m}^{-2} = (M \times P/RT) \times \text{ppb}$

2 where, M is the gas molar mass in gram per mol, P is the air pressure fixed at 1013×10^2 Pa, R is the
3 perfect gas constant ($8.31 \text{ J K}^{-1} \text{ mol}^{-1}$) and T is the absolute (K) air temperature in the chamber
4 headspace, measured during the gas accumulation. There were few gaps in N_2O flux measurements
5 due to management practice, poor quality data and instrumental failure. During the ploughing events,
6 the chambers were generally removed for three days. N_2O flux measurements were checked taking
7 CO_2 flux as reference, and with abnormal measured CO_2 flux, N_2O flux measurements were
8 discarded.

9 *2.7. DailyDayCent model description:*

10 The model DailyDayCent is the daily time-step version of the CENTURY biogeochemical
11 model, simulates daily exchanges of carbon, nutrients and trace gases among the atmosphere,
12 vegetation and soil (Parton et al., 1998; Del Grosso et al., 2001, 2011). Key sub-models include plant
13 production, decomposition of dead plant material and soil organic matter, soil water and temperature
14 dynamics, and N gas fluxes. Flows of C and N between the different soil organic matter pools are
15 controlled by the size of the pools, C/N ratio and lignin content of material, and abiotic
16 water/temperature factors. The land surface sub-model simulates soil water and temperature for each
17 horizon throughout the defined depth of the soil profile. The soil water sub-model particularly
18 simulates soil water content and water fluxes (e.g., run off, leaching, evaporation and transpiration).
19 Saturated water flow occurs on days that receive rainfall, irrigation, or snow melt, and unsaturated
20 flow occurs on all days that do not have water inputs sufficient to saturate the profile and can be up
21 or down the profile depending on matric and gravitational potentials. The plant growth sub-model
22 simulates plant productivity as a function of genetic potential, phenology, temperature, soil water,
23 nutrient availability, shading and solar radiation (i.e. energy biomass conversion factor). Net primary
24 productivity is divided among leafy, woody, and root compartments on the basis of plant type and

1 phenology. The root/shoot ratio of NPP allocation is a function of soil water content and nutrient
2 availability. **Plant** germination date could either be specified or calculated as a function of soil
3 temperature; similarly harvesting date could either be specified or calculated as a function of
4 accumulated growing degree days since germination. Management and disturbance events (e.g.
5 cultivation, fertilization, grazing, cutting, fire, irrigation etc.) can easily be implemented. The death
6 rate of plant compartments is controlled by soil water, temperature, season, and plant-specific
7 senescence parameters. Dead plant material is divided into structural (high C/N) and metabolic (low
8 C/N) components. In the SOM submodule, soil organic matter (SOM) is divided into three pools
9 (active, slow, and passive) based on their turnover rates. SOM is simulated in the top 20 cm soil
10 layer as a sum of dead plant matter and three SOM pools on the basis of their decomposition rates.
11 Decomposition of litter and soil organic matter mineralization are functions of substrate availability,
12 substrate quality (lignin content, C/N ratio), and water and temperature stress, soil texture and tillage
13 intensity. Soil nitrate (NO_3^-) is distributed throughout the soil profile and available for leaching into
14 the sub-soils. Nitrate movement and leaching are largely controlled by soil water flow and plant N
15 uptake. Soil ammonium (NH_4^+) is assumed to be immobile and distributed entirely in the top 15 cm
16 layer of soil layer. The N gas sub-model simulates soil N_2O and NO_x gas emissions from
17 nitrification and denitrification, as well as N_2 emissions from denitrification. Nitrifying microbes
18 oxidise NH_4^+ to NO_3^- , with some N_2O and NO_x released during intermediate steps. N gas emissions
19 from nitrification is calculated on a daily basis, based on soil NH_4^+ concentration, water content, pH,
20 texture and the temperature in the top 15 cm layer. Denitrification is an anaerobic process in which
21 heterotrophic microbes reduce NO_3^- to NO_x , N_2O and N_2 . Daily denitrification is calculated for each
22 soil layer based on soil NO_3^- concentration, heterotrophic respiration (available labile carbon), soil
23 water content and soil physical properties related to texture, which influences gas diffusivity. The
24 model calculates $\text{N}_2+\text{N}_2\text{O}$ emissions from denitrification by assuming that the process is controlled

1 by the input (NO_3^- , respiration, WFPS) that is most limiting. N_2O emissions are calculated from
2 $\text{N}_2+\text{N}_2\text{O}$ gas emissions and a $\text{N}_2/\text{N}_2\text{O}$ ratio adjustment coefficient (*n2n2oadj*). The current
3 DailyDayCent model allows the user to vary *n2n2oadj* along with other soil N dynamic parameters
4 viz. maximum daily nitrification amount (*MaxNitAmt*), fraction of new net mineralization that goes
5 to NO_3^- (*netmn_to_no3*), maximum proportion of nitrified N that is lost as N_2O at field capacity
6 (*N2Oadjust_fc*), and minimum proportion of nitrified N that is lost as N_2O at wilting point
7 (*N2Oadjust_wp*). These above five important soil N parameters can be found in “sitepar.in” file.
8 Daily maximum/minimum air temperature and precipitation, soil texture by horizon, land cover/use
9 data, and timing and information of field and crop management events are needed as primary model
10 inputs. Model simulated outputs include daily N-gas flux (N_2O , NO_x , N_2), CO_2 flux from
11 heterotrophic soil respiration, soil organic C and N, NPP, soil NH_4^+ in top 15 cm soil, NO_3^- , water
12 content, WFPS and temperature by soil horizon, H_2O and NO_3^- leaching, and other ecosystem
13 parameters. A more detailed description of the model can be found elsewhere (Parton et al., 1998,
14 2001; Del Grosso et al., 2001, 2008b, 2011, Nectpálová et al., 2015).

15 *2.8. Model set-up, parameterization, calibration and simulation:* DailyDayCent was set-up using
16 site specific parameters viz. texture, bulk density (BD), field capacity (FC), wilting point (WP),
17 hydraulic conductivity, SOC, pH etc., measured or estimated in 2005 (Table 2). Soil water
18 characteristics (FC, WP and saturated hydraulic conductivity) were estimated from texture and
19 organic matter using the algorithm developed by Saxton and Rawls (2006). But, soil water content
20 (SWC) was found from preliminary model run to be overestimated in our site. All three estimated
21 soil water characteristics were tested for possible model overestimation of SWC, and a reasonable
22 model simulation of SWC was obtained when FC was reduced by 10%. To reduce any uncertainty
23 originating from the estimation of soil water characteristics, in simulation of SWC, WFPS and
24 subsequently N_2O emissions, estimated FC was calibrated by reducing the value by 10% in our

1 model set-up, according to the recommendation of the DailyDaycent developer (Del Grosso et al.,
2 2011).

3 As N₂O emissions are sensitive to SOC and prior land-use, and all the SOC pools including
4 different nutrients are rarely known at the beginning of a current experiment of interest, simulation
5 of native vegetation followed by historical land uses are generally recommended for the
6 DailyDayCent model to establish a modern-day base line (Del Grosso et al., 2006, 2011). To
7 establish a modern-day base line at the starting of our main experiment in 2005, model simulations
8 were performed in three time blocks according to historical records and published literature *viz.* (1)
9 native temperate-deciduous forest (AD 1 to plough out-1750), (2) historical land use – (a) grass
10 grazing (1751-1845), (b) ley-arable rotation (1846-1980), and (3) modern day agriculture with
11 known ley-arable rotation (1981-2004) (Mather et al., 1999; Chabbi et al., 2009; Kaplan et al., 2009;
12 Senapati et al., 2014). Thirty years (1975-2004) of available daily weather data, as mentioned in the
13 meteorological measurement section, was used to run the model from AD 1 to 2004. A spin-up
14 simulation (native forest) of at least 1600 years was needed to achieve relatively stable SOC pools
15 before implementing the base simulation (plough out and historical land use). The equilibrium
16 simulation suggested that the SOC pool in the top 20 cm soil layer under the native temperate-
17 deciduous forest (~81 Mg C ha⁻¹) decreased by 42% within 100 years of agricultural use (~47 Mg C
18 ha⁻¹) by 1850 (Fig. 3). From 1850 onwards, SOC further decreased to 37-39 Mg C ha⁻¹ in 2005,
19 representing another 17-21% loss within 155 years compared to the level in 1850. The equilibrium
20 simulation was consistent with the literature, indicating a mean SOC stock in the top 30 cm soil layer
21 under various native forest of 60-94 Mg C ha⁻¹ in France (Arrouays et al., 2001; Martin et al., 2011;
22 Meersmans et al., 2012), and a loss in SOC ranging from 30-70% due to land use change from native
23 forest to agriculture in France (Arrouays and Pelissier, 1994; Balesdent et al., 1998). Other studies
24 around the world also reported a 30-60% loss in SOC after clearing of native forest followed by

1 agricultural uses (Guo and Gifford, 2002; Poeplau et al., 2011). Simulated SOC stocks in 2005 were
2 similar to our field measurements in the same year in mown-grassland (38.9 Mg C ha⁻¹) and grain-
3 cropland (36.6 Mg C ha⁻¹) (Fig. 3).

4 In the plant growth sub-model, temperate mown-grass was simulated as a perennial plant
5 with dynamic C allocation, whereas the three grain crops (corn, wheat and barley) were simulated as
6 grain filling annuals with growing degree day (GDD) and dynamic C allocation. The plant growth
7 sub-model parameters were adjusted based on literature values, previous model experience,
8 preliminary model runs and field measurements (Del Grosso et al., 2011; Chang et al., 2013; Rafique
9 et al., 2014; Necpálová et al., 2015). The parameters related to plant growth and biomass
10 accumulation in the present study are listed in Table 3. The simulated harvested C in the mown-
11 grassland, and simulated grain and straw C in the cropland were manually converted to dry matter by
12 dividing the C with the measured C concentrations in hay (41%), grain (45%) and straw (41%).
13 Table 3 also shows five default soil N dynamics parameters used in the “sitepar.in” file. No other
14 model parameter was modified or adjusted. After establishing the modern-day base line in 2005 for
15 model simulation in our experiment, as described above, the model run was continued in both
16 mown-grassland and grain-cropland until 2014, using field management practices and climatic
17 variables as drivers.

18 2.8. Statistical analysis

19 The following tests were used to evaluate the performance of the DailyDayCent model:
20 sample correlation coefficient (r), root mean square error ($RMSE$) and mean error (ME), as defined
21 in Smith et al. (1996, 1997) and summarized in Smith and Smith (2007). The significance of r was
22 tested using a F -test ($P = 0.05$), whereas significance of ME was evaluated using Student's t -test
23 (two-tailed, critical at 2.5%). On the other hand, $RMSE$ was tested by comparing to its value at 95%
24 confidence intervals ($RMSE_{95\%}$) (Table 4). The statistic r tests the correlation between measured and

1 simulated values, and thus describes to what extent the dynamics or variability can be captured by
2 the model irrespective of any systematic errors. On the other hand *RMSE* and *ME* evaluate the
3 coincidence, and thus quantify the difference between simulated and measured values. Replication
4 values of some measured variables, such as WFPS and soil temperature, were not available in our
5 experiment, but the same were available for other measurements (N₂O flux, soil mineral N
6 concentration, SOC and plant yield). For this reason, two different coincidence analysing statistics
7 (*ME* and *RMSE*) were used to exploit the advantage of replicated measurements whenever available
8 in our experiment. For an ideal fit, *r* equals 1, and *ME* and *RMSE* equal zero.

9 2.9. Sensitivity analysis

10 (Model sensitivity to a total of 14 parameters (2-climatic input parameters, 7-soil
11 parameters, fertilizer N quantity, and 5-soil N-dynamics parameters in “sitepar.in” file) was
12 conducted by altering one parameter at a time (local sensitivity analysis;Smith and Smith, 2007;
13 Table 5). Sensitivities of simulated variables were examined by changing daily air temperature by
14 $\pm 1^{\circ}\text{C}$ and pH by ± 1 unit, whereas sensitivity of model simulations to all other parameters were
15 examined by changing $\pm 10\%$ of the parameter base values. Sensitivity was expressed as percentage
16 change in the simulated variable compared to its original base simulation over the experimental
17 period 2011-2014. The sensitivities $>10\%$, 5-10% and $<5\%$ were considered high, moderate and
18 weak in our present study. Additionally, to test whether those changes ($\pm 1^{\circ}\text{C}$ in air temperature,
19 ± 1 unit in pH and $\pm 10\%$ in others) in parameter/inputs had a significant influence on model
20 performance, the influence of the individual parameter error or uncertainty on model performance
21 was tested against measurements (Table 5). **3. Results**

22 3.1. Modelling soil water (water filled pore space) and temperature

23 Over the experimental period, significant agreement was obtained ($r = 0.86$, $ME = -2.5\%$)
24 between modelled and measured WFPS at 10 cm soil depth in mown-grassland (Fig. 4 and Table 4).

1 The model successfully simulated seasonal dynamics, and the processes of soil drying and wetting
2 during summer and autumn, respectively (Fig. 4). However, some discrepancies were found between
3 simulation and measurements during different seasons. For example, the model moderately
4 overestimated WFPS (9-27%) during summer-autumn; in contrast WFPS was slightly
5 underestimated (8%) during spring. Model performance for WFPS was not evaluated in grain-
6 cropland due to the unavailability of measured data. However, averaged over mown-grassland and
7 grain-cropland, simulated WFPS at 10 cm soil depth was high (60-61%) during winter and low in
8 summer (35-41%) (Fig. 4). The simulated WFPS reached the highest point (92%) in winter, and was
9 lowest (11%) during summer. Simulated WFPS under mown-grassland and grain-cropland was
10 almost equal during winter and autumn, but some discrepancy was found from spring to summer. In
11 2011, WFPS was relatively higher under corn compared to mown-grass during spring; on the other
12 hand, WFPS was lower under corn during late-summer to early autumn. Interestingly, WFPS was
13 higher under wheat and barley during summer compared to mown-grass in 2012 and 2013,
14 respectively. Averaged over the whole experimental period, simulated WFPS at 10 cm soil depth
15 was 49% in mown-grassland, whereas WFPS was 4.5% greater in cropland compared to grassland
16 (Fig. 4).

17 The simulated soil temperature at 10 cm soil depth was highly correlated ($r = 0.96$) with
18 measurements over the study period in mown-grassland, with non-significant simulation error ($ME =$
19 -0.63°C) (Fig. 5 and Table 4). DailyDaycent also accurately captured the seasonal pattern of soil
20 temperature, both in terms of time and magnitude. However, the model moderately overestimated
21 soil temperature by 21% during late-summer to winter. Model performance for soil temperature was
22 not evaluated in grain-cropland for to the unavailability of measured data. Averaged over of the two
23 systems, mean simulated soil temperature across the experimental period at the 10 cm soil depth was
24 14.1°C (Fig. 5). Summer soil temperature peaked up to 25°C , whereas minimum temperature

1 lowered down to 0.78°C during winter. Simulated soil temperature was higher in cropland during
2 spring compared to mown-grassland in 2011, but it was lower during late summer–early autumn in
3 the same year. In contrast, an opposite trend in simulated soil temperature was found in 2012 and
4 2013. Averaged simulated soil temperature at the 10 cm soil depth was higher in grain-cropland, by
5 around 1°C, compared to mown-grassland.

6 .

7 *3.2. Modelling plant production, nitrogen uptake and nitrogen leaching*

8 Over the simulation period of three years, DailyDayCent simulated cumulative hay
9 production efficiently ($r = 0.99$, $ME = -1.40$ Mg DM ha⁻¹) in mown-grassland (Fig. 6-7 and Table 4).
10 Over all three grain-crops in cropland, simulated plant production was reasonable ($r = 0.88$, $ME =$
11 1.22 Mg DM ha⁻¹). The model simulated total above-ground biomass, grain and straw yield
12 satisfactorily for wheat and barley, but the model underestimated corn production significantly (Fig.
13 7 and Table 4). On each mowing events in grassland, simulated above-ground live biomass
14 decreased sharply on mowing dates (Fig. 6). . The growth of winter wheat and barley in cropland
15 was slow at the beginning, due to lower winter temperature, and thereafter picked-up with increasing
16 air temperature (Fig. 6). Simulated cumulative plant N-uptake over the three year period was almost
17 similar in magnitude in both mown-grassland and grain-cropland (355-413 kg N ha⁻¹). Simulated
18 cumulative total N-leaching over the same period was found in the range 163-517 kg N ha⁻¹, and the
19 result indicates that total leaching loss of N from grassland was 2.2 times greater than cropland (Fig
20 6).

21 *3.3. Modelling soil organic carbon and soil mineral nitrogen*

22

1 Significant coincidence between measured and modelled SOC stocks in the top 20 cm soil
2 layer was found in both systems (Fig. 2 and Table 4). The measured and modelled SOC were close,
3 but with a non-significant ($p < 0.05$) correlation between them. The results show that the model
4 efficiently simulated the magnitude of SOC, but was not so well able to simulate SOC dynamic.
5 However, both measured and simulated values demonstrated that SOC remained relatively constant
6 over the experimental period under both the agro-ecosystems.

7 Overall, reasonable model prediction of soil NH_4^+ in top 15cm soil layer ($r = 0.23-0.29$, ME
8 $= 0.01-0.42$ mg N kg^{-1} soil) was achieved in both the ecosystems (Fig. 8 and Table 4). Significant
9 coincidence was found between measured and simulated NH_4^+ in both systems, but no significant
10 correlation was obtained between them. The model significantly underestimated soil NO_3^-
11 concentration ($ME = 5.5-16.4$ mg N kg^{-1} soil) in the top 30 cm soil layer under both systems, and no
12 significant correlation ($r = -0.19$ to -0.22) was obtained between modelled and measured soil NO_3^-
13 (Fig. 8 and Table 4). ..,=. Simulated soil mineral N concentration was mainly driven by N-
14 fertilization events. There were sharp peaks in simulated NH_4^+ concentration after each of the
15 fertilization events, depending on the amount of applied fertilizer-N. Similarly, simulated NO_3^-
16 concentration followed the same trends as of NH_4^+ , but the peaks of NO_3^- concentration were
17 relatively blunt compared to that of NH_4^+ . Comparing the two systems, averaged simulated soil
18 mineral N concentration in mown grassland was 1.1-2.5 times greater compared to cropland.
19 Averaged measured soil NH_4^+ concentration was 1.03 times greater in mown-grassland compared to
20 grain-cropland, but measured NO_3^- was 0.55 times greater in cropland compared to mown-grassland.

21 3.4. Modelling nitrous oxide flux

22 In mown-grassland, the model simulated the dynamics and the magnitude of N_2O flux
23 reasonably well ($r = 0.63$, $ME = -0.65$ g N ha^{-1} day^{-1}) over the whole experimental period from

1 March 2011 to February 2014 (Fig. 9 and Table 4). Significant correlation ($p < 0.05$) was obtained
2 between measured and modelled daily N₂O fluxes, but among the two coincidence analysing
3 statistics *viz.* *ME* and *RMSE*, only *RMSE* was found to be significant at the 95% confidence limit,
4 indicating significant simulation error for N₂O emission when only accounting for measurement
5 error. Model simulations of N₂O flux in different seasons and years showed variability. In 2011, two
6 fertilization events were immediately followed by two simulated small N₂O flux peaks in spring.
7 The model simulated the timing and the magnitude of measured N₂O peaks correctly throughout the
8 year 2011. Three simulated N₂O peaks were found after three fertilization events during spring-early
9 summer in 2012. But, no peak was observed in the measurements after the first and third fertilization
10 events in March and July, respectively. The model overestimated N₂O emission during the main
11 grass growing period in spring, but correctly predicted an extended measured peak of 5-10 g N ha⁻¹
12 day⁻¹ in autumn. The year 2013 was marked with four mowing and five fertilization events during
13 late-winter to early-autumn. The model reasonably simulated the dynamics and magnitude of N₂O
14 flux in 2013, but the model overestimated emissions in early spring. N-fertilizer was applied at the
15 highest rate of 90 kg-N ha⁻¹ in February, but only a small peak was found in both simulation and
16 measurement after the fertilization event. Two moderate N₂O peaks were measured in May after the
17 second N-fertilizer application of 60 kg-N ha⁻¹, and the both peaks were simulated satisfactorily. But
18 after the third fertilization event (60 kg-N ha⁻¹) in June, the model failed to simulate the largest
19 measured peak of about 250 g N ha⁻¹ day⁻¹, and the measured peaks were 3-4 times greater and late
20 by around one week compared to the simulated peaks. There were two more moderate simulated
21 N₂O peaks (36-56 g N ha⁻¹ day⁻¹), after the last two fertilization events in 2013; but the model
22 overestimated the N₂O peak after the last fertilization event. Interestingly, some small negative N₂O
23 fluxes (> -10 g N ha⁻¹ day⁻¹) were found in measurements under mown-grassland during May-July in
24 2011 and August-October in 2012. However, no negative flux was simulated by DailyDayCent.

1 In cropland, significant agreement between measured and simulated daily N₂O fluxes was
2 obtained over the whole experimental period (Fig. 9 and Table 4). A significant correlation ($r =$
3 0.16) was obtained between measured and simulated fluxes at $P < 0.05$, and there was no significant
4 simulation error at $P < 0.025$ or 95% confidence limit. In general, almost every N-fertilization event
5 was immediately followed by a simulated peak in N₂O emissions, irrespective of season and year.
6 Both measurement and simulation showed a small N₂O peak (8-9 g N ha⁻¹ day⁻¹) during March-
7 April, after the first tillage operation and before sowing of corn. In the corn production season during
8 April-September in 2011, significance correlation was obtained between measured and simulated
9 N₂O fluxes, but the model overestimated N₂O emissions over the corn season (Fig. 9 and Table 4).
10 The model simulated a moderately high N₂O peak after the first fertilization event in early May, but
11 no such peak was observed in the measurements. There were some small negative measured peaks
12 (> -1.2 g N ha⁻¹ day⁻¹) during July-September, but no negative N₂O flux was found in the simulation.
13 Overall, in the wheat growing period from November 2011 to July 2012, the model successfully
14 simulated N₂O emissions, but correlation between measured and simulated flux values was low (Fig.
15 9 and Table 4). There were three simulated N₂O peaks after three N-fertilization events in wheat
16 seasons, but no peak was observed after the third fertilization event in measurements. In contrast, the
17 model was inefficient in capturing two measured N₂O peaks during winter before the first
18 fertilization event. Some small negative measured fluxes were found in measurements during wheat
19 growing season, mostly in late winter to early summer, but the model did not simulate any negative
20 N₂O flux during the same time. There were some interesting N₂O flux activities in 2012 during the
21 fallow period between harvesting of wheat in July and sowing of barley in October. During this
22 fallow period, some positive and negative fluxes in the range -8 to 11 g N ha⁻¹ day⁻¹ were observed in
23 measurements, but DailyDayCent was unable to simulate them both precisely, where the model
24 underestimated the flux during late-summer, but overestimated during early autumn (Fig. 9).

1 DailyDayCent was also unable to predict N₂O uptake in the fallow period, unlike the measurements.
2 Significant correlation between measured and simulated N₂O fluxes was obtained over the barley
3 growing period from October 2012 to July 2013, but the model significantly underestimated N₂O
4 emissions in the same period (Fig. 9 and Table 4). N-fertilizer was applied twice in the barley
5 season, and the model reasonably simulated the timing and magnitude of the measured peak after the
6 first fertilization, but underestimated the measured peak after the second fertilization event. A few
7 other discrepancies between simulated and measured N₂O fluxes were also observed during the
8 barley production season (Fig. 9). For example, the model failed to simulate two small measured
9 N₂O peaks during winter. The model was also unable to simulate any measured peak (~10-60 g N
10 ha⁻¹ day⁻¹) during May-June before the harvesting of barley, where the model mostly underestimated
11 measured large N₂O fluxes. There was a fallow period after harvesting of barley in July, 2013 until
12 February, 2014. The model predicted N₂O emissions satisfactorily during this fallow period, but
13 there was some underestimation in August and November, and overestimation in September (Fig. 9).

14 Both in mown-grassland and grain-cropland, overall N₂O peaks were driven by precipitation
15 and fertilization events, and the main simulated and measured N₂O peaks were seen during the main
16 plant growing period from spring–early autumn, whereas emissions were low in winter. Over a
17 period of three years, simulated cumulative N₂O emissions were 5.90 and 3.72 kg N ha⁻¹ in grassland
18 and cropland, respectively (Figure 9). This indicates an annual N₂O emission of 1.97 and 1.24 kg N
19 ha⁻¹ year⁻¹ from mown-grassland and grain-cropland, respectively. Results also showed that
20 simulated daily and cumulative N₂O emissions from grassland were 59% greater compared to
21 cropland.

22 3.5. Sensitivity analysis

23 Model simulations of N₂O emissions, WFPS, soil temperature, plant production and soil
24 mineral N concentrations were examined for their sensitivities to a total of 14 parameters. In this

1 section, model sensitivity is described as averaged over mown-grassland and grain-cropland, and
2 then simulation sensitivity is compared between the two contrasting agro-systems.

3 Among the 14 parameters, DailyDayCent was mostly sensitive to four soil properties (BD,
4 FC, SOC and pH), amount of applied fertilizer-N, one soil N-dynamics parameters in the
5 “sitepar.in” file (*N₂Oadjust_fc*) and two climatic inputs (air temperature and precipitation) (Table 5).
6 Among different model output variables, WFPS was highly sensitive to changes in FC and BD,
7 whereas sensitivity was lower to other parameters. Simulated soil temperature was only moderately
8 sensitive to air temperature. DailyDayCent exhibited a low sensitivity in simulation of plant yield to
9 different parameters *viz.* SOC, FC, fertilizer-N quantity, air temperature and precipitation. Model
10 prediction of soil NH₄⁺ concentration was highly sensitive to changes in BD and pH, whereas the
11 same had a moderate sensitivity to fertilizer-N quantity, SOC and air temperature. In contrast, model
12 simulation of soil NO₃⁻ concentration had high sensitivity to changes in fertilizer-N quantity and BD,
13 with a lower sensitivity to changes in air temperature, precipitation and SOC. Sensitivity of
14 simulated N₂O emissions was high to changes in BD and FC, moderate to SOC, *N₂Oadjust_fc* and
15 air temperature, and weak to fertilizer-N and daily precipitation. A change in air temperature by
16 ±1°C resulted in changes in simulated plant production, soil temperature, NH₄⁺ and NO₃⁻
17 concentration, and N₂O emissions by 1.6, 6.9, 7.9, 3.7 and 7.2%, respectively. Similarly, changing
18 daily precipitation by ±10% altered simulated plant production, WFPS, NH₄⁺ and NO₃⁻
19 concentration, and N₂O by 1.3, 2.0, 1.3, 4.2 and 4.1%, respectively. Effects of an increase in air
20 temperature were positive on soil temperature, soil NO₃⁻ concentration and N₂O emissions, but
21 negative on soil NH₄⁺ concentration and plant production. On the other hand, decreasing daily
22 precipitation had negative effects on WFPS, plant production and N₂O emissions, but increased soil
23 mineral N concentrations. Increasing FC by 10% led to an increase in simulated WFPS and N₂O
24 emissions by 10.5 and 17.2%, respectively. Similarly, decreasing BC by 10% led to a decrease in

1 WFPS and N₂O emissions by 9.9 and 16.5%. A 10% decrease in BD increased soil mineral N
2 concentrations by 10.6-11.8%, but decreased WFPS and soil mineral N concentration by 10.2 and
3 15.0%, respectively. Increasing the baseline SOC level by 10% led to an increase in crop production
4 (4%), soil NH₄⁺ concentration (6.4%), soil NO₃⁻ concentration (3.9%) and N₂O emissions (9.2%),
5 whereas decreasing baseline SOC level by an equal magnitude decreased equally the crop
6 production (4.1%), soil NH₄⁺ concentration (6.1%), soil NO₃⁻ concentration (3.7%) and N₂O
7 emissions (8.8%). A one unit increase in soil pH from 6.4 to 7.4 led to 4.7% decrease in soil NH₄⁺
8 concentration, whereas a one unit decrease in soil pH from 6.4 to 5.4 led to 3 times greater increase
9 in soil NH₄⁺ concentration (19.7%). Interestingly, there was no significance impact of change in soil
10 pH (± 1 unit) on other model simulations, including N₂O emissions. Increasing fertilizer-N
11 application by 10% resulted in an increase in crop production, soil NH₄⁺, soil NO₃⁻ concentration
12 and N₂O emissions by 3.1, 9.2, 11.3 and 4.8%, respectively. On the other hand, decreasing fertilizer-
13 N application by 10% decreased those model simulations by similar respective levels.

14 When mown-grassland system was compared with grain-cropland, model sensitivity was
15 found, in general, to be nearly equal under both systems, but a few differences were seen. For
16 example, simulated hay production was insensitive to baseline SOC and N-fertilizer, but changing
17 both parameters by 10% altered grain-crop production by 3-4%. Simulated crop yield was 10% more
18 sensitive to temperature than hay production, and the negative effect of increase in air temperature
19 was greater on crop yield compared to hay production. Sensitivity of simulated soil NO₃⁻
20 concentration was greater to air temperature by 3.5 times and SOC by 1.1 times in cropland
21 compared to mown-grassland. Finally, N₂O emissions were 1-1.6 times greater sensitive to SOC, air
22 temperature and BD in cropland compared to grassland.

23 All the above 14 parameters were also examined for their influence on model performances,
24 along with sensitivity analysis (Table 5). A 10% decrease in FC or BD led significant

1 underestimation for WFPS in mown-grassland. Similarly, decreasing air temperature input variable
2 by 1°C resulted in significance underestimation for soil temperature in grassland. Changes in daily
3 air temperature (1°C), precipitation, FC, SOC and fertilizer-N quantity (10%) altered significantly
4 model performances for soil NO₃⁻ concentration in grassland (Table 5). On the other hand, changing
5 air temperature and soil pH by ±1°C and ± 1 unit, respectively, or changing other parameters by 10%
6 did not influence model performance for simulation of N₂O emissions, but they had potentials to
7 reduce simulation errors to some extent.

8 **4. General Discussion**

9

10 *4.1. Testing model performance*

11 Use of dynamic system models for simulation of N₂O emission has increased rapidly in
12 recent years. These models are now being used not only for prediction of N₂O emissions from
13 different agro-ecosystems, but estimation of N₂O inventories on national, regional and global scales,
14 and assessing climate change impacts and mitigation strategies (Del Grosso et al., 2006, 2009; EPA,
15 2006). However, to ensure that these model predictions are reliable enough in a new environment,
16 model performance needs to be tested first with different data streams from real world experiments.
17 To our knowledge, the present study is one of the first of its kind to rigorously test the DailyDayCent
18 model against high frequency field measurements for not only daily N₂O emission, but also for daily
19 soil water (WFPS) and soil temperature, including SOC, plant production and soil mineral nitrogen
20 concentration at different temporal frequency, over a relatively long time period (three years) in two
21 contrasting ecosystems together *viz.* mown-grassland and grain-cropland.

22 The model DailyDayCent simulates nitrification as a function of soil NH₄⁺ concentration,
23 water content, temperature and pH; whereas the model assumes denitrification is a function of NO₃⁻

1 concentration (e^- acceptor), labile C availability (e^- donor) and O_2 availability (competing e^-
2 acceptor), where O_2 availability is calculated as a function of WFPS, O_2 demand and soil properties
3 that control gas diffusivity (Parton et al., 2001; Del Grosso et al., 2008b). For the above reasons, as
4 correct simulations of WFPS, soil temperature, plant production, SOC and soil mineral N
5 concentration are a prerequisite for successful model simulation of N_2O emissions (Del Grosso et al.,
6 2011), model performance for WFPS, soil temperature, plant production SOC, soil mineral N and at
7 last N_2O emissions are discussed below.

8 *4.1.1. Modelling water filled pore space and soil temperature*

9 In the present study, the DailyDaycent simulated WFPS and soil temperature efficiently in mown-
10 grassland, although some minor discrepancies were found in individual seasons. Model performance
11 for WFPS and soil temperature in cropland was not tested due to unavailability of measurements.
12 However, model simulations of WFPS and soil temperature in croplands were different to those for
13 mown-grassland, probably due to the different plant growth and management practices. As mown-
14 grassland and grain-cropland were in adjacent fields, with very similar soil characteristics, and
15 almost the same model parameterization was used for both (except plant and management practices),
16 a similarly efficient model performance for WFPS and soil temperature was expected in the grain-
17 cropland. Some studies obtained accurate predictions of soil water and temperature (Del Grosso et
18 al., 2008a; Jarecki et al., 2008; Scheer et al., 2014), though a few others found some discrepancy in
19 simulation of WFPS during winter and summer due to the way in which internal drainage and
20 hysteresis effects are simulated in the model, dew formation in summer, and accumulation, drifting
21 and melting of snow, which are not accounted for in the model (Parton et al., 2001; Del Grosso et al.,
22 2002; Stehfest and Müller, 2004). However, correct estimation of FC was found to be one of the
23 most critical factors for the successful simulation of WFPS in our study.

1 *4.1.2. Modelling plant production*

2 The simulated plant growth curves were reasonable (Fig. 6), and good agreements between
3 measured and simulated hay production, and overall crop yield were obtained in the present
4 experiment. DailyDayCent has been successfully applied for simulation of plant production across
5 grain-croplands and grassland (Stehfest et al., 2007; Del Grosso et al., 2008a; Abdalla et al., 2010;
6 Lee et al., 2012; Chang et al., 2013). However, the model significantly underestimated plant
7 production for corn in our study. In our present experiment, only 36 kg fertilizer-N was applied
8 during the corn season. Most of the N demand, as estimated by PC-AZOTE for corn, was
9 supposedly met through decomposition of grass biomass incorporated at the time of ploughing
10 before sowing of corn in spring 2011, during the land-use conversion from mown-grassland to grain-
11 cropland. However, a minimum dose of N-fertilizer at the rate of 110 kg N ha⁻¹ is quite common in
12 the study region (Kunrath et al., 2015). One additional model simulation with the above minimum
13 N-fertilization, keeping all other inputs the same as the original model simulation, produced
14 favourable results for corn production, with no significant effect on overall N₂O emission (Table 4).
15 Thus, our results demonstrate that the corn production was most probably limited by N-deficiency
16 within the model, indicating inability of the model to precisely simulate plant available N from plant
17 residue decomposition.

18 *4.1.3. Modelling soil organic carbon and soil mineral nitrogen*

19 Reasonable agreements between measured and modelled SOC stocks indicate that the baseline SOC
20 and its dynamic were simulated reasonably in our experimental site as recommended by the model
21 developer. The carbon sub-model of DailyDaycent is based on the Century model, and the family of
22 models is well known for their good capacity to simulate SOC dynamics (Chang et al., 2013;
23 Congreves et al., 2015; Xuan et al., 2016). Regarding modelling soil mineral N at the site, simulation
24 of soil NH₄⁺ concentration was close, but the model significantly underestimated soil NO₃⁻

1 concentration in both the systems. A similar underestimation of soil NO_3^- level by the
2 DailyDayCent model was found by other studies (Del Grosso et al., 2008a; Jarecki et al., 2008).
3 Systematic significant disagreements between measured and modelled soil mineral N is an issue
4 with the present model, and various studies have reported similar concern when using the model
5 (Parton et al., 2001; Stehfest and Müller, 2004; Del Grosso et al., 2008a; Jarecki et al., 2008; Scheer
6 et al., 2014), even after site specific calibration (Necpálová et al., 2015). Systematic discrepancy
7 between measured and simulated soil mineral N is an issue for different ecosystem models, such as
8 the CoupModel (Conrad and Fohrer, 2009), DNDC (Smith et al., 2008), and EPIC, NLEAP, NTRM
9 and CERES (Beckie et al., 1995). Reasonable simulation of soil NH_4^+ concentration, but
10 underestimation of NO_3^- in the present study with DailyDayCent indicates some discrepancy in
11 nitrification/denitrification process within the model, for example a lower nitrification rate, or
12 overestimation of denitrification rate, or some direct but significant loss of NO_3^- from soil. As N_2O
13 flux is calculated by the model from simulated aggregated flux of $\text{N}_2+\text{N}_2\text{O}$ and an $\text{N}_2/\text{N}_2\text{O}$ ratio
14 adjustment coefficient (*n2n2oadj*), a greater sensitivity of N_2O emissions to *n2n2oadj* along with an
15 overall incorrect simulation of N_2O emissions could contribute to the possible under/overestimation
16 of nitrification/denitrification process. However, the overall satisfactory simulation of N_2O emission
17 and the insensitivity of simulated N_2O emissions to the parameter ‘*n2n2oadj*’ do not support the
18 hypothesis that nitrification was underestimated or that denitrification rate was overestimated. One
19 reason for poor model performance for soil NO_3^- concentration in the present experiment could be
20 inappropriate model simulation of leaching loss of soil N. The testing of DailyDayCent for N-
21 leaching has been relatively limited (Stehfest and Müller, 2004; Del Grosso et al., 2005). Annual
22 simulated N-leaching from the mown-grassland was 2.2 times higher compared to cropping system.
23 Leaching loss of N was not measured in our present experiment, but from the similar adjacent
24 experiments, Kunrath et al. (2015) reported in contrast an annual leaching loss of N from the

1 cropping system 3-4 times greater than grassland. Applied annual fertilizer-N in our grassland was
2 1.2 times higher compared to the cropland, but simulated similar annual N-uptake in both systems
3 might provide a larger excess N in mown-grassland, and this excess N could be lost through leaching.
4 Successful simulations of plant productions in the present study indicate reliable simulation of plant
5 N-uptake, whereas Kunrath et al. (2015) used a simple computational procedure for estimating
6 annual leaching loss of N from qualitative measurements, without capturing other components of N
7 cycle. However, contrasting results on N-leaching suggest the need for more field experiments,
8 model testing and subsequent model development for correct simulation of leaching loss of N and
9 soil NO_3^- concentration. Surprisingly in our sensitivity analysis, none of the soil N-dynamics
10 parameters in “sitepar.in” file influenced significantly, nor improved, the model performance for
11 simulation of soil NO_3^- concentration. Thus, concentration of simulated soil NO_3^- was relatively
12 insensitive to variation in soil N-dynamics parameters in “sitepar.in” file within the model structure.
13 Necpálová et al. (2015) observed the inability of an inverse modelling algorithm to improve
14 simulation of soil NO_3^- , when the same improved model performance for other components of N
15 cycle, and concluded that the poor performance of the DailyDayCent model for soil mineral N is
16 probably due to the result of excessively restrictive parameter constraints within the model
17 parameterization, or that the model structure simply does not allow accurate simulation of the
18 observed phenomenon due to some model structural error. Thus, the current exercise suggests that
19 the DailyDayCent sub-model responsible for N transformations might need to be improved for a
20 better simulation of soil mineral N, particularly soil NO_3^- concentration.

21 *4.1.4. Modelling overall N_2O emissions*

22 When DailyDayCent was tested for the simulation of the overall daily N_2O emission,
23 significant correlations between measured and simulated N_2O fluxes were found over the entire
24 experimental period, both in mown-grassland ($r = 0.63$) and grain-cropland ($r = 16$). Although the

1 correlation was much lower in cropland, but was still statistically significant at $P < 0.05$. Results of
2 the present experiment demonstrate that the model has the ability to simulate significantly the overall
3 dynamics of the daily N₂O flux in contrasting agroecosystems. Different studies with the same
4 model have found a range of correlations from weak to strong ($r \sim 0-0.72$) across different
5 agroecosystems. Parton et al. (2001) found correlation between daily measured vs. simulated N₂O
6 emissions, ranging from 0 to 0.44, from a variety of five different grassland sites in the United
7 States. Scheer et al. (2014) obtained a better correlation ($r = 0.72$) from a cotton-wheat crop
8 rotational experiment. When analysing total simulation error for modelling daily N₂O emissions over
9 the entire experimental period, no significant error was obtained under grain-cropping, but
10 significant simulation error (*RMSE*) was found at the 95% confidence limit in mown-grassland.
11 However, *ME* was not significant at $P < 0.025$, thus model performance was considered reasonable
12 for the mown-grassland, when mean daily measurements of N₂O flux were used. However, when the
13 measurement error generated from spatial replications was accounted for, simulation error (*RMSE*)
14 became significant. Thus, our result supports the view that high spatial variation in measured data of
15 N₂O flux, or uncertainties inherent in measurements, can contribute to apparent poor model
16 performance (Del Grosso et al., 2001; Rafique et al., 2014). Different studies demonstrate that
17 performance of the DailyDayCent model for N₂O emissions decreases when model performance is
18 tested against daily measured flux, instead of cumulative seasonal or annual emissions (Parton et al.,
19 2001; Del Grosso et al., 2002, 2008a, 2008b, 2011; Abdalla et al., 2010). Other ecosystem models
20 also face similar difficulties in simulation of daily N₂O emissions (Yeluripati et al., 2015). Different
21 studies demonstrated model performance for overall daily N₂O emissions from poor to reasonable
22 using different models including DailyDayCent (Smith et al., 2002, 2008; Del Grosso et al., 2008;
23 Jarecki et al., 2008; Abdalla et al., 2010; van Oijen et al., 2011; Rafique et al., 2013; He et al. 2016).
24 In our present study, overall reasonable model performance was obtained for modelling daily N₂O

1 emissions in mown-grassland and grain-cropland. Recently, similar overall favourable performance
2 for daily N₂O emission was obtained by Scheer et al. (2014) from a cotton-wheat cropping system in
3 Australia. Scheer et al. (2014) explained their overall successful model simulation for N₂O emissions
4 by the high-frequency data set, used for initial model calibration and model testing, whereas we
5 found overall good model performance for the same due to the ability of the DailyDayCent model to
6 successfully simulate WFPS, soil temperature, SOC, plant production and soil mineral N,
7 particularly NH₄⁺, which all together control nitrification and denitrification processes directly or
8 indirectly. Our results demonstrate that DailyDayCent has potential for successfully simulating
9 overall daily N₂O emissions in different agro-ecosystems in the study region, and the model would
10 be a good tool for projection of N₂O emissions under different management and climate change
11 scenarios, and evaluation of different mitigation strategies for overall N₂O emission.

12 The simulated annual N₂O emissions of the present study *viz.* 1.24-1.97 kg N ha⁻¹ yr⁻¹ with
13 applied fertilizer-N 95-210 kg N ha⁻¹ yr⁻¹, were within the range of measured emissions of 0.65-2.9
14 kg N ha⁻¹ yr⁻¹ as reported by other researchers from similar agro-ecosystems around France
15 (Gabrielle et al., 2006; Laville et al., 2011). Annual N₂O emissions from our managed grassland and
16 cropland were also in line with different studies in other European countries (1-3.9 kg N ha⁻¹ yr⁻¹),
17 depending on the quantity of applied fertilizer-N (0-350 kg N ha⁻¹ yr⁻¹) (Abdalla et al., 2010; Fitton
18 et al., 2014b). A greater range of N₂O emissions from 2-35 kg N ha⁻¹ yr⁻¹ was also found around the
19 world, but with a higher N-fertilization of 135-432 kg N ha⁻¹ yr⁻¹ (Cardenas et al., 2010; Rafique et
20 al., 2011; Abdalla et al., 2014). In general, N₂O emissions from agricultural systems have been
21 found to increase with increasing N-input, either linearly (Flechard et al., 2007; Beek et al., 2009) or
22 exponentially (Eckard et al., 2006; Rafique et al., 2011). The positive correlation of N₂O emissions
23 with the quantity of applied N, and a 120% greater application of N-fertilizer could explain the 59%
24 higher N₂O emissions from the mown-grassland system compared to the grain-cropping. In the

1 present experiment, averaged simulations of WFPS and soil temperature were greater by 4.5% and
2 1°C, respectively in grain-cropland compared to mown-grassland, but soil mineral N concentrations
3 (NH_4^+ and NO_3^-) were 1.1-2.5 times greater in mown-grassland compared to cropland, which leads
4 to higher N_2O emissions from mown-grass than grain cropping system.

5 *4.1.5. Modelling N_2O emissions on day-by-day basis*

6 High frequency measurements in the present study provided the opportunity to analyse in
7 detail the performance of the model for N_2O emissions on a daily basis. Some inconsistencies were
8 found under both mown-grassland and grain-cropland. Although, most of the discrepancies between
9 measured and model simulation of N_2O flux were found after a precipitation or N-fertilization event,
10 no definite pattern was obtained over the course of the three year experiment. In the present
11 simulation, discrepancies between measured and modelled N_2O flux were found mainly in five
12 categories *viz.* a) the model failed to capture some large N_2O fluxes, b) the model simulated some
13 peaks that were not found in the measurements, c) the model failed to simulate some measured
14 peaks, d) general underestimation of large fluxes, but overestimation of small fluxes and e) some
15 negative N_2O fluxes, observed in the measurements that were not found in the simulation.
16 DailyDayCent was unable to simulate some large measured N_2O peaks both in mown-grassland
17 ($150\text{-}250 \text{ g N ha}^{-1} \text{ day}^{-1}$) and grain-cropland ($\sim 10\text{-}60 \text{ g N ha}^{-1} \text{ day}^{-1}$) during June, 2013. One possible
18 reason for this could be the slight underestimation of WFPS by the model during the month June in
19 2013 (Fig. 4). However, underestimation of WFPS alone could not explain the inability of the model
20 to capture large N_2O peaks, as model underestimation of WFPS was merely XX%. Another possible
21 reason could be the inability of the model to carry over the residual mineral N from previous N-
22 fertilizer applications ($90\text{-}150 \text{ kg N ha}^{-1}$) during February-April in the same year. A similar
23 phenomenon with the same model was observed by other researchers (Abdalla et al., 2010). Other
24 explanations could be the systematic underestimation of soil NO_3^- in our experiments or the

1 description of N transformation processes in the model or structural error in the model (Smith et al.,
2 2008, van Oijen et al. 2011). Similar weaknesses of the DailyDayCent model in capturing large N₂O
3 peaks have been reported in different studies (Del Grosso et al., 2008a; Rafique et al., 2013;
4 Necpálová et al., 2015). Inability to simulate very large, infrequent N₂O peaks is also common
5 across other ecosystem models. For example, van Oijen et al. (2011) found that no model, even after
6 calibration, explained infrequent events of very high nitrogenous emission rate when applying a set
7 of four models with different complexity viz. BASFOR, DayCent, Mobile-DNDC and CoupModel.
8 Regarding simulation of extra N₂O peaks in our experiment, Del Grosso et al. (2008a) also found
9 similar extra peaks what were not observed in their measurements. As in the present experiment,
10 Jarecki et al. (2008) and Del Grosso et al. (2008a) also found similar underestimation and
11 overestimation of N₂O flux by the DailyDayCent model at high and low ranges, respectively. Thus,
12 simulation of N₂O flux on a day-by-day basis is a concern with the DailyDayCent model (Parton et
13 al., 2001; Del Grosso et al., 2002, 2005; Jarecki et al., 2008; Rafique et al., 2013). The poor model
14 performance for N₂O flux on day-to-day basis is a common concern for most process-based models.
15 Most ecosystem models commonly simulate total or overall N₂O emissions correctly, or at least
16 reasonably, but inaccuracy in the timing of emissions and over/under-estimations of individual N₂O
17 peaks are common concerns with different models, for example DNDC (Smith et.al, 2002, 2008),
18 CERES (Gabrielle et al, 2006), PaSim (Calanca et al. 2007) and CoupModel (Hongxing et. al 2016).
19 There could be several reasons for the overall systematic disagreements for DailyDayCent model in
20 simulation of daily N₂O emissions. These disparities could not be explained by poor model
21 performance, or any small simulation discrepancy for WFPS, soil temperature, SOC, soil NH₄⁺
22 concentration, or plant production (N-uptake) in our experiments - unlike in other studies (Parton et
23 al., 1998; Del Grosso et al., 2002; Stehfest and Müller, 2004; Scheer et al., 2014), as the dynamics of
24 those variables were simulated by the model correctly, or at least reasonably well, in the present

1 experiment. Additionally, no regular pattern was found in those day-to-day N₂O flux discrepancies,
2 unlike some regular but minor seasonal simulation discrepancies obtained in simulation of some of
3 the above variables. Significant difference between predicted and measured soil NO₃⁻ concentrations,
4 as found in our study, could be a possible factor. The current exercise suggests that the
5 DailyDayCent sub-module responsible for N transformations might need to be improved for a better
6 simulation of soil mineral N, as discussed earlier, and also for better simulation of N₂O emissions on
7 a daily basis. Similar conclusions have also been drawn in other studies (Stehfest and Müller, 2004;
8 Del Grosso et al., 2008a; Jarecki et al., 2008; Necpálová et al., 2015). For simulation of soil mineral
9 N and N₂O emissions with higher precision and accuracy, overall improvement in model algorithms
10 and parameterization controlling nitrification and denitrification processes, modifications in the
11 nitrification and denitrification subroutines, and improvement in the model structure could be
12 beneficial (Jarecki et al., 2008; Del Grosso et al. 2008a, 2010; van Oijen et al., 2011; Necpálová et
13 al., 2015). Other reasons for model disagreement with measurements on a daily basis could be due
14 to the local emission hot spots, which might be formed due to N deposition (N-fertilization),
15 producing high peaks, which could perhaps be captured in measurements, but not by the model, as
16 DailyDayCent assumes all the model inputs are uniform spatially (Del Grosso et al., 2008a).
17 Emissions of N₂O might also be influenced by heterogeneity of the soil surface, but spatial variation
18 is a limitation of the model, as the model counts soil as a uniform system (Rafique et al., 2014).
19 Effects of topography, aspect, wind, humidity, microsite heterogeneity, gas diffusion, and other
20 factors on soil water and temperature, which are not included in DailyDayCent, could be also critical
21 for precise simulation of N₂O emissions on a daily basis (Del Grosso et al., 2005). The lack of depth-
22 dependence in the denitrifying microbial community and their composition are another limitation in
23 the DailyDayCent model. Denitrification rates may vary with soil depth as denitrifying microbial
24 biomass and their species composition vary with soil depth (Venterea et al., 2005; Paul, 2006). Thus,

1 microbial biomass and species composition may be important controls for N₂O emission in field
2 soils (Del Grosso et al., 2000). Del Grosso et al. (2008a) suggested that the model could be improved
3 by accounting for the impacts of soil depth-dependent changes in microbial community on
4 denitrification rate. The DailyDayCent model failed to simulate any of the observed negative fluxes
5 ($\leq -8 \text{ g N ha}^{-1} \text{ day}^{-1}$) in our experiment. The classical microbial denitrification pathway of
6 atmospheric N₂O to N₂ at the surface layer of soils could be an explanation to negative N₂O flux or
7 N₂O uptake by agricultural soils (Yu et al., 2000; Wrage et al., 2004). Negative N₂O fluxes have
8 been found in various agroecosystems across different seasons ranging from -1 to -55 g N ha⁻¹ day⁻¹
9 (Flechard et al., 2005; Rafique et al., 2011; Zhang et al., 2013). In contrast, from a recent
10 investigation, Cowan et al., (2014) has suggested that the bulk of negative N₂O fluxes reported from
11 agricultural fields are most likely due to instrument noise or limits in detection of a particular flux
12 measurement methodology, but not a result of microbiological activity consuming atmospheric N₂O.
13 However, it remains plausible that various microbial processes in soils are able to remove N₂O from
14 the atmosphere under a range of aerobic and anaerobic soil conditions, but different influential
15 factors, the mechanisms, and the triggers for N₂O uptake need to be studied further to understand
16 these factors and processes precisely (Wrage et al., 2001; Chapuis-Lardy et al., 2007). Because the
17 mechanism of soil uptake of N₂O is unclear, the DailyDayCent model does not simulate the uptake
18 of N₂O. Although measured cumulative negative flux was small and the model simulated overall
19 N₂O emissions satisfactorily without the above N₂O uptake mechanism, incorporation of the above
20 mechanism in the present model may be helpful to represent real world systems more precisely.

21 *4.2. Sensitivity analysis:*

22 Sensitivity analysis is important as it elucidates many aspects, importance and implications
23 for the present modelling study. For example, sensitivity analysis demonstrated that N₂O emissions
24 from agricultural systems (mown-grass and grain-cropping) may increase by 5-13% if air

1 temperature increases by just 1°C in the near future. In contrast, decreasing precipitation of 10%
2 would decrease N₂O emission by 4%. Sensitivity analysis of the present study demonstrated that
3 sensitivity of N₂O emissions to changes in air temperature and precipitation is most likely the results
4 of combined sensitivities of WFPS, soil temperature, plant production and soil mineral N
5 concentrations, which control nitrification and denitrification processes. We tested the influence of
6 an increase in air temperature and a decrease in precipitation uniformly throughout the year, whereas
7 it is quite possible that future temperature increase or precipitation decrease would not be uniform
8 throughout the year. In any case, increased N₂O emissions due to future climate change could
9 enhance climate change further. Our findings on sensitivity of N₂O emissions to climate change are
10 in the line to those of other researchers. Using the DailyDayCent model in a wheat experiment, UK,
11 Fitton et al. (2014b) reported 6-17% increases and 2-3% decreases in annual N₂O emissions due to
12 an increase in temperature by 1°C and decrease of daily precipitation by 1mm, respectively. Our
13 results also show that an average error or uncertainty of 1°C or 10% in the inputs of average daily air
14 temperature and precipitation, respectively, would not influence model performance significantly for
15 at least N₂O emissions. We found three out of six soil properties *viz.* FC, BD and SOC, were the
16 most influential parameters in determining N₂O emissions. A 10% change or uncertainty in these
17 three parameters individually could introduce on an average 4-12% error in simulated WFPS and
18 soil mineral N concentration, and ultimately 9-17% uncertainty in N₂O emissions. In general,
19 changing FC, BD and SOC influence N transformations by altering soil pore spaces, WFPS, oxygen
20 demand, gas diffusivity, availability of soil mineral N and microbial activity; most of these processes
21 are also accounted by DailyDayCent (Abbasi and Adams, 2000; Parton et al., 2001). Although N₂O
22 emissions were moderate to highly sensitive to FC, BD and SOC, a 10% error or uncertainty in
23 these three soil properties did not influence model performance significantly for N₂O emissions. But,
24 a 10% error or uncertainty in these three parameters significantly changed the model performance

1 for WFPS and soil mineral N concentration. Additionally a 10% reduction in error or uncertainty in
2 measurement of FC, BD and SOC has the potential to reduce simulation error to some extent also for
3 N₂O emissions (Table 5), hence these three parameters were considered as important for modelling
4 N₂O emissions. s Thus our results demonstrated the importance of measuring different soil
5 properties correctly, particularly FC, BD and SOC, for simulation of N₂O emissions. Similar
6 conclusions had also been reported by other studies (Abdalla et al., 2009; Fitton et al., 2014a). In the
7 present study (soil pH~6.4), simulated soil NH₄⁺ concentration was highly sensitive to changes in
8 soil pH, and effect of one unit decrease in soil pH was greater compared to a one unit pH increase.
9 However simulated soil NO₃⁻ concentration and N₂O emissions were not sensitive to soil pH. Fitton
10 et al. (2014b) found N₂O emissions to be most sensitive to soil pH, and sensitivity was an order of
11 magnitude greater compared to FC and BD. They argued that a decrease of soil pH by 1 unit in their
12 slightly acidic soils (pH~6) might contribute to the movement of C and N through different pools,
13 interaction between pH and low temperature, specific change in N-compounds, and ultimately the
14 creation of conditions favourable for denitrification. As pH is logarithmic, any effect of one unit
15 increase in soil pH is not the same as a one unit decrease. For the same reason, effects of change in
16 soil pH (increase/decrease) in different sites with different soil pH are not comparable. However, in
17 the nitrification sub-module of DailyDayCent, soil pH directly influence nitrification rate, and there
18 is no direct influence of the parameter on denitrification (Parton et al., 2001). Thus, high sensitivity
19 of N₂O emissions to soil pH may need to be investigated further using measurements and the model.
20 Sensitivity analysis indicated that there might be some trade-offs between plant production and N₂O
21 emissions when changing baseline SOC levels. Our results indicated that increasing the baseline
22 SOC by 10% would increase grain-crop yield by 4%, but also may increase N₂O emissions up to
23 12%. Sensitivity analysis illustrated the possible scope for reducing N₂O emissions by reducing the
24 quantity of N-fertilizer in mown-grasslands without any reduction in hay production, although doing

1 the same in grain-cropping systems could reduce the crop yield. The results are explained by the
2 yield saturation observed in hay production system, and an unsaturation in grain-crop yield. The
3 scope for yield optimization with increasing N-fertilizer in cropping system is narrow and would
4 come at the cost of higher N₂O emissions. However, as discussed earlier, DailyDayCent
5 underestimated plant production only for corn, mainly due to the lower availability of simulated
6 mineral N from mineralization of grass biomass incorporated during land use change from
7 temporary grassland to grain-cropland just before sowing of corn. Taking the above facts into
8 consideration, model performance with respect to plant production can be considered reasonable
9 (Lemaire et al., 2008; Kunrath et al., 2015).

10 Sensitivity of model simulations to five soil N parameters in the '*sitepar.in*' file was also
11 tested in the present study. It is not generally recommended that these parameters be tuned arbitrarily
12 to improve the model fit (Del Grosso et al., 2011). However, N₂O emissions have been found to be
13 highly sensitive to *MaxNitAmt* in recent studies (Rafique et al., 2013; Necpálová et al., 2015). In
14 contrast, N₂O emissions were not seen to be sensitive to *MaxNitAmt* in our study. The former two
15 studies were complex inverse modelling studies, with data assimilation/optimization to determine the
16 optimized values of the parameter ranging from 0.28-1.91 g N m⁻². In our study, the default
17 parameter value of 0.4 g N m⁻² was used, and the sensitivity analysis tested one parameter at a time,
18 keeping other parameters constant. According to the developer, users should not use parameter
19 values in DailyDayCent that improve model performance unless they make sense biologically.
20 However, as our present study demonstrated an insensitivity of N₂O emissions to *MaxNitAmt*, ;
21 further experiments may be needed to examine the above parameter value and its sensitivity. In the
22 older version of the DailyDayCent model, only one parameter was used to control the proportion of
23 nitrified N that is lost as N₂O (*nitrified_n*), and different studies demonstrated low to medium
24 sensitivity of N₂O emissions to the parameter (Rafique et al., 2013; Rafique et al., 2014; Necpálová

1 et al., 2015). The model developer also observed similar results, and recommend that a relationship
2 may need to be developed to predict the above proportion based on the O₂ availability or other
3 variables (Del Grosso et al., 2008a). In the new version of the DailyDayCent, the same proportion is
4 controlled by two different parameters, *N₂Oadjust_fc* i.e. the maximum proportion of nitrified N that
5 is lost as N₂O at field capacity , and *N₂Oadjust_wp* i.e. the minimum proportion of nitrified N that is
6 lost as N₂O at wilting point (). However, only *N₂Oadjust_fc* was found to be a critical parameter, as
7 N₂O emissions were sensitive to it in our study, and the results also pointed out that the default
8 values of these soil N-dynamics parameters in “sitepar.in” file might need site-specific calibration
9 for a better model simulation of N₂O emissions from different agricultural systems. Our results show
10 that overall model sensitivity was slightly different between mown-grassland and grain-cropland.
11 The main reasons for this difference could be the different management practices (e.g. tillage vs.
12 mowing,), biomass production (C input to soil), plant growth stage and growing period, and soil
13 cover, which in turn influence soil mineral N, labile C, WFPS, O₂ demand and supply, and
14 ultimately modified N₂O emissions (Del Grosso et al., 2011).

15 **5. Conclusion**

16 In the present study, the DailyDayCent model was applied to simulate N₂O emissions from
17 two contrasting agro-ecosystems *viz.* mown-grassland and grain-cropland. Model performance was
18 tested against high frequency data sets and a local sensitivity analysis was performed using 14 model
19 parameters. Our modelling study shows 59% greater annual N₂O emission from the mown-grassland
20 compared to the grain-cropping system, mainly due to higher N-fertilization (120%) in the former
21 system. Our results demonstrated that DailyDayCent has the potential for successful simulation of
22 overall daily N₂O emissions from two contrasting agro-ecosystems in the study region, and the
23 model would be a good tool, or at least a reasonable means for estimation of N₂O inventory,
24 projection of N₂O emissions under different scenarios, and evaluation of different mitigation

1 strategies against overall N₂O emissions in the region. The model can simulate WFPS, soil
2 temperature, SOC, soil NH₄⁺ and plant production accurately which is a prerequisite for the
3 successful simulation of N₂O emission. Our study indicated that higher variation in measurements
4 of N₂O flux could contribute to poor fit between model outputs and measurements. Further
5 experimental and model improvement might be required to track N from decomposition of plant
6 residue to plant uptake. Systematic discrepancies between measured and modelled N₂O fluxes were
7 obtained on a daily basis, but no definite pattern was obtained over the course of three year
8 experiment. Significant differences between predicted and measured soil NO₃⁻ concentration was the
9 most probable reason for such discrepancies. The current exercise suggests that the DailyDayCent
10 sub-module responsible for N transformations might need to be improved for better simulation of
11 soil mineral N, particularly soil NO₃⁻, and N₂O emission on a daily basis. There is still space for
12 more model improvement for N₂O flux on a daily basis, potentially by incorporating a range of other
13 factors, which the model still does not account for, such as N₂O uptake, spatial distribution of
14 applied fertilizer-N, soil heterogeneity, depth distribution and composition of denitrifying microbes
15 etc.

16 Sensitivity analysis showed that a total of four out of 14 parameters (FC, BD, SOC and
17 *N₂Oadjust_fc*) were critical for simulation of N₂O emissions, hence the need for careful estimation
18 or site-specific calibration for successful modelling of N₂O emission in the study region. Sensitivity
19 analysis indicated that baseline SOC has a trade-off effect between plant production and N₂O
20 emissions. Our results also pointed out that an average error or uncertainty of 1°C or 10% in the
21 inputs of daily air temperature and precipitation, respectively, would not influence model
22 performance for daily N₂O emissions significantly. Sensitivity estimation also shows possible effects
23 of future change in air temperature and precipitation on overall N₂O emissions. Sensitivity analysis
24 illustrated the opportunity of reducing N₂O emissions by reducing the quantity of fertilizer-N in

1 mown-grasslands without any reduction in hay production, though doing the same in the grain-
2 cropping system could reduce the yield marginally.

3 Our present study is limited in application of one model only. Using other models together
4 would be useful to test the quality of the input as well as model testing data, which are important for
5 successful evaluation of model performance. A future multi-model approach on daily data would
6 also be helpful for model improvement, by comparing different individual process/variables within
7 the models against measurements. In our study, a local sensitivity analysis was performed; a full
8 global sensitivity assessment and parameter estimation, including analysis of parameter correlation
9 structure would be interesting and will be the subject of further study.

10 **Acknowledgement**

11 The lead author, Nimai Senapati (Post doc), was funded by the European community's
12 Seventh Framework programme (FP2012-2015) under grant agreement no. 262060 (ExpeER). The
13 research leading to these results has received funding principally from the ANR (ANR-11-INBS-
14 0001), AllEnvi, CNRS-INSU. We would like to thank the National Research Infrastructure 'Agro-
15 écosystèmes, Cycles Biogéochimique et Biodiversité (SOERE-ACBB [http://www.soere-
17 acbb.com/fr/](http://www.soere-
16 acbb.com/fr/)) for their support in field experiment. We are deeply indebted to Christophe de
18 Berranger, Xavier Charrier for their substantial technical assistance and Patricia Laville for her
valuable suggestion regarding N₂O flux estimation.

19 **Compliance with ethical standards**

20 We declare that we do not have any conflict of interest.

21 **References**

- 1 Abbasi, M.K., Adams, W.A., 2000. Gaseous N emission during simultaneous nitrification–
2 denitrification associated with mineral N fertilization to a grassland soil under field conditions.
3 *Soil Biol. Biochem.* 32, 1251-1259.
- 4 Abdalla, M., Hastings, A., Helmy, M., Prescher, A., Osborne, B., Lanigan, G., et al., 2014.
5 Assessing the combined use of reduced tillage and cover crops for mitigating greenhouse gas
6 emissions from arable ecosystem. *Geoderma* 223–225, 9-20.
- 7 Abdalla, M., Jones, M., Yeluripati, J., Smith, P., Burke, J., Williams, M., 2010. Testing DayCent and
8 DNDC model simulations of N₂O fluxes and assessing the impacts of climate change on the
9 gas flux and biomass production from a humid pasture. *Atmos. Environ.* 44, 2961-2970.
- 10 Abdalla, M., Wattenbach, M., Smith, P., Ambus, P., Jones, M., Williams, M., 2009. Application of
11 the DNDC model to predict emissions of N₂O from Irish agriculture. *Geoderma* 151: 327-337.
- 12 Angevin, F., 1999. Raisonement de la fertilisation azotée. Le logiciel PCazote enPoitou-Charentes.
13 *Oléoscope* 54, 32–34.
- 14 Arrouays, D., Deslais, W., Badeau, V., 2001. The carbon content of topsoil and its geographical
15 distribution in France. *Soil Use and Manage.* 17, 7-11.
- 16 Arrouays, D., Pelissier, P., 1994. Changes in carbon storage in temperate humic loamy soils after
17 forest clearing and continuous corn cropping in France. *Plant Soil* 160, 215-223.
- 18 Balesdent, J., Besnard, E., Arrouays, D., Chenu, C., 1998. The dynamics of carbon in particle-size
19 fractions of soil in a forest-cultivation sequence. *Plant Soil* 201, 49-57.
- 20 Beek, C.L., Pleijter, M., Jacobs, C.M.J., Velthof, G.L., Groenigen, J.W., Kuikman, P.J., 2009.
21 Emissions of N₂O from fertilized and grazed grassland on organic soil in relation to
22 groundwater level. *Nutr. Cycl. Agroecosyst.* 86, 331-340.

- 1 Butterbach-Bahl, K., Baggs, E.M., Dannenmann, M., Kiese, R., Zechmeister-Boltenstern, S., 2013.
2 Nitrous oxide emissions from soils: How well do we understand the processes and their
3 controls? *Phil. Trans. R. Soc. B Biol. Sci.* 368.
- 4 Cardenas, L.M., Thorman, R., Ashlee, N., Butler, M., Chadwick, D., Chambers, B., et al., 2010.
5 Quantifying annual N₂O emission fluxes from grazed grassland under a range of inorganic
6 fertiliser nitrogen inputs. *Agric. Ecosyst. Environ.* 136, 218-226.
- 7 Chabbi, A., Kögel-Knabner, I., Rumpel, C., 2009. Stabilised carbon in subsoil horizons is located in
8 spatially distinct parts of the soil profile. *Soil Biol. Biochem.* 41, 256-261.
- 9 Chang, K.H., Warland, J., Voroney, P., Bartlett, P., Wagner-Riddle, C., 2013. Using DayCENT to
10 simulate carbon dynamics in conventional and no-till agriculture. *Soil Sci. Soc. Am. J.* 77, 941-
11 950.
- 12 Chapuis-Lardy, L., Wrage, N., Metay, A., Chotte, J.L., Bernoux, M., 2007. Soils, a sink for N₂O? A
13 review. *Glob. Change Biol.* 13, 1-17.
- 14 Congreves, K.A., Grant, B.B., Campbell, C.A., Smith, W.N., VandenBygaart, A.J., Kröbel, R., et al.,
15 2015. Measuring and modeling the long-term impact of crop management on soil carbon
16 sequestration in the semiarid Canadian prairies. *Agron. J.* 107, 1141-1154.
- 17 Cowan, N.J., Famulari, D., Levy, P.E., Anderson, M., Reay, D.S., Skiba, U.M., 2014. Investigating
18 uptake of N₂O in agricultural soils using a high-precision dynamic chamber method. *Atmos.*
19 *Meas. Tech.* 7, 4455-4462.
- 20 Crutzen, P.J., Ehhalt, D.H., 1977. Effects of nitrogen fertilizers and combustion on the stratospheric
21 ozone layer. *Ambio* 6, 112-117.
- 22 Čuhel, J., Šimek, M., Laughlin, R.J., Bru, D., Chèneby, D., Watson, C.J., et al., 2010. Insights into
23 the effect of soil pH on N₂O and N₂ emissions and denitrifier community size and activity.
24 *Appl. Environ. Microbiol.* 76, 1870-1878.

- 1 Das, S., Adhya, T.K., 2014. Effect of combine application of organic manure and inorganic fertilizer
2 on methane and nitrous oxide emissions from a tropical flooded soil planted to rice. *Geoderma*
3 213, 185-192.
- 4 Davidson, E.A., 2009. The contribution of manure and fertilizer nitrogen to atmospheric nitrous
5 oxide since 1860. *Nature Geosci.* 2, 659-662.
- 6 Del Grosso, S.J., Halvorson, A.D., Parton, W.J., 2008a. Testing DAYCENT model simulations of
7 corn yields and nitrous oxide emissions in irrigated tillage systems in Colorado. *J. Environ.*
8 *Qual.* 37, 1383-1389.
- 9 Del Grosso, S.J., Mosier, A.R., Parton, W.J., Ojima, D.S., 2005. DAYCENT model analysis of past
10 and contemporary soil N₂O and net greenhouse gas flux for major crops in the USA. *Soil Till.*
11 *Res.* 83, 9-24.
- 12 Del Grosso, S.J., Ogle, S.M., Parton, W.J., Breidt, F.J., 2010. Estimating uncertainty in N₂O
13 emissions from U.S. cropland soils. *Glob. Biogeochem. Cycles* 24, GB1009.
- 14 Del Grosso, S., Ojima, D., Parton, W., Mosier, A., Peterson, G., Schimel, D., 2002. Simulated
15 effects of dryland cropping intensification on soil organic matter and greenhouse gas
16 exchanges using the DAYCENT ecosystem model. *Environ. Pollut.* 116, S75-S83.
- 17 Del Grosso, S.J., Ojima, D.S., Parton, W.J., Stehfest, E., Heistemann, M., DeAngelo, B., et al., 2009.
18 Global scale DAYCENT model analysis of greenhouse gas emissions and mitigation strategies
19 for cropped soils. *Glob. Planet. Change* 67, 44-50.
- 20 Del Grosso, S.J., Parton, W.J., Keough, C.A., Reyes-Fox, M., 2011. Special features of the DayCent
21 modeling package and additional procedures for parameterization, calibration, validation, and
22 applications. In: Ahuja, L.R., Ma, L. (Eds.), *Methods of Introducing System Models into*
23 *Agricultural Research*. American Society of Agronomy, Crop Science Society of America, Soil
24 Science Society of America, Madison, WI 53711-5801, USA, pp. 155-176.

- 1 Del Grosso, S.J., Parton, W.J., Mosier, A.R., Hartman, M.D., Brenner, J., Ojima, D.S., et al., 2001.
2 Simulated interaction of carbon dynamics and nitrogen trace gas fluxes using the DAYCENT
3 model. In: Shaffer, M.J., Ma, L., Hansen, S. (Eds.), *Modeling Carbon and Nitrogen Dynamics*
4 *for Soil Management*. CRC Press, Boca Raton, Florida, pp. 303-332.
- 5 Del Grosso, S.J., Parton, W.J., Mosier, A.R., Ojima, D.S., Kulmala, A.E., Phongpan, S., 2000.
6 General model for N₂O and N₂ gas emissions from soils due to denitrification. *Glob.*
7 *Biogeochem. Cycles* 14, 1045-1060.
- 8 Del Grosso, S.J., Parton, W.J., Mosier, A.R., Walsh, M.K., Ojima, D.S., Thornton, P.E., 2006.
9 DAYCENT national-scale simulations of nitrous oxide emissions from cropped soils in the
10 United States. *J. Environ. Qual.* 35, 1451-1460.
- 11 Del Grosso, S.J., Parton, W.J., Ojima, D.S., Keough, C.A., Riley, T.H., Mosier, A.R., 2008b.
12 DAYCENT simulated effects of land use and climate on county level N loss vectors in the
13 USA. In: Hatfield, J.L., Follett, R.F. (Eds.), *Nitrogen in the Environment: Sources, Problems,*
14 *and Management*. Publications from USDA-ARS/UNL Faculty, pp. 571-595.
- 15 Denman, K.L., Brasseur, G., Chidthaisong, A., Ciais, P., Cox, P.M., Dickinson, R.E., et al., 2007.
16 Couplings between changes in the climate system and biogeochemistry. In: Solomon, S., Qin,
17 D., Manning, M., Chen, Z., Marquis, M., Averyt, K.B., et al. (Eds.), *Climate Change 2007: The*
18 *Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of*
19 *the Intergovernmental Panel on Climate Change*. Cambridge University Press, Cambridge,
20 United Kingdom and New York, NY, USA, pp. 500-587.
- 21 Duru, M., 2004. Simplified nitrogen assessment of orchardgrass swards. *Agron. J.* 96, 1598–1605.
- 22 Eckard, R., Johnson, I., Chapman, D., 2006. Modelling nitrous oxide abatement strategies in
23 intensive pasture systems. *Int. Congr. Ser.* 1293, 76-85.

1 EPA, 2006. Inventory of U.S. Greenhouse Gas Emissions and Sinks: 1990-2004. United States
2 Environmental Protection Agency, Washington, DC, USA.

3 EPA, 2010. Methane and Nitrous Oxide Emissions from Natural Sources. United States
4 Environmental Protection Agency, Washington, DC, USA.

5 EPA, 2012. Global Anthropogenic Non-CO₂ Greenhouse Gas Emissions: 1990-2030. Office of
6 Atmospheric Programs Climate Change Division, U.S. Environmental Protection Agency,
7 1200 Pennsylvania Avenue, NW, Washington, DC 20460.

8 EPA, 2013. Inventory of U.S. Greenhouse Gas Emissions and Sink: 1990-2011. U.S. Environmental
9 Protection Agency, Washington, DC, USA.

10 Farrugia, A., Gastal, F., Scholefield, D., 2004. Assessment of the nitrogen status of grassland.
11 Grass Forage Sci. 59, 113-120.

12 Fitton, N., Datta, A., Hastings, A., Kuhnert, M., Topp, C.F.E., Cloy, J.M., et al., 2014a. The
13 challenge of modelling nitrogen management at the field scale: simulation and sensitivity
14 analysis of N₂O fluxes across nine experimental sites using DailyDayCent. Environ. Res. Lett.
15 9, 095003 (pp.15).

16 Fitton, N., Datta, A., Smith, K., Williams, J.R., Hastings, A., Kuhnert, M., et al., 2014b. Assessing
17 the sensitivity of modelled estimates of N₂O emissions and yield to input uncertainty at a UK
18 cropland experimental site using the DailyDayCent model. Nutr. Cycl. Agroecosyst. 99, 119-
19 133.

20 Flechard, C.R., Ambus, P., Skiba, U., Rees, R.M., Hensen, A., van Amstel, A., et al., 2007. Effects
21 of climate and management intensity on nitrous oxide emissions in grassland systems across
22 Europe. Agric. Ecosyst. Environ. 121, 135-152.

1 Flechard, C.R., Neftel, A., Jocher, M., Ammann, C., Fuhrer, J., 2005. Bi-directional soil/atmosphere
2 N₂O exchange over two mown grassland systems with contrasting management practices.
3 Glob. Change Biol. 11, 2114-2127.

4 Forster, P., Ramaswamy, V., Artaxo, P., Berntsen, J., Betts, R., Fahey, D.W., et al., 2007. Changes
5 in atmospheric constituents and in radiative forcing. In: Solomon, S., Qin, D., Manning, M.,
6 Chen, Z., Marquis, M., Averyt, K., et al. (Eds.), Climate Change 2007 : The Physical Science
7 Basis: Contribution of Working Group I to the Fourth Assessment Report of the
8 Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge, United
9 Kingdom and New York, NY, USA, pp. 130-234.

10 Gabrielle, B., Laville, P., Duval, O., Nicoullaud, B., Germon, J.C., Hénault, C., 2006. Process-based
11 modeling of nitrous oxide emissions from wheat-cropped soils at the subregional scale. Glob.
12 Biogeochem. Cycles 20, GB4018.

13 Groffman, P.M., Butterbach-Bahl, K., Fulweiler, R.W., Gold, A.J., Morse, J.L., Stander, E.K., et al.,
14 2009. Challenges to incorporating spatially and temporally explicit phenomena (hotspots and
15 hot moments) in denitrification models. Biogeochemistry 93, 49-77.

16 Guo, L.B., Gifford, R.M., 2002. Soil carbon stocks and land use change: a meta analysis. Glob.
17 Change Biol. 8, 345-360.

18 IPCC, 2006. 2006 IPCC Guidelines for National Greenhouse Gas Inventories, Volume 4:
19 Agriculture, Forestry and other Land Use. The Intergovernmental Panel on Climate Change,
20 National Greenhouse Gas Inventories Programme [Eggleston, H.S., Buendia, L., Miwa, K.,
21 Ngara, T., Tanabe, K. (Eds.)], Kanagawa, Japan.

22 IPCC, 2007. Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to
23 the Fourth Assessment Report of the Intergovernmental Panel on Climate Change [Solomon,

1 S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K.B., et al. (Eds.)], Cambridge
2 University Press Cambridge, United Kingdom and New York, USA.

3 Jarecki, M.K., Parkin, T.B., Chan, A.S.K., Hatfield, J.L., Jones, R., 2008. Comparison of
4 DAYCENT-simulated and measured nitrous oxide emissions from a corn field. *J. Environ.*
5 *Qual.* 37, 1685-1690.

6 Jeuffroy, M.H., Baranger, E., Carrouée, B., de Chezelles, E., Gosme, M., Hénault, C., et al., 2013.
7 Nitrous oxide emissions from crop rotations including wheat, oilseed rape and dry peas.
8 *Biogeosciences* 10, 1787-1797.

9 Kamphake, L.J., Hannah, S.A., Cohen, J.M., 1967. Automated analysis for nitrate by hydrazine
10 reduction. *Water Res.* 1, 205-216.

11 Kaplan, J.O., Krumhardt, K.M., Zimmermann, N., 2009. The prehistoric and preindustrial
12 deforestation of Europe. *Quat. Sci. Rev.* 28, 3016-3034.

13 Kim, D.G., Rafique, R., Leahy, P., Cochrane, M., Kiely, G., 2014. Estimating the impact of
14 changing fertilizer application rate, land use, and climate on nitrous oxide emissions in Irish
15 grasslands. *Plant Soil* 374, 55-71.

16 Kunrath, T.R., de Berranger, C., Charrier, X., Gastal, F., de Faccio Carvalho, P.C., Lemaire, G., et
17 al., 2015. How much do sod-based rotations reduce nitrate leaching in a cereal cropping
18 system? *Agric. Water Manage.* 150, 46-56.

19 Laville, P., Lehuger, S., Loubet, B., Chaumartin, F., Cellier, P., 2011. Effect of management, climate
20 and soil conditions on N₂O and NO emissions from an arable crop rotation using high temporal
21 resolution measurements. *Agric. For. Meteorol.* 151, 228-240.

22 Lee, J., Pedroso, G., Linqvist, B.A., Putnam, D., van Kessel, C., Six J., 2012. Simulating switchgrass
23 biomass production across ecoregions using the DAYCENT model. *GCB Bioenergy* 4, 521-
24 533.

- 1 Lemaire, G., Jeuffroy, M.H., Gastal F., 2008. Diagnosis tool for plant and crop N status in vegetative
2 stage: Theory and practices for crop N management. *Eur. J. Agron.* 28, 614-624.
- 3 Linn, D.M., Doran, J.W., 1984. Effect of water-filled pore space on carbon dioxide and nitrous oxide
4 production in tilled and nontilled soils. *Soil Sci. Soc. Am. J.* 48, 1267-1272.
- 5 Liu, C., Wang, K., Meng, S., Zheng, X., Zhou, Z., Han, S., et al., 2011. Effects of irrigation,
6 fertilization and crop straw management on nitrous oxide and nitric oxide emissions from a
7 wheat-maize rotation field in northern China. *Agric. Ecosyst. Environ.* 140, 226-233.
- 8 Liu, X.J., Mosier, A.R., Halvorson, A.D., Zhang, F.S., 2006. The impact of nitrogen placement and
9 tillage on NO, N₂O, CH₄ and CO₂ fluxes from a clay loam soil. *Plant Soil* 280, 177-188.
- 10 Martin, M.P., Wattenbach, M., Smith, P., Meersmans, J., Jolivet, C., Boulonne, L., et al., 2011.
11 Spatial distribution of soil organic carbon stocks in France. *Biogeosciences* 8, 1053-1065.
- 12 Mather, A.S., Fairbairn, J., Needle, C.L., 1999. The course and drivers of the forest transition: The
13 case of France. *J. Rural Stud.* 15, 65-90.
- 14 Mathieu, O., Lévêque, J., Hénault, C., Milloux, M.J., Bizouard, F., Andreux, F., 2006. Emissions
15 and spatial variability of N₂O, N₂ and nitrous oxide mole fraction at the field scale, revealed
16 with ¹⁵N isotopic techniques. *Soil Biol. Biochem.* 38, 941-951.
- 17 Meersmans, J., Martin, M., Laccarce, E., De Baets, S., Jolivet, C., Boulonne, L., et al., 2012. A high
18 resolution map of French soil organic carbon. *Agron. Sustain. Dev.* 32, 841-851.
- 19 Moni, C., Chabbi, A., Nunan, N., Rumpel, C., Chenu, C., 2010. Spatial dependence of organic
20 carbon-metal relationships. A multi-scale statistical analysis, from horizon to field. *Geoderma*
21 158, 120-127.
- 22 Mosier, A., Kroeze, C., 2000. Potential impact on the global atmospheric N₂O budget of the
23 increased nitrogen input required to meet future global food demands. *Chemosphere Glob.*
24 *Change Sci.* 2, 465-473.

- 1 Necpálová, M., Anex, R.P., Fienen, M.N., Del Grosso, S.J., Castellano, M.J., Sawyer, J.E., et al.,
2 2015. Understanding the DayCent model: Calibration, sensitivity, and identifiability through
3 inverse modeling. *Environ. Model. Softw.* 66, 110-130.
- 4 Omonode, R.A., Smith, D.R., Gál A, Vyn, T.J., 2011. Soil nitrous oxide emissions in corn following
5 three decades of tillage and rotation treatments. *Soil Sci. Soc. Am. J.* 75, 152-163.
- 6 Parton, W.J., Hartman, M., Ojima, D., Schimel, D., 1998. DAYCENT and its land surface submodel:
7 Description and testing. *Glob. Planet. Change* 19, 35-48.
- 8 Parton, W.J., Holland, E.A., Del Grosso, S.J., Hartman, M.D., Martin, R.E., Mosier, A.R., et al.,
9 2001. Generalized model for NO_x and N₂O emissions from soils. *J. Geophys. Res.* 106, 17403-
10 17419.
- 11 Paul, E.A., 2006. *Soil Microbiology and Biochemistry*: 3rd ed. Academic Press.
- 12 Poeplau, C., Don, A., Vesterdal, L., Leifeld, J., Van Wesemael, B.A.S., Schumacher, J., et al., 2011.
13 Temporal dynamics of soil organic carbon after land-use change in the temperate zone –
14 carbon response functions as a model approach. *Glob. Change Biol.* 17, 2415-2427.
- 15 Rafique, R., Fienen, M., Parkin, T., Anex, R., 2013. Nitrous oxide emissions from cropland: a
16 procedure for calibrating the DayCent biogeochemical model using inverse modelling. *Water
17 Air Soil Pollut.* 224, 1-15.
- 18 Rafique, R., Hennessy, D., Kiely, G., 2011. Nitrous oxide emission from grazed grassland under
19 different management systems. *Ecosystems* 14, 563-582.
- 20 Rafique, R., Kumar, S., Luo, Y., Xu, X., Li, D., Zhang, W., et al., 2014. Estimation of greenhouse
21 gases (N₂O, CH₄ and CO₂) from no-till cropland under increased temperature and altered
22 precipitation regime: A DAYCENT model approach. *Glob. Planet. Change* 118, 106-114.
- 23 Ravishankara, A.R., Daniel, J.S., Portmann, R.W., 2009. Nitrous oxide (N₂O): The dominant ozone-
24 depleting substance emitted in the 21st century. *Science* 326, 123-125.

1 Saxton, K.E., Rawls, W.J., 2006. Soil water characteristic estimates by texture and organic matter
2 for hydrologic solutions. *Soil Sci. Soc. Am. J.* 70, 1569–1578.

3 Scheer, C., Del Grosso, S.J., Parton, W.J., Rowlings, D.W., Grace, P.R., 2014. Modeling nitrous
4 oxide emissions from irrigated agriculture: Testing DayCent with high-frequency
5 measurements. *Ecol. Appl.* 24, 528-538.

6 Senapati, N., Chabbi, A., Gastal, F., Smith, P., Mascher, N., Loubet, B., et al., 2014. Net carbon
7 storage measured in a mowed and grazed temperate sown grassland shows potential for carbon
8 sequestration under grazed system. *Carbon Manage.* 5, 131-144.

9 Shan, J., Yan, X., 2013. Effects of crop residue returning on nitrous oxide emissions in agricultural
10 soils. *Atmos. Environ.* 71, 170-175.

11 Signor, D., Cerri, C.E.P., 2013. Nitrous oxide emissions in agricultural soils: a review. *Pesq.*
12 *Agropec. Trop.* 43, 322-338.

13 Smith, J., Smith, P., 2007. *Environmental Modelling: An Introduction*. Oxford University Press,
14 New York, USA.

15 Smith, J.U., Smith, P., Addiscott, T.M., 1996. Quantitative methods to evaluate and compare soil
16 organic matter (SOM) models. In: Powlson, D.S., Smith, P., Smith, J.U. (Eds.), *Evaluation of*
17 *Soil Organic Matter Models Using Existing Long-Term Datasets*. NATO ASI Series I: Global
18 *Environmental Change*, Vol. 38. Springer-Verlag, Berlin Heidelberg, pp. 181-199.

19 Smith, P., Albanito, F., Bell, M., Bellarby, J., Blagodatskiy, S., Datta, A., et al., 2012. Systems
20 approaches in global change and biogeochemistry research. *Phil. Trans. R. Soc. B* 367, 311-
21 321.

22 Smith, P., Smith, J.U., Powlson, D.S., McGill, W.B., Arah, J.R.M., Chertov, O.G., et al., 1997. A
23 comparison of the performance of nine soil organic matter models using datasets from seven
24 long-term experiments. *Geoderma* 81, 153-225.

- 1 Stehfest, E., Heistermann, M., Priess, J.A., Ojima, D.S., Alcamo, J., 2007. Simulation of global crop
2 production with the ecosystem model DayCent. *Ecol. Model.* 209, 203-219.
- 3 Stehfest, E., Müller, C., 2004. Simulation of N₂O emissions from a urine-affected pasture in New
4 Zealand with the ecosystem model DayCent. *J. Geophys. Res.* 109, D03109.
- 5 Syakila, A., Kroeze, C., 2011. The global nitrous oxide budget revisited. *Greenhouse Gas Measure.*
6 *Manage.* 1, 17-26.
- 7 Trost, B., Prochnow, A., Drastig, K., Meyer-Aurich, A., Ellmer, F., Baumecker, M., 2013. Irrigation,
8 soil organic carbon and N₂O emissions. A review. *Agron. Sustain. Dev.* 33, 733-749.
- 9 Venterea, R.T., Burger, M., Spokas, K.A., 2005. Nitrogen oxide and methane emissions under
10 varying tillage and fertilizer management. *J. Environ. Qual.* 34, 1467–1477.
- 11 WMO, 2010. Greenhouse Gas Bulletin No. 6: The state of greenhouse gases in the atmosphere
12 based on observations through 2009. World Meteorological Organization, Geneva.
13 <http://www.wmo.int/pages/prog/arep/gaw/ghg/GHGbulletin.html>
- 14 WMO, 2014. Greenhouse Gas Bulletin: The State of Greenhouse Gases in the Atmosphere Based on
15 Global Observations through 2013. World meteorological Organization, Geneva.
16 <http://www.wmo.int/pages/prog/arep/gaw/ghg/GHGbulletin.html>
- 17 Wrage, N., Lauf, J., del Prado, A., Pinto, M., Pietrzak, S., Yamulki, S., et al., 2004. Distinguishing
18 sources of N₂O in European grasslands by stable isotope analysis. *Rapid Commun. Mass*
19 *Spectrom.* 18, 1201-1207.
- 20 Wrage, N., Velthof, G.L., van Beusichem, M.L., Oenema, O., 2001. Role of nitrifier denitrification
21 in the production of nitrous oxide. *Soil Biol. Biochem.* 33, 1723-1732.
- 22 Xuan, Z, Li-yong, X., Li-ping, G., Jing-wei, F., 2016. Modelling the changes of soil organic carbon
23 under different management practices using Daycent model in North China. *Chin. J. Appl.*
24 *Ecol.* 27, 539-548.

- 1 Yu, K., Chen G, Struwe, S., Kjøller, A., 2000. Production and reduction of nitrous oxide in
2 agricultural and forest soils. *J. Appl. Ecol.* 11, 385-389.
- 3 Zhang, Y., Qian, Y., Bremer, D.J., Kaye, J.P., 2013. Simulation of nitrous oxide emissions and
4 estimation of global warming potential in turfgrass systems using the daycent model. *J.*
5 *Environ. Qual.* 42, 1100-1108.

6 **Figure caption**

7 **Fig. 1.** SOERE-ACBB long-term experiment, Lusignan, France.

8 **Fig. 2.** Daily air temperature and precipitation during the experimental period March 2011 to
9 February 2014.

10 **Fig. 3.** Simulated soil organic carbon (SOC) under native vegetation (equilibrium-run,) past land use
11 changes and present conditions in the top 20 cm soil layer in mown-grassland and grain-cropland
12 (upper), and current measured and simulated SOC in the top 20 cm soil layer in mown-grassland and
13 grain-cropland (lower).

14 **Fig. 4.** Simulated water filled pore space (WFPS) at 10 cm soil depth in mown-grassland and grain-
15 cropland during 2011-2014 (top), and measured and simulated WFPS at 10 cm soil depth in mown-
16 grassland during 2011-2013.

17 **Fig. 5.** Simulated soil temperature at 10 cm soil depth in mown-grassland and grain-cropland during
18 2011-2014 (top), and measured and simulated soil temperature at 10 cm soil depth in mown-
19 grassland during 2011-2013.

20 **Fig. 6.** Simulated above-ground live biomass, total nitrogen uptake and nitrogen leaching in mown-
21 grassland and grain-cropland during the experimental period March 2011 to February 2014. C:
22 mowing event, T: tillage, S: sowing, H: harvesting, 36-90: amount of fertilizer nitrogen (kg N ha^{-1}).

1 **Fig. 7.** Measured and simulated cumulative hay production in mown-grassland (upper), and
2 measured and simulated total above ground biomass, grain and straw yield of corn, wheat and barley
3 in cropland during the experimental period March 2011 to February 2014.

4 **Fig. 8.** Measured and simulated ammonium (NH_4^+) and nitrate (NO_3^-) concentrations in mown-
5 grassland (top two) and grain-cropland (bottom two) during the experimental period March 2011 to
6 February 2014. C: mowing event, T: tillage, S: sowing, H: harvesting, 36-90: amount of fertilizer
7 nitrogen (kg N ha^{-1}).

8 **Fig. 9.** Simulated cumulative N_2O flux in mown-grassland and grain-cropland (top), measured and
9 simulated N_2O flux in mown-grassland with all measured values (second top) and excluding six
10 larger measured fluxes for elucidating N_2O flux on finer scale (second bottom) , and measured and
11 simulated N_2O flux in grain-cropland (bottom) during the experimental period March 2011 to
12 February 2014. C: mowing event, T: tillage, S: sowing, H: harvesting, 36-90: amount of fertilizer
13 nitrogen (kg N ha^{-1}).