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► To cite this version:

Marcio dos Reis Martins, Magdalena Necpalova, Christof Ammann, Nina Buchmann, Pierluigi Calanca, et al.. Modeling N₂O emissions of complex cropland management in Western Europe using DayCent: Performance and scope for improvement. *European Journal of Agronomy*, 2022, 141, pp.126613. <10.1016/j.eja.2022.126613>. <hal-03771026>

HAL Id: hal-03771026

<https://institut-agro-dijon.hal.science/hal-03771026v1>

Submitted on 27 May 2025

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Modeling N₂O emissions of complex cropland management in Western Europe using DayCent: Performance and scope for improvement

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ARTICLE INFO

Keywords:

Model
Denitrification
Greenhouse gas
IPCC Tier 3
Trace gas

ABSTRACT

Under the United Nations Framework Convention on Climate Change (UNFCCC), industrialized countries and countries with economies in transition (so called Annex 1 countries) are encouraged to move towards more sophisticated approaches for national greenhouse gas reporting. To develop a model-based approach for estimating nitrous oxide (N₂O) emissions from agricultural soils, model calibration is one of the first important steps. Extensive multisite field observations are necessary for this purpose, as agricultural management in Western Europe is complex (e.g., diverse crop rotations, different types of fertilizer and soil tillage). In the present study, we used ca. 24,000 daily N₂O flux observations from six cropland sites, two in France and four in Switzerland, to conduct an automatic data-driven calibration of the biogeochemical model DayCent. This model is planned to be used for greenhouse gas reporting in the entire European Union as well as in Switzerland. After a site-specific calibration, a leave-one-out (LOO) cross-evaluation was conducted to assess the model's ability to predict N₂O emissions for sites it was not calibrated for. Mean observed N₂O fluxes for 54 interactions of crop cycles, field studies and treatments were used to evaluate the model. The LOO cross-evaluation resulted in a R² of 0.63 for the

Abbreviations: AF, alfalfa (*Medicago sativa* L.); BIOORG, organic farming with manure and slurry as N fertilization; CC, cover crop; CL, clover (*Trifolium* spp.); CONFYM, conventional farming with manure plus additional mineral fertilization; CONMIN, conventional farming with only mineral fertilization; cr, cover crushing; DayCent, Daily CENTURY Model; EF, emission factor; F, synthetic fertilizer; FB, faba bean (*Vicia faba* L.); GC, grass+clover ley; GHG, greenhouse gas; GM, green manure; hb, herbicide; IPCC, Intergovernmental Panel on Climate Change; LOO, leave-one-out; M, manure compost; MAP, mean annual precipitation; MAT, mean annual temperature; MaxNitAmt, maximum daily nitrification amount (g N m⁻²); mod, modeled value; $\overline{\text{mod}}$, average of the modeled values; MU, mustard (*Sinapis alba* L.); MZ, maize (*Zea mays* L.); n, number of observations; N₂N₂Oadj, N₂:N₂O ratio adjustment coefficient; N₂Oadj_{fc}, maximum proportion of nitrified N lost as N₂O at field capacity; N₂Oadj_{wp}, minimum proportion of nitrified N lost as N₂O at wilting point; Ncoeff, minimum water and temperature limitation coefficient for nitrification; netmn_{to_no3}, fraction of new net mineralization that goes to NO₃; NOFERT, unfertilized control with four replicates each; OA, oats (*Avena sativa* L.); obs, observed value; $\overline{\text{obs}}$, average of the observed values; PE, peas (*Pisum sativum* L.); PEST, Model-Independent Parameter Estimation; pl, moldboard plowing; PO, potato (*Solanum tuberosum* L.); Q₁, middle value between the minimum value and the median; Q₃, middle value between the median and the maximum value; R², coefficient of determination; rl, rolling; RMSE, root mean square error; RP, rapeseed (*Brassica napus* L.); RPIQ, the ratio of performance to interquartile distance; rRMSE, relative root mean square error; rt, rotary tillage; RY, rye (*Secale cereale* L.); S, slurry; S1, reference system with conventional tillage; S2, no-tillage system; S3, integrated weed management system; S5, a fully integrated weed management system; SB, summer barley (*Hordeum vulgare* L.); SF, sunflower (*Helianthus annuus* L.); SOC, soil organic carbon; SP, spelt (*Triticum spelta* L.); st, shallow tillage; SY, soybeans (*Glycine max* (L.) Merr); TR, triticale (*Triticale hexaploide* Lart.); WB, winter barley (*Hordeum vulgare* L.); wfpsdnitadj, adjustment on inflection point for water-filled pore space effect on denitrification; WW, winter wheat (*Triticum aestivum* L.).

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<https://doi.org/10.1016/j.eja.2022.126613>

Received 4 April 2022; Received in revised form 17 August 2022; Accepted 19 August 2022

Available online 2 September 2022

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prediction of mean N₂O fluxes per crop cycle, compared to an R^2 of 0.51 obtained with default parameterization. Our results showed that the improvement in N₂O predictions was associated with the adjustment of only seven parameters controlling the N cycle in soil (e.g., the maximum daily nitrification amount and the inflection point for the effect of water-filled pore space on denitrification) out of several hundred parameters. These parameters showed a wide range of values between sites, revealing an important challenge for calibration-based improvement of N₂O simulations. Despite the remaining uncertainty, our model-based estimates of N₂O emission per crop cycle (2.64 kg N ha⁻¹) were clearly closer to measurements (2.67 kg N ha⁻¹) than commonly used emission factor approaches (1.60–1.71 kg N ha⁻¹). Based on extensive field observations, our results suggest that, after data-driven calibration of only few N cycle parameters, DayCent simulations are useful for reporting N₂O emissions of complex cropland management. These model based-estimates were more accurate, because they consider key drivers that are disregarded by simpler approaches. Moving towards more complex methods of N₂O reporting, is therefore expected to improve the accuracy and additionally allows to assess mitigation options.

1. Introduction

The global emissions of nitrous oxide (N₂O), a potent greenhouse and ozone-depleting gas, increased from approximately 11 Tg N yr⁻¹ in the pre-industrial era to 17 Tg N yr⁻¹ in recent decades (Müller, 2021). Agriculture is the main anthropogenic source of global N₂O emissions, which is associated with the input of reactive forms of N to the soil (Hergoualc'h et al., 2019), originating from synthetic fertilizers, animal excreta, biological N₂ fixation, soil organic N mineralization and atmospheric deposition. The assessment of the important sources and potential mitigation options are necessary to define policies for curbing soil N₂O emissions. However, large-scale estimates of soil N₂O emissions are still highly uncertain. A main reason for this uncertainty is the spatially and temporally dynamic nature of nitrification, denitrification, and N₂O reduction to N₂, which are the major processes controlling soil N₂O fluxes (Ibraim et al., 2019; Verhoeven et al., 2019; Gallarotti et al., 2021). Disregarding the key drivers of those processes is the main problem of national-scale N₂O emission reports based on generic approaches that rely on emission factors (EF). The EF concept considers the ratio of N losses as N₂O to N inputs as a fixed proportion. The EF-based estimates of soil N₂O emissions, usually performed for an aggregated time-scale (e.g., a year), do not take into account the variation in N use efficiency by different crops, soil properties, soil management, and climate (Hergoualc'h et al., 2019; Del Grosso et al., 2020). This is an important issue for mitigation policies, which depend on accurate estimates of the greenhouse gas (GHG) budget of the region for policy implementation. Process-based modeling that includes our current mechanistic understanding of the C and N cycles can be an adequate option for the assessment of critical soil, management and weather conditions influencing N₂O emissions from soils at regional scales (Lugato et al., 2018).

Biogeochemical models help to overcome the difficulty to conduct extensive, and thereby expensive, field measurements of N₂O over time (e.g., decades) and over geographic regions (e.g., ecoregions). Among the biogeochemical models, DayCent has been successfully applied for reporting N₂O emissions in the national GHG inventory of the U.S. (US-EPA, 2022). It has been employed also to simulate the impact of different management practices or climate change scenarios on GHG emissions and to do life-cycle analysis (Álvarez-Fuentes et al., 2017; Lugato et al., 2018; Del Grosso et al., 2019). However, the success of using process-based models like DayCent relies on the calibration and further evaluation of the model against reliable field measurements (Deng et al., 2018; Ogle et al., 2019). Although there have been key studies focused on the improvement of model estimates of GHG emissions from croplands in Switzerland and other regions of temperate Europe (e.g., Necpálová et al., 2018; Lugato et al., 2018; Revill et al., 2019; Lee et al., 2020a,2020b), there is still a lack of studies focusing on the model evaluation based on multisite measurements of N₂O emissions. More specifically, DayCent's performance has not been widely tested against field measurements of N₂O covering different pedoclimatic conditions and management practices in temperate Europe.

A particular challenge of estimating N₂O fluxes in agricultural

systems with diverse cropping and management practices over time are legacy effects, such as the amount of N returned as crop residues and left in soil from one cropping season to the next. Those legacy effects influence background N₂O fluxes, which represent a major fraction of the total emissions in complex farming systems, and are difficult to predict (Hansen et al., 2019). Therefore, for croplands with higher diversity of crop rotations and management, process-oriented models could provide more accurate estimates, which are unattainable by using simpler approaches. For instance, the assessment of the additive or interactive effects of different mitigation practices in N₂O emissions can be improved by using process-based models.

There is a clear lack of studies with multisite data-driven calibration of model parameters controlling N transformation by nitrification and denitrification in soil and determining the model's predictive ability for N₂O emissions. This is considered one of the main bottlenecks in modeling soil N₂O emissions (Del Grosso et al., 2020). The calibration of N cycle parameters depends on reliable field data covering different crops, soil type and interannual variability of climatic variables. This is particularly important in regions with complex interaction of diverse crop rotations (e.g., integration of ley, presence of legumes, number of crops), different N sources, and different soil management practices including full inversion tillage.

The objective of this study was to evaluate the performance of DayCent to estimate soil N₂O emissions from several crop cycles in six field studies in Western Europe. A specific aim was to assess the range of values of critical parameters controlling nitrification and denitrification in soil that directly affect the simulation of N₂O emissions. Further, we compared the N₂O estimates based on DayCent for crop cycles against estimates using the commonly applied EF approach.

2. Materials and methods

2.1. DayCent model

DayCent is an abbreviation for "Daily CENTURY Model" (Hartmann et al., 2018). The processes in the soil-plant system are simulated by integrated submodels, including vegetation growth (forest, grassland and cropland), decomposition of plant residues and soil organic matter pools, soil water and soil temperature dynamics, N transformation by nitrification and denitrification determining NO₃ leaching and gaseous losses of N, methane oxidation and methanogenesis (Del Grosso et al., 2011; Hartmann et al., 2018). The DD17centEVI version of DayCent was used in the present study (Hartmann et al., 2018). Additional description of the model is provided in the Appendix.

2.2. Field data

The measurement data of six field studies were used for the calibration and evaluation of the DayCent model (Fig. 1). The most important soil and weather characteristics of the field studies are presented in Table 1. Soil properties available at the plot level were used as input for each modeled treatment. Soil hydraulic properties were

estimated using pedotransfer functions (see Appendix). Approximately 24,000 daily N₂O flux observations were included in the present study considering the frequency of sample collection and the number of chambers per treatment in each field study. Some details of the N₂O flux measurements in the different field studies are presented in Table 2. The studies using chambers meet the set of criteria defined by Rochette and Eriksen-Hamel (2008) for quality control of N₂O flux measurements (e. g., minimum chamber height, insertion in soil, sampling time). The crops used in the field studies are among the most important in terms of harvested area in Western Europe (FAOSTAT, 2021). The N rates per crop cycle during the N₂O flux monitoring across different field studies and treatments ranged from 0 to 335 kg N ha⁻¹. Details of the crop rotations at each field study are presented in Table 2.

The long-term field study in Bretenière, located in Eastern France, was set up to assess agronomical and environmental effects of different weed management cropping systems (Chikowo et al., 2009; Ugarte Nano et al., 2015, 2016; Vermue et al., 2016). It involves different crop rotations, intensities of tillage and herbicide application. Originally, five different treatments were applied in different plots, without replication (Chikowo et al., 2009). Measurements of N₂O were performed in four treatments representing different management systems (Vermue et al., 2016), including (i) S1, a reference system with conventional tillage, crop rotation and use of herbicides; (ii) S2, a no-tillage system with less herbicide use than in the reference; (iii) S3, an integrated weed management system in which tillage was carried out for weed control only when necessary; and (iv) S5, a fully integrated weed management system with weed control based on cultural practices, soil cultivation when necessary and without herbicides. Soil N₂O emissions were measured using 6 chambers per treatment.

The long-term field study known as EFELE is located in Le Rheu, Northwestern France. It has been conducted to assess the effect of long-term repeated application of organic N derived from animal production (INRAE, 2021). This study is part of the French National Observatory

SOERE PRO, which is a network focused on long-term environmental impacts of organic waste products on cropping systems (INRAE, 2021). Soil N₂O fluxes have been measured for eight sequential years in two treatments applied in field plots (no replicates) fertilized with different N sources: (i) ammonium nitrate, and (ii) pig slurry. Measurements of soil N₂O emissions were performed using 3 chambers per treatment.

The long-term field study known as DOK is located in Therwil, Switzerland. DOK is the German acronym for “*Dynamisch, Organisch, Konventionell*”. This study has been conducted on an area of 2 ha to compare different farming systems characterized by fertilization strategies and plant protection management (Mäder et al., 2002; Mayer et al., 2015; Skinner et al., 2019). The treatments considered for simulations were: (i) BIOORG, organic farming with manure and slurry as N fertilization, (ii) CONFYM, conventional farming with manure plus additional mineral fertilization, (iii) CONMIN, conventional farming with only mineral fertilization, and (iv) NOFERT, unfertilized control with four replicates each. The biodynamic treatment was not included in the present study. Plant protection in the organic and the unfertilized system is based on mechanical weeding, indirect disease control measures and plant extracts together with bio-controls against insects, while in the non-organic systems herbicides, fungicides and pesticides are applied.

The long-term field study in Frick, Switzerland, was set up to compare management factors related to the type of organic fertilization, soil tillage and biodynamic preparations (Berner et al., 2008; Gadermaier et al., 2012; Krauss et al., 2017). Nitrous oxide fluxes were measured in four treatments based on a combination of two different types of organic fertilizer and two types of tillage, with four replicates (Krauss et al., 2017, dataset: doi.org/10.5281/zenodo.1566066). The effect of biodynamic preparations was not included in the N₂O monitoring. The organic fertilization treatments were (i) cattle slurry alone (Slurry) and cattle manure compost plus slurry (Manure compost). The soil tillage treatments were (i) conventional tillage (15–18 cm,

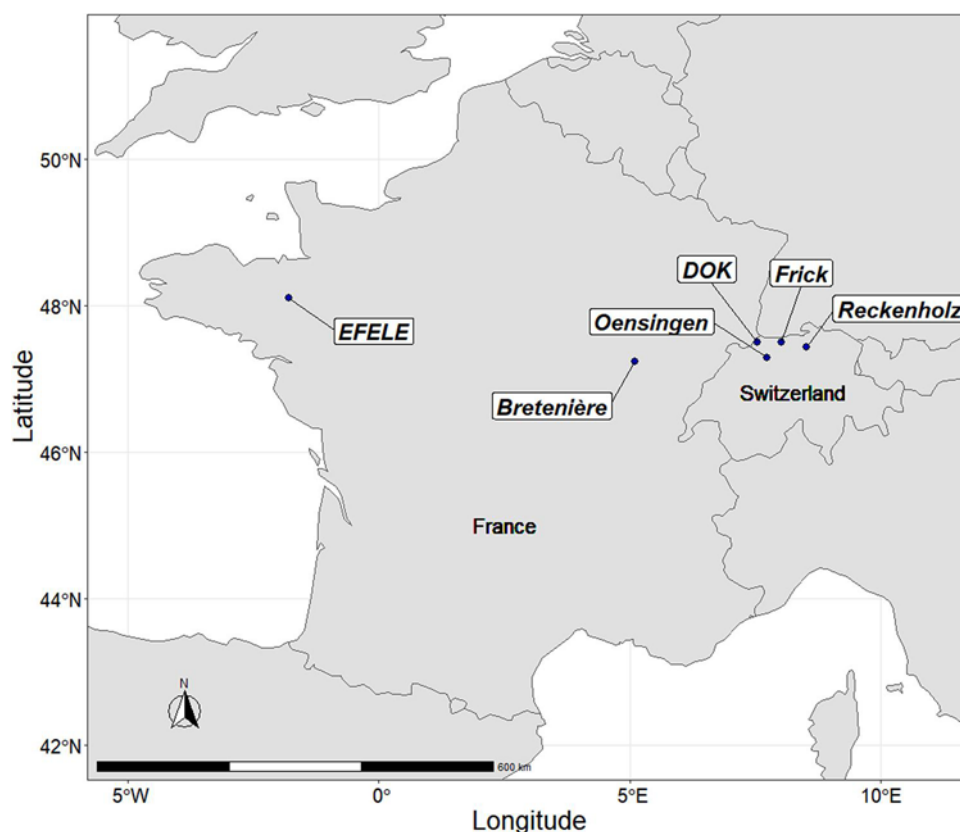


Fig. 1. Location of the field studies used for the calibration and evaluation of the DayCent model.

inversion) and (ii) reduced tillage (7–10 cm, non-inversion). The amounts of N input in different fertilization treatments were determined by the N content in slurry and manure compost multiplied by application rates (Gadermaier et al., 2012).

In the long-term field study in Oensingen, Switzerland, which is part of the Swiss FluxNet (database code CH-Oe2; for details, see Emmel et al., 2018), the ecosystem-scale N₂O fluxes were measured in 2019 at high temporal resolution (10 Hz) using the eddy-covariance technique (Mair and Buchmann, 2019). For the present study, the N₂O fluxes were averaged to daily values. This field study is managed with intensive crop rotations following the Swiss Integrated Pest Management regime, known as IP-SUISSE. Various types of N inputs have been used since the beginning of the field study. Mineral N inputs were mostly ammonium nitrate-based fertilizers. Organic N inputs were slurry, cattle manure and cattle manure compost. Typical conventional soil tillage practices used in Switzerland were applied at this site, including ploughing (chisel and moldboard), cultivation and rolling for seedbed preparation.

The field study in Reckenholz was conducted for one cropping season in 2014 to test the effect of biochar and limestone application on N₂O emissions from a soil under maize (Hüppi et al., 2015). The treatments were the type of additions to soil before maize sowing, including (i) biochar, (ii) limestone control, and (iii) a control without additions. Three replicated plots were used per treatment. The field was sown with maize for grain production in 2014. Ammonium nitrate-based fertilizer was applied 18, 39 and 69 days after sowing at rates of 40, 80 and 40 kg N ha⁻¹, respectively.

2.3. Meteorological data

Meteorological data for the field studies were obtained from stations located at the field experiments or from nearby stations (*i.e.*, at distances up to 5 km) for gap-filling. Data from nearby stations in Switzerland (Basel-Benningen, Wynau, and Reckenholz) were available on the IDAWEB portal of the Swiss Federal Office of Meteorology and Climatology (<https://gate.meteoswiss.ch/idaweb>) and in France (Dijon and Rennes) on the CLIMATIK portal provided by INRAE (https://intranet.inrae.fr/climatik_v2). Simulations for each field study were performed using the DayCent's extra climate driver's mode with six meteorological variables at a daily resolution. The variables were maximum and minimum air temperature, precipitation, solar radiation, relative air humidity, and wind speed.

2.4. Initialization of the model

The initialization of the model consisted of a simulation of the C and N cycling over many centuries to define the size of different soil organic matter pools before starting simulations for the recent experimental period. For this model initialization, an overall land-use history in Switzerland and France during the last two millennia was assumed as

proposed by Necpálová et al. (2018) based on literature of the history of land-use in Western Europe (*e.g.*, Vannière et al., 2003; Bürgi, 2016). We considered the presence of a deciduous forest until the end of the 15th century. The definition of parameters for this “medieval forest phase” was mostly based on default parameters for deciduous forests from the DayCent library. Some adjustments were made in these forest parameters by accounting for litter composition measurements performed in European forests (*e.g.*, Jacob et al., 2010). We assumed that agriculture was established after forest clearing and has undergone different stages according to the development of farming technology (Necpálová et al., 2018). The first agricultural phase was from 1500 to 1750 (pre agricultural revolution), the second phase from 1751 to 1850 (agricultural revolution), the third phase from 1851 to 1950 (agriculture intensification), and the fourth phase from 1951 to the year before the beginning of the field study (modern agriculture). Gradual increments in N inputs, diversity of crops, and yields were considered over these phases. The meteorological data from each field study (see Section 2.3 above) were used with recursion for the initialization of the model.

2.5. Assessment of DayCent's performance

The model's predictive ability for N₂O emissions was assessed using a leave-one-out (LOO) cross-evaluation (Efron and Tibshirani, 1994; Wallach et al., 2018). The cross-evaluation was based on splitting the six datasets in five “calibration” sites and one “evaluation” site. In this way, the simulations for each site were carried out by averaging the values of calibrated parameters obtained at remaining sites. It means that for a given site the values of the calibrated parameters obtained for this site were excluded from the calculation of the average values of parameters used to test the model's performance. Only the crops for which a calibration was performed at least for one independent site were included in the cross-evaluation.

The model calibration at each site was performed by coupling DayCent with PEST (Fig. 2). PEST is an abbreviation for “Model-Independent Parameter Estimation”. It is a statistical tool based on inverse modeling for iterative selection of the best set of parameter values based on best fit, *i.e.*, minimization of difference between the modeled and observed values (Doherty, 2020). For the calibration, the PEST code executes DayCent runs several times with variations of the parameters. The parameter estimation is based on a gradient optimization using a Jacobian matrix of sensitivities of model outputs to parameters (Doherty, 2020). This process is performed by sequentially varying the parameter values in the input files, running DayCent, recording the output values and comparing them with the observed values. The Gauss-Marquardt-Levenberg algorithm is used by PEST to iteratively select the parameter values minimizing the difference between model outputs and observed values. The parameter estimation process is conducted until no improvement occurs between two sequential iterations (Doherty, 2020).

Table 1

Climate and soil^a characteristics of the six field studies used for simulations with DayCent.

Field study	Location	Coordinates	Altitude (m. a.s.l.)	MAP (mm)	MAT (°C)	Soil Class (FAO-WRB, 2014)	Clay (%)	Silt (%)	Sand (%)	pH	SOC (%)	Bulk density (g cm ⁻³)
Bretenière	Bretenière, France	47°14'N, 5°6'E	211	770	10.5	Hypereutric Cambisol	41	53	5	6.9	1.91	1.49
EFELE	Le Rheu, France	48°6'N, 1°48'W	40	754	12.0	Stagnic Luvisol	14	71	15	6.1	1.16	1.32
DOK	Therwil, Switzerland	47°30'N, 7°32'E	306	791	9.5	Haplic Luvisol	16	71	11	6.1	1.43	1.32
Frick	Frick, Switzerland	47°30'N, 8°01'E	350	1000	8.9	Vertic Cambisol	45	27	28	7.1	2.20	1.11
Oensingen	Oensingen, Switzerland	47°17'N, 7°44'E	452	1086	9.8	Eutri-stagnic Cambisol	43	47	10	6.4	2.12	1.23
Reckenholz	Zürich, Switzerland	47°26'N, 8°31'E	437	1054	9.4	Eutric Mollic Gleysol	36	27	37	6.3	2.62	1.30

^a Average of plots used for the simulations (plough layer). MAP: mean annual precipitation; MAT: mean annual temperature; SOC: soil organic carbon.

Table 2Crop rotations and details regarding N₂O measurements of the six field studies used for simulations with DayCent.

Field studies	Period of the study ^a	Crop rotation in the last ten years used for simulation ^b	Period of N ₂ O flux measurements	Method of N ₂ O flux measurements	References
Bretonnière	2000–2013	<i>Treatment S1:</i> WB ₀₄ –RP ₀₅ –WW ₀₆ –WB ₀₇ –RP ₀₈ –WW ₀₉ –WB ₁₀ –RP ₁₁ –WW ₁₂ –WB ₁₃ ; <i>Treatment S2:</i> RP ₀₄ –WW ₀₅ –OA ₀₅ –SB ₀₆ –SY ₀₇ –WW ₀₈ –RP ₀₉ –SY ₁₀ –WW ₁₁ – SB₁₂–OA₁₂–SY₁₃ ; <i>Treatment S3:</i> MU ₀₃ –WW ₀₄ –RP ₀₅ –TR ₀₆ –SY ₀₇ –WW ₀₈ –RP ₀₉ –TR ₁₀ –RP ₁₁ – WW₁₂–CC₁₂–SY₁₃ ; <i>Treatment S5:</i> WB ₀₄ –FB ₀₅ –TR ₀₆ –RP ₀₇ –WW ₀₈ –WB ₀₉ –CC ₀₉ –FB ₁₀ –WW ₁₁ – AF₁₂–MZ₁₃ <i>All treatments:</i> WW₁₃–CC₁₄–MZ₁₄–WW₁₅–CC₁₆–MZ₁₆–WW₁₇–CC₁₈–MZ₁₈–WW₁₉–CC₂₀–MZ₂₀	Mar. 2012–Apr. 2013	Chambers with automated sampling	Chikowo et al. (2009); Ugarte Nano et al., (2015, 2016); Vermue et al. (2016)
EFELE	2012–2020	<i>All treatments:</i> WW₁₃–CC₁₄–MZ₁₄–WW₁₅–CC₁₆–MZ₁₆–WW₁₇–CC₁₈–MZ₁₈–WW₁₉–CC₂₀–MZ₂₀	Mar. 2013–Sep. 2020	Chambers with automated sampling	INRAE (2021)
DOK	1977–2014	<i>All treatments:</i> GC ₀₅ –MZ ₀₆ –WW ₀₇ –GM ₀₈ –SY ₀₈ –RY ₀₉ –PO ₀₉ –WW ₁₀ –GC ₁₁ – GC₁₂–MZ₁₃–GM₁₄	Aug. 2012–Mar. 2014	Chambers with manual sampling	Mäder et al. (2002); Mayer et al. (2015); Skinner et al. (2019)
Frick	2002–2014	<i>All treatments:</i> SP ₀₅ –GC ₀₆ –GC ₀₇ –MZ ₀₈ –WW ₀₉ –CC ₁₀ –SF ₁₀ –SP ₁₁ – GC₁₂–GC₁₃–WW₁₄–CC₁₅	Aug. 2012–Oct. 2014	Chambers with manual sampling	Berner et al. (2008); Gadermaier et al. (2012); Krauss et al. (2017)
Oensingen	2003–2020	WW ₁₁ –WB ₁₂ –RP ₁₃ –WW ₁₄ –WB ₁₅ –PE ₁₆ –WW ₁₇ –RP ₁₈ – WW₁₉–WB₂₀	Jan. 2019–Jan. 2020	High resolution eddy covariance system	Emmel et al. (2018); Maier and Buchmann (2019)
Reckenholz ^c	2014	<i>All treatments:</i> MZ₁₄	Mar. 2014–Dec. 2014	Chambers with automated sampling	Hüppi et al. (2015)

^a Period from the beginning of the experiment to the last year of simulations, *i.e.*, not necessarily to the end of the experiment.

^b Letters indicate the crop and subscript numbers indicate the last two digits of the year of crop harvest or termination (cover crop, catch crop or green manure); AF = alfalfa (*Medicago sativa* L.), CC = catch or cover crop, CL = clover (*Trifolium* spp.), FB = faba bean (*Vicia faba* L.), GC = grass+clover ley, GM = green manure, MZ = maize (*Zea mays* L.), MU = mustard (*Sinapis alba* L.), OA = oats (*Avena sativa* L.), PE = peas (*Pisum sativum* L.), PO = potato (*Solanum tuberosum* L.), RP = rapeseed (*Brassica napus* L.), RY = rye (*Secale cereale* L.), SB = summer barley (*Hordeum vulgare* L.), SF = sunflower (*Helianthus annuus* L.), SP = spelt (*Triticum spelta* L.), SY = soybeans (*Glycine max* (L.) Merr), TR = triticale (*Triticale hexaploide* Lart.), WB = winter barley, and WW = winter wheat (*T. aestivum* L.); bold abbreviations indicated the crop cycles in which the N₂O fluxes were measured.

^c Please note that the simulations for EFELE and Reckenholz field studies were performed for less than 10 years.

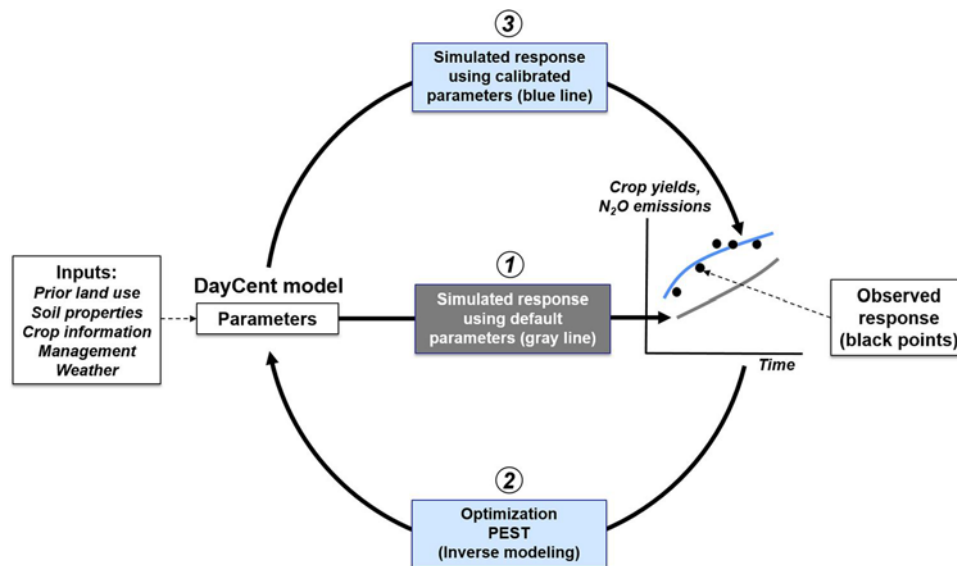


Fig. 2. Procedure for calibration of DayCent using inverse modeling based on field observations.

To perform the calibration, we selected the same plant and management parameters sensitive to measured data as found by Necpálová et al. (2018). Considering the significant correlation between many parameters found by these authors, we also followed independent sequential stages for calibration of the model parameters, but with an additional stage for the calibration of the N cycle parameters. Parameters calibrated in previous stages were kept at their optimized values for

the calibration of parameters in a subsequent stage. The five sequential stages are:

- *Stage I:* the parameter denoting the photosynthetic radiation-use efficiency in the forest phase was calibrated during model initialization based on initial soil organic C (SOC) stocks observations in the top arable layer at a 20 cm depth at each field study.

- *Stage II*: crop parameters were calibrated based on yield data.
- *Stage III*: the tillage parameters, which control the effect of tillage on different SOC and soil N pools, were calibrated based on measurements of SOC stocks over time.
- *Stage IV*: for the sites with organic N inputs, we performed a calibration of parameters determining decomposition of organic inputs (manure, manure compost and slurry) based on measured SOC stocks and crop yield data.
- *Stage V*: N cycle parameters controlling nitrification and denitrification were calibrated based on observed cumulative N₂O emissions over time.

Linear interpolation was used for gap filling of daily measured N₂O fluxes to calculate the cumulative emissions. Long gaps in measured daily fluxes (≥ 4 d) after fertilization or tillage events were not filled to avoid errors in the calibration process related to the calculation of cumulative N₂O emissions. Therefore, the modeled daily N₂O fluxes corresponding to the unfilled gaps were also excluded from the modeled cumulative N₂O emissions used in the calibration process. Thus, for coupling DayCent and PEST for calibration of N cycle parameters at the stage V described above, new selective datasets were created with simulated N₂O emission data coincident to the available gap-filled data. Additional details of the inverse modeling for calibration of DayCent parameters using the PEST tool are given by Rafique et al. (2013) and Necpálová et al., (2015, 2018).

By selecting only crop cycles with entire gap-filled management periods for N₂O flux measurements, we made a comparison of DayCent estimates against EF approaches commonly used in IPCC Tier 1. The latter represents the most basic method for national inventories of greenhouse gas emissions and hardly includes country specific data. Two EF approaches were considered for this comparison with model estimates. The first approach is the use of an aggregated EF with a general value of 1% of the N losses as N₂O from N inputs (Klein et al., 2007). The second approach is a refinement of the Tier 1 approach based on the use of disaggregated EFs, which means that the percentage of N loss as N₂O depends on the type of N input, with 1.6% for synthetic fertilizers and 0.6% for other inputs (Hergoualc'h et al., 2019). Further detailed procedures for estimates based on EF approaches were described in the Appendix.

In addition to the observed N₂O emissions for each site, we used observed crop yield data to evaluate the overall performance of the model, *i.e.*, as a general quality control of the model outputs (Del Grosso et al., 2020). Evaluating crop yields in the different stages was also an attempt to reduce the risk of a good model performance for N₂O emissions due to errors in parameters not directly related to the N cycle. More insights on the equifinality, *i.e.*, good model fit obtained for the wrong reasons, was given by Beven (2006). For the cross evaluation, the average of parameters was obtained in a more generic way, which would be the approach most likely applied for simulating N₂O emission over large regions (*e.g.*, for national inventories). For example, plant parameters were averaged at a species level rather than at a cultivar level.

2.6. Statistical metrics

Linear regressions of modeled against observed crop yields and mean daily N₂O fluxes over a crop cycle were used to assess the overall model's performance. To calculate the mean fluxes, a crop cycle was considered to begin at the seedbed preparation or pre-plant fertilizer application or only sowing in some cases (*e.g.*, no-tillage), *i.e.*, any of these events occurring first. Therefore, the occurrence of one of these events was also considered as the end of a previous cycle. In this way, the post-harvest period was included in the crop cycle with the effect of crop residue decomposition on N₂O emissions, as recommended by IPCC (Hergoualc'h et al., 2019). The winter period was also included in the cycles of some crops (*e.g.*, winter wheat and ley). The combination of different crop cycles, treatments and field studies resulted in n of 54 for

mean N₂O fluxes and 236 for crop yields. Average values were used for treatments with field replicates (see Section 2.2 above). In addition to the coefficient of determination (R^2), we also used the relative root mean square error (*rRMSE*), the ratio of performance to interquartile distance (*RPIQ*), and the *bias* as a statistical metrics for the regressions. The *rRMSE* and the *RPIQ* value is calculated based on the root mean square error (*RMSE*), which is defined as:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (obs - mod)^2}$$

where n is the number of measurements, *obs* is the observed value and *mod* is the modeled value. The *rRMSE* value is calculated as follows:

$$rRMSE = \frac{RMSE}{\overline{obs}}$$

where \overline{obs} is the average of the observed values. Smaller values of *rRMSE* indicates greater accuracy in the predictions (Wallach et al., 2018). The *RPIQ* value is calculated as:

$$RPIQ = \frac{Q_3 - Q_1}{RMSE}$$

where Q_3 is the third quartile of the observed values, *i.e.*, the middle value between the median and the maximum value of the observed data set, and Q_1 is the first quartile of the observed values, *i.e.*, is the middle value between the minimum value and the median of the observed data set. An advantage of *RPIQ* is that it takes in account the degree of variation in observed values (Bellon-Maurel et al., 2010). It denotes a comparison of the level of dispersion in the observed data set with the prediction error. The higher the value of *RPIQ*, the better the model's predictive ability. The *bias* is calculated as follows:

$$bias = \overline{mod} - \overline{obs}$$

where \overline{mod} is the average of the modeled values. The value of *bias* indicates systematic errors in the model estimates.

The integrated development environment R studio (Campbell, 2020) was used to develop a script to run DayCent for each site and instantaneously obtain the graphics and data outputs for assessing DayCent's performance during calibration and evaluation stages.

3. Results

3.1. Site-specific calibration and simulation of daily N₂O fluxes

DayCent's ability to reproduce daily N₂O fluxes before and after calibration is illustrated in Fig. 3 in an exemplary way by showing the simulation results of two treatments at two sites. The simulations of daily N₂O fluxes for all the remaining studies and treatments are presented as Appendix (Fig. A.1–A.6). Site-specific calibration effectively increased the adjustability of the modeled to observed daily N₂O fluxes as affected by crop types, N inputs and soil tillage for both sites (Fig. 3a–d). With the uncalibrated model, simulations performed at the Bretenièrre site showed some fertilizer-induced N₂O pulses up to 34 g N ha⁻¹ d⁻¹ during the wheat-growing season under conventional tillage (reference treatment), while the observed fluxes stayed below 10 g N ha⁻¹ d⁻¹ (Fig. 3a). Conversely, the uncalibrated model significantly underestimated the high N₂O fluxes in the no-tillage treatment, which were up to 246 g N ha⁻¹ d⁻¹ after barley fertilization (Fig. 3b). The site-specific calibration substantially improved DayCent's ability to capture the effects of these contrasting managements on N₂O emissions (Fig. 3b). This improvement is evident by comparing the observed and modeled cumulative N₂O emissions (lower panels in Figs. 3a and 3b). The observed cumulative N₂O emissions were 0.1 kg N ha⁻¹ in the reference treatment and 4.9 kg N ha⁻¹ in the no-tillage treatment. Before calibration, the

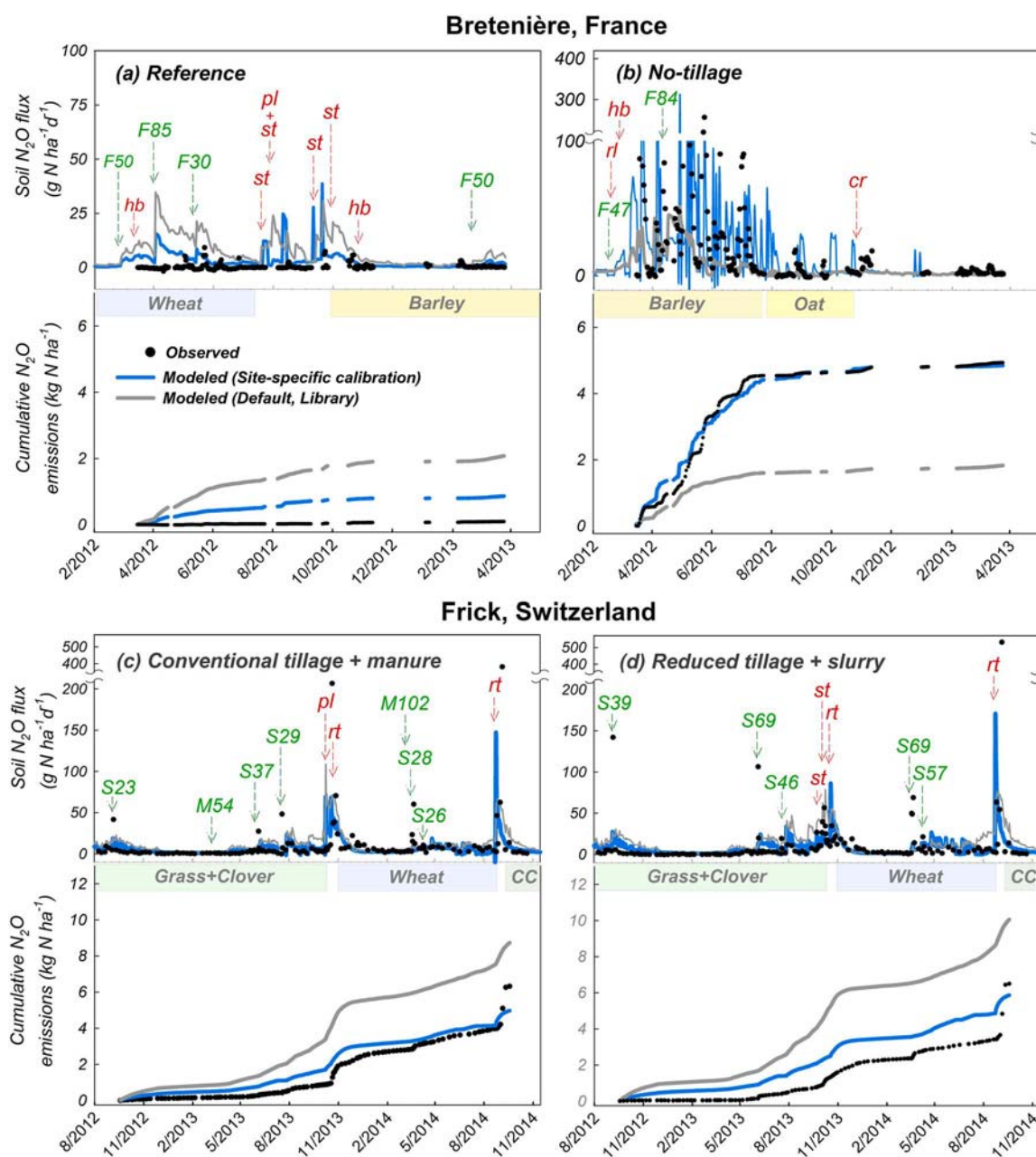


Fig. 3. Modeled (lines) versus observed (symbols) daily soil N₂O fluxes (top panels) and cumulative N₂O emissions (lower panels) from the ‘Reference’ (a) and the ‘No-tillage’ (b) treatments in Bretenièrre (France) and from the ‘Conventional tillage + manure’ (c) and the ‘Reduced tillage + slurry’ (d) treatments in Frick (Switzerland). Arrows associated with lowercase letters indicate cultivation events (*cr* = cover crushing, *hb* = herbicide, *pl* = moldboard plowing, *rl* = rolling, *rt* = rotary tillage, *st* = shallow tillage). Arrows associated with uppercase letters followed by values indicate N inputs, including fertilization type (*F* = synthetic fertilizer, *S* = slurry, *M* = manure compost) and rates, in kg N ha⁻¹, respectively (e.g., *F50* indicates an application of synthetic fertilizer at a rate of 50 kg N ha⁻¹). Please note the scale and breaks in the Y-axis. The crop growing periods from sowing to harvest or termination are indicated below the X-axis of the upper panels. CC = cover crop.

differences of the modeled and the observed values were 2.0 kg N ha⁻¹ for the reference and - 3.1 kg N ha⁻¹ for the no-tillage treatment. After calibration, the agreement between modeled and observed cumulative N₂O emissions were much better, with differences of 0.8 kg N ha⁻¹ for the reference and - 0.1 kg N ha⁻¹ for the no-tillage.

Also at the Frick site, the site-specific calibration clearly improved simulations of DayCent by reducing overpredicted cumulative N₂O emissions (Figs. 3c and 3d). Although some N₂O pulses associated with slurry applications (labeled *S*) and rotary tillage (labeled *rt*) were underpredicted by DayCent, the modeled cumulative emissions were significantly better adjusted after the site-specific calibration (Figs. 3c and 3d). Overall, this improvement in the adjustment for cumulative

N₂O emissions was also found for the other field studies (Appendix, Fig. A.1–A.6). The two exceptions to this were the fully integrated weed management treatment at the Bretenièrre site (Fig. A.1) and the ammonium nitrate treatment at the EFELE site (Fig. A.2). It is also worth noting that for BIOORG, CONMIN, CONFYM, treatments at DOK field study, even the uncalibrated model simulated the cumulative emissions well (Fig. A.3). On the other hand, in this field study, we observed the largest relative deviation between modeled and observed N₂O emissions in the control treatment (NOFERT), even after model calibration. Despite the underestimation, the lower modeled N₂O fluxes in this treatment are consistent with no N-fertilizer inputs for several decades (Mayer et al., 2015; Skinner et al., 2019). A possible explanation for this

underestimation of N_2O emissions is a systematic overestimation of crop yields for the NOFERT treatment (result not shown). This results in overestimation of N uptake by plants derived from N sources other than N-fertilizer (e.g., soil organic matter mineralization). Therefore, the model likely underestimated the amounts of soil N available to microorganisms that produce N_2O .

3.2. Average model calibration and evaluation

Regressions of modeled against observed crop yields and N_2O

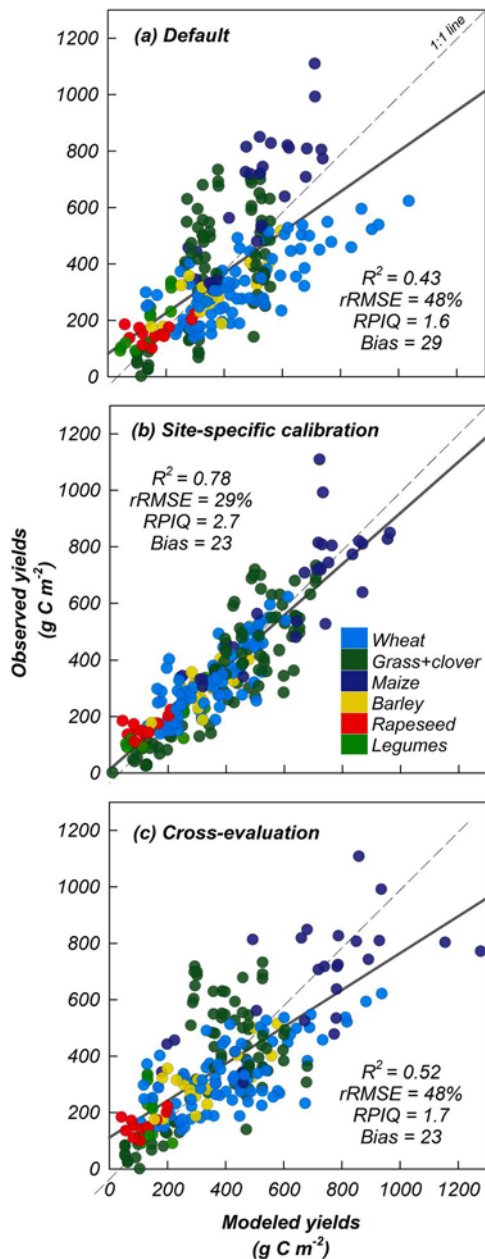


Fig. 4. Modeled against observed crop yields for six different field studies in Switzerland and France. Model performance was assessed for default parameterization (a), site-specific calibration (b), and leave-one-out cross-evaluation, i.e., the mean parameter value of all other sites except the one simulated was used (c). Each symbol stands for a harvest event of a specific treatment and site. Different crop types are indicated by different colors. The agreement between modeled and measured data is described by the coefficient of determination (R^2), the relative root mean square error ($rRMSE$), ratio of performance to interquartile distance ($RPIQ$) and *bias*.

emissions from crop cycles at the six sites were used to assess DayCent's performance (Figs. 4 and 5). It is possible to observe how much improvement in the estimates of crop yields and N_2O emissions was possible to attain by site-specific calibration (Figs. 4b and 5b) instead of using default parameters (Figs. 4a and 5a). Site-specific calibration increased the R^2 values from 0.22 to 0.78 for crop yields and from 0.51 to 0.78 for mean N_2O fluxes. The $RPIQ$ values also clearly indicate a better fit, increasing from 1.6 to 2.7 for crop yields and from 1.3 to 2.1 for mean N_2O fluxes. Values of $rRMSE$ declined from 75% to 29% for crop yields and from 88% to 54% for mean N_2O fluxes. Positive bias

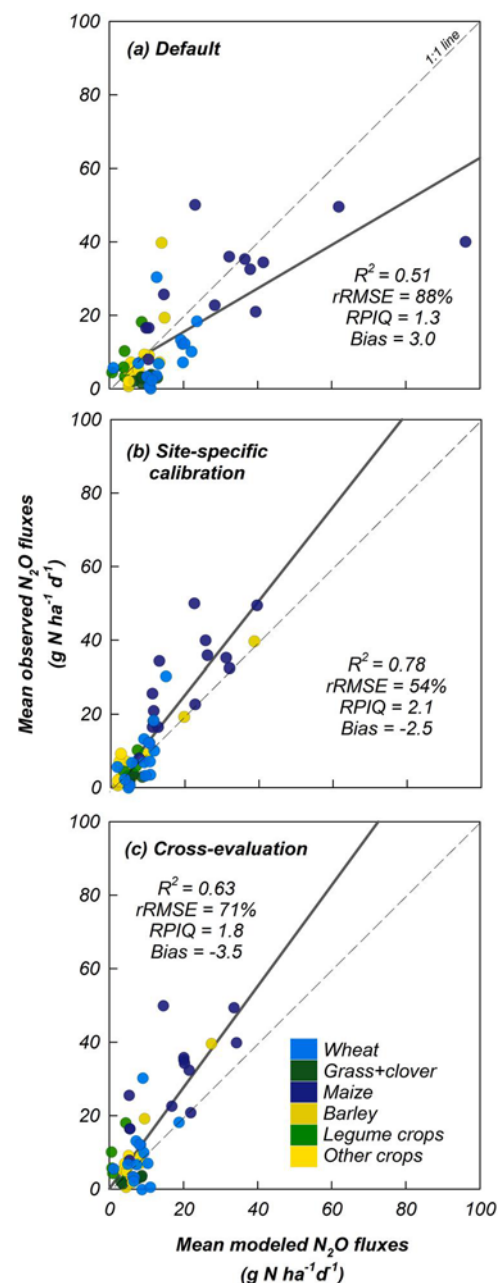


Fig. 5. Mean modeled versus observed soil N_2O fluxes during different crop cycles of six sites in Switzerland and France. Model performance was assessed for default parameterization (a), site-specific calibration (b), and leave-one-out cross-evaluation, i.e., the mean parameter value of all other sites except the one simulated was used (c). Each symbol stands for a crop cycle of a specific treatment and site. Please note that N_2O measurements were usually only performed during a few single crop cycles of the entire long-term experiments, explaining the lower number of symbols compared to Fig. 4.

slightly decreased for crop yields (29–23 g C m⁻²) and turned into negative bias for N₂O emissions (3.0 to -2.5 g N ha⁻¹ d⁻¹) after site-specific calibration.

The LOO cross-evaluation also showed a slight improvement in the model performance compared to the default (Figs. 4a and 4c), although it was, as expected, lower compared to site-specific calibration (Figs. 4b and 4c). For crop yields, the improvement in the model performance compared to using default parameters is shown by an increase of R^2 from 0.43 to 0.52. The use of plant parameters averaged at a species-level for the LOO cross-evaluation instead of using cultivar-specific parameterization limited further improvement of model estimates of crop yields. It is important to consider that when the model is applied for simulations over regions (e.g., country), field activity data at a cultivar level (e.g., share of land area with a specific cultivar) is often not available at large scales. Therefore, averaging parameter values at a species level is necessary for model simulations covering large regions. The LOO cross-evaluation for N₂O emissions showed an R^2 of 0.63, which was still higher than 0.51 obtained using the default parameters (Figs. 5a and 5c). The values of $rRMSE$ and $RPIQ$ also showed better model performance in the LOO cross-evaluation compared to the use of default parameters.

The best performance of the model for predicting N₂O emissions in the LOO cross-evaluation was achieved by adjusting the model parameters controlling nitrification and denitrification (Fig. 6). When these N cycle parameters were kept at their default values and other parameters

related to plant growth and management were adjusted, we observed only a slight improvement of the model's predictive ability for N₂O emissions (Fig. A.7).

In the LOO cross-evaluation, some of the N cycle parameters deviated significantly from the default value. This was evident, for example, for the maximum daily nitrification amount ($MaxNitAmt$) and the inflection point for the effect of water-filled pore space on denitrification ($wfpsdnitadj$). Other parameters ended by presenting LOO averages close to the default values, like the N₂:N₂O ratio adjustment coefficient ($N2N2Oadj$), even presenting site-specific values deviating significantly from the default value (Fig. 6).

3.3. DayCent model versus emission factor approaches

For a comparison of modeled and EF approaches, we estimated the mean cumulated N₂O emissions for crop cycles with all management periods (N fertilization and tillage) covered by measurements with gap-filling, including winter (See Section 2.5). This was possible for 23 interactions of crop cycles and treatments from three field studies (DOK, Frick, EFELE) for winter wheat, silage maize and grass-clover ley. The observed N₂O emissions for the selected crop cycles presented a wide range of values (0.7–7.0 kg N ha⁻¹) with a mean of 2.7 kg N ha⁻¹ (Fig. 7). The N₂O emissions estimated using the aggregated EF approach, i.e., considering 1% of N losses from N inputs (Klein et al., 2007), presented a

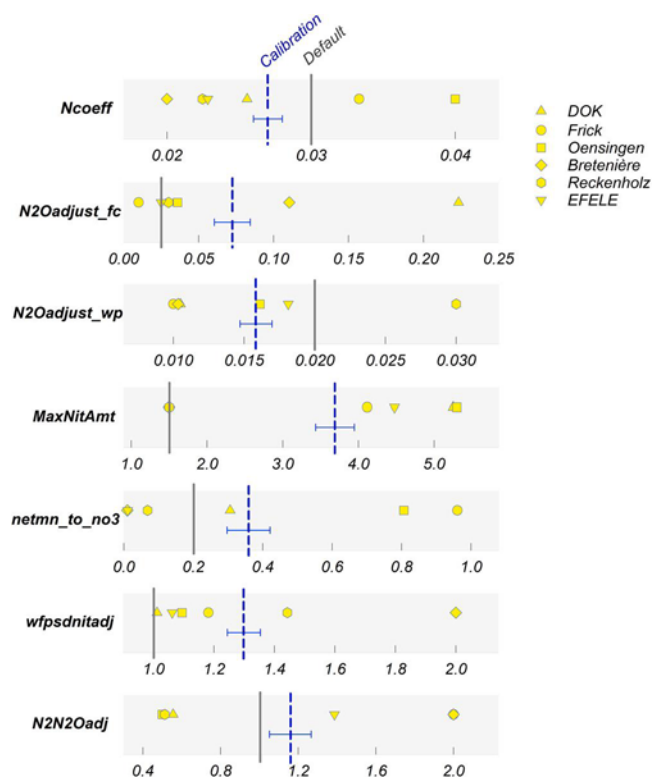


Fig. 6. DayCent parameters controlling soil N₂O emissions before and after calibration based on data from six cropland field studies in Switzerland and France. The gray solid vertical lines indicate the original default model values of the parameter, the dashed blue lines indicate the value of the average calibration using all six sites with horizontal blue bars indicating the confidence interval of the leave-one-out values for $\alpha = 0.05$. The yellow symbols indicate the values from the individual site-specific calibrations. $Ncoeff$ = minimum water and temperature limitation coefficient for nitrification, $N2Oadjust_fc$ = maximum proportion of nitrified N lost as N₂O at field capacity, $N2Oadjust_wp$ = minimum proportion of nitrified N lost as N₂O at wilting point, $MaxNitAmt$ = maximum daily nitrification amount (g N m⁻²), $netmn_to_no3$ = fraction of new net mineralization that goes to NO₃, $wfpsdnitadj$ = adjustment on inflection point for water-filled pore space effect on denitrification, $N2N2Oadj$ = N₂:N₂O ratio adjustment coefficient.

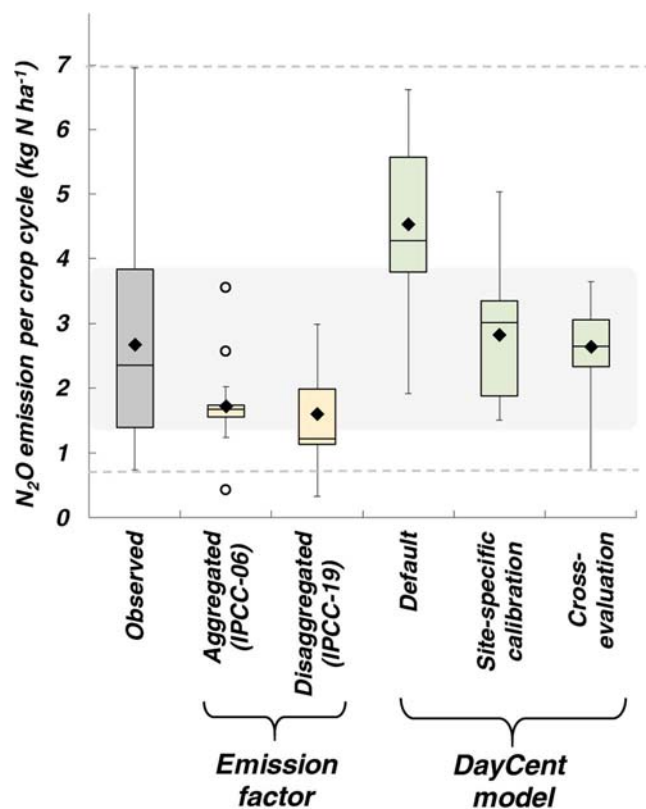


Fig. 7. Box plots of cumulative N₂O emissions and N inputs per crop cycle in field studies ($n = 23$ crop cycles). Different approaches were compared with observed N₂O emissions including IPCC emission factor (EF) and modeling. Two types of EF approaches were considered: *Aggregated (IPCC-06)* means that 1% of the N inputs are lost as N₂O (Klein et al., 2007); *Disaggregated (IPCC-19)* is a refinement of the previous EF approach and means that the percentage of N loss as N₂O depends on the type of N input, with 1.6% for synthetic fertilizers and 0.6% for other inputs (Hergoualc'h et al., 2019). The range from the first to the third quartile are indicated by boxes. The horizontal lines within the boxes indicate median values and diamond symbols indicate mean values. The upper and lower extremes are represented by whiskers and the outliers by circles. The dotted lines and the gray area indicate extremes and interquartile range of observed emissions, respectively.

37% lower mean value (1.7 kg N ha^{-1}). Besides this, the variation of emission estimates using this aggregated EF approach was much narrower, ranging from 1.2 to 2.0 kg N ha^{-1} (Fig. 7). The use of disaggregated EFs, i.e., 1.6% for synthetic fertilizers and 0.6% for other inputs (Hergoualc'h et al., 2019) resulted in a wider range of emissions (0.3 – 3.0 kg N ha^{-1}) and a mean estimated emission of 1.6 kg N ha^{-1} , also clearly lower than mean value of observed emissions (Fig. 7). The model estimates with either site-specific calibration or LOO average of parameters were significantly better than the EF approaches, although the interquartile range of estimates is narrower. This indicates that the adjustment of model parameters by site-specific site calibration or LOO average made the model more parsimonious for prediction of extreme N_2O emissions.

4. Discussion

Based on an extensive set of N_2O flux observations we identified which parameters of the biogeochemical model DayCent are most critical for improving the prediction of N_2O emissions from cropland soils (Figs. 3, 5 and 6). The data set included measurements from six different sites with various crop rotations, soil management and fertilization types. Our results indicate a significant variability in N cycle parameter values for different sites. This was a limiting factor for the improvement of the model's predictive ability by using an average parameterization strategy. On the other hand, we were able to show that, in the LOO cross-evaluation, some of the N cycle parameters deviated significantly from the default value, like *MaxNitAmt* and *wfspdntadj* (Fig. 6). This implies that even the application of average values for these parameters helped to enhance the model's performance in the LOO cross-evaluation (Figs. 5a and 5c). This result suggests that experimental efforts to assess these parameters that directly affect nitrification and denitrification could contribute to improve the process-based modeling of N_2O emissions.

The simulation of gaseous N losses using biogeochemical models includes some steps that are particularly challenging. A recent study emphasized the difficulty to improve simulations of the denitrification process due to a lack of measurement data to support modeling (Del Grosso et al., 2020). For example, measurements of N_2 emissions are scarce due to the difficulty of determining N_2 fluxes from soils because of the high atmospheric concentrations (78%). The partitioning between N_2 and N_2O in the denitrification process driven by N-NO_3 is taken into account to simulate N_2O in DayCent (Hartmann et al., 2018; Del Grosso et al., 2020). In our study, the parameter related to this partitioning is the $\text{N}_2:\text{N}_2\text{O}$ ratio adjustment coefficient (*N2N2Oadj*). Similar as discussed above for other N cycle parameters, this coefficient also presented high variability between sites, but it ended by presenting LOO average values close to default values (Fig. 6). Therefore, the restricted offset of the LOO average values of *N2N2Oadj* could not contribute significantly to improve the overall model's prediction ability. A more in-depth knowledge of the drivers of $\text{N}_2:\text{N}_2\text{O}$ stoichiometry would contribute to improve the simulation of N_2O emissions. The reduction of N_2O to N_2 is the main process determining the proportion of the two gases (Ibraim et al., 2019; Verhoeven et al., 2019; Gallarotti et al., 2021). Improving the simulation of the N_2O reduction process in biogeochemical models could increase accuracy in simulations of N_2O fluxes. For instance, a better sub-model structure for soil water dynamics could improve this step in the simulation of N_2O emissions (Smith et al., 2020).

Accurate predictions of N_2O emissions are not only determined by the simulation of soil N transformations. Ensuring reasonable model performance for predicting plant growth and yield also has positive consequences for modeling N_2O emissions. Part of the errors in model predictions of crop growth in the LOO cross-evaluation (Fig. 4c) likely contributed to the errors in the model prediction of N_2O emissions (Fig. 5c). This is consistent with the slight improvement of modeled N_2O emissions associated with the adjustment of only plant growth

parameters in the LOO cross-evaluation (Fig. 5a, Fig. A.7a). Better prediction of plant growth reduces the errors in key model outputs caused by a "cascade effect" and the possibility of obtaining a good model performance caused by biased parameterization is diminished (Houska et al., 2017; Sima et al., 2020). For example, errors in estimates of crop growth affect predictions of N uptake during a crop cycle, as well as the amount of N in plant residues after harvest. Consequently, this impacts the predicted N_2O emissions derived from residue decomposition. Further improvements of model simulations of crop growth would also contribute to improve the simulations of cropland N_2O emissions.

A particularly challenging point in simulating N_2O emissions in conventional tillage-based croplands is the model's ability to capture the N_2O pulses induced by soil physical disturbance. Conventional tillage with regular full-inversion and seedbed preparation is representative for croplands in Western Europe and is reflected by treatments in the present study. Overall, the model was able to reproduce reasonably well the post-tillage N_2O pulses over time (Fig. 3 and Fig. A.1–A.6). The ability of DayCent to capture these physical soil disturbance effects is likely one of the main reasons why simulations outperformed estimates by the EF approach (Fig. 7). Our results showed that DayCent was able to mimic soil physical disturbance effects on N mineralization and increases of easily decomposable C, which supply energy for denitrification (Zhu et al., 2013). Occasional underestimation of fluxes induced by tillage, like observed in Frick (Figs. 3c and 3d), can be attributed to the fact that models of intermediate complexity do not fully reproduce the interaction of organic pools with dynamic soil physical variables. Among physical variables, soil aggregation is usually not explicitly represented by ecosystem models. However, it plays an important role in the protection of soil organic pools and therefore controls dynamics of soil C and N (Six et al., 1999, 2004).

By considering crop cycles with entire gap-filled management periods for N_2O flux measurements, we were able to show that model estimates can provide more accurate estimates of cropland N_2O emissions compared to EF approaches (Fig. 7). This result can be partially explained by the fact that N fertilizer inputs, which are the major predictor used in EF estimates, did not present large variation, showing an interquartile range of 102 – 138 kg N ha^{-1} per crop cycle. A more general comparison of the model and EF approaches would require N_2O data for a wide range of soil, climate, and crop types. Overall, measurements of N_2O emissions in Western Europe have usually been performed for the most important crops such as winter wheat and maize that cover large areas (e.g., Sehy et al., 2003; Oorts et al., 2007; Maier et al., 2022). There is a lack of N_2O flux measurements for other important crops, such as sugar beets, potatoes, sunflowers and secondary small-grained cereals, such as rye and triticale (FAOSTAT, 2021). Furthermore, N_2O flux measurements are rarely performed over many seasons in long-term field studies, which are extremely valuable for modeling (Coleman et al., 1997). Still N_2O emissions have generally been measured more often compared to other types of N losses that would be just as important (e.g., NO_3 leaching and N_2 emissions). An intensive monitoring of daily N_2O fluxes is necessary to cope with the high variability due to the spatially and temporally dynamic nature of nitrification, denitrification and N_2O reduction (Chadwick et al., 2014; Barton et al., 2015; Hörtnagl et al., 2018).

Despite the potential calibration-based improvement we identified, our results suggest that DayCent is an adequate model for reporting cropland N_2O emissions for Western Europe with complex soil management and diverse crop rotations (Fig. 7). The main advantage over commonly used EF approaches is that DayCent takes into account key drivers not considered by simple estimates. Estimates based on EF do not explicitly account for the impact of tillage or the long-lasting effect of crop residues on the interseasonal variability of background N_2O emissions, which has been recognized as a major contribution to the total emission (Hansen et al., 2019). Other important factors, such as N and water use efficiency of crops are not accounted by EF approaches. Considering the influence of these factors is crucial to forecast the

impact of climate change on N₂O emissions. Management alternatives towards emission abatement can also only be tested by considering the major processes involved, which are simulated by ecosystem models such as DayCent.

5. Conclusions

Our results showed that predictions of N₂O emissions could be improved by adjusting only a few parameters controlling the soil N cycle, such as the maximum daily nitrification amount and the inflection point for the effect of water-filled pore space on denitrification. Experimental efforts to assess these parameters directly affecting nitrification and denitrification could support the process-based modeling of N₂O emissions. Further systematic multisite N₂O monitoring covering different soils and weather conditions would also contribute to additional calibration-based improvement of model estimates. Overall our results showed that DayCent simulations were clearly more accurate than EF approaches. Based on extensive field observations, our results suggest that, even with scope for further improvement, DayCent simulations are useful for reporting cropland N₂O emissions under complex soil management by considering key drivers affecting the N transformation in soil.

CRedit authorship contribution statement

Marcio dos Reis Martins: Conceptualization, Methodology, Formal analysis, Writing – original draft, Visualization. **Magdalena Necpalova:** Software, Writing – review & editing. **Christof Ammann:** Methodology, Writing – review & editing. **Nina Buchmann:** Resources, Writing – review & editing. **Pierluigi Calanca:** Software, Writing – review & editing. **Christophe R. Flechard:** Resources, Writing – review & editing. **Melannie D. Hartman:** Software. **Maïke Krauss:** Resources, Writing – review & editing. **Philippe Le Roy:** Investigation. **Paul Mäder:** Resources, Writing – review & editing. **Regine Maier:** Investigation, Writing – review & editing. **Thierry Morvan:** Investigation. **Bernard Nicolardot:** Resources, Writing – review & editing. **Colin Skinner:** Investigation, Writing – review & editing. **Johan Six:** Resources, Writing – review & editing. **Sonja G. Keel:** Conceptualization, Writing – review & editing, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This study was supported by the Swiss Federal Office for the Environment (FOEN, LACHSIM project - 6510355). The EFELE field experiment forms part of the SOERE-PRO, which is a network of long-term experiments dedicated to the study of impacts of organic waste product recycling and it is certified by ALLENI (“Alliance Nationale de Recherche pour l’Environnement”) and integrated as a service of the “Le Programme d’Investissement d’Avenir” infrastructure AnaEE-France, overseen by the French National Research Agency (ANR-11-INBS-0001). Nitrous oxide measurements performed at the Bretenière site were granted by Burgundy region. We thank the staff of the INRAE experimental unit who supported the field management of the cropping systems and the technicians of Agroecology unit who contributed to field measurements or soil characterization. The N₂O measurements in the DOK experiment were granted by the Swiss Federal Office for the Environment (FOEN) and the Swiss Federal Office of Agriculture (FOAG). The N₂O measurements in the Frick experiment were part of the TILMAN-ORG project supported by the Funding Bodies of the FP7 ERA-Net project CORE Organic II. The N₂O measurements at Oensingen were supported by the

Swiss National Science Foundation (SNSF), within the framework of the National Research Programme “Sustainable Economy: resource-friendly, future-oriented, innovative” (NRP 73), in the InnoFarm project, Grant-N° 407340_172433. We thank Lukas Hörtnagl and Markus Staudinger from ETH for their support in data processing and technical support, respectively. We thank Luca Nembrini for the support in the model simulations, Robing Giger for the soil sampling and chemical analysis for the Oensingen site, and Marlies Sommer for the analyses of hydraulic properties of the same site.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.eja.2022.126613](https://doi.org/10.1016/j.eja.2022.126613).

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